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MATHEMATICAL MODELING OF RF PLASMA FLOW WITH METASTABLE ATOMS AT LOW PRESSURE

A. YU. SHEMAKHIN[1] AND V. S. ZHELTUKHIN[2]

[1] Kazan Federal University
Kremlyovskaya 18, 420008 Kazan, Tatarstan, Russia
e-mail: shemakhin@gmail.com

[2] Kazan National Research Technological University
Karl Marx Street 68, 420015 Kazan, Tatarstan, Russia

Summary. The mathematical model of the rf plasma flow at a pressure of 0.15–150 Pa in both free-molecule and transition flow at Knudsen $0.03 \leq \mathrm{Kn} \leq 3$ is described. The model is based on the statistical approach for the neutral component together with the continuum model for electron and metastable components of the rf plasma. Results of plasma flow calculations for electrons and metastables density, distributions of electron temperature, neutral component velocity, pressure and temperature at a prescribed electric field are presented.

1 INTRODUCTION

Radio frequency plasma discharges at low pressures ($p = 0.15$–150 Pa) is used successfully for the modification of various materials: dielectric, conducting, semiconducting [1, 2]. The plasma has the following properties: ionization degree is from 10^{-7} up to 10^{-5}, electron density n_e is from 10^{15} up to 10^{19} m^{-3}, electron temperature T_e is from 1 up to 4 eV, temperature of atoms and ions T_a is in range of $(3\text{–}4) \times 10^3$ K in the plasma bunch and the ones is in range of $T_a = (3.2\text{–}10) \times 10^2$ K in a plasma stream.

The plasma equipment is shown on figure 1(a). The special feature of low pressure rf is that the plasma jet has length top up to 0.5 m. Figure 1(b) shows the plasma jet. A hybrid mathematical model, combining a kinetic model for the carrier gas flow at Knudsen $0.03 \leq$ $\mathrm{Kn} \leq 3$ and the continuous model for charged particles and metastables is developed.

2 MATHEMATICAL MODEL OF LOW PRESSURE RF PLASMAS STREAM

Mathematical model of the low pressure rf plasma stream is constructed by neglecting the Hall effect, electron pressure gradient, the radiation energy loss [3], the electron attachment, the excitation of atoms, bulk recombination, formation of multiply charged ions and electron attachment. A direct electron impact as the basic mechanism of charged particles appearance [3] is assumed. We assume that the ion density is equal to the electron ones, the ion temperature coincides with the temperature of the neutral atoms. The first models was developed in [4–6]. Let us designate the radius of the cylindrical vacuum chamber as R_{vk}, the length of ones as L_{vk},

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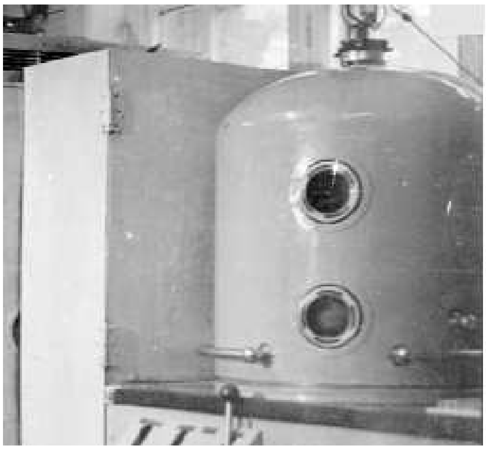
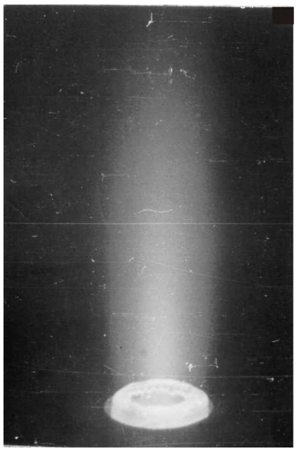


(*a*)



(*b*)

Figure 1: (*a*) Plasma equipment and (*b*) plasma jet.

the radius of the plasma torch outlet as R_{rk}, subscripts inlet, outlet, body, walls will used for parameter value on inlet and outlet of the chamber, on the walls of the sample and the vacuum chamber, respectively.

The model includes:

- the Boltzmann's transport equation for neutral atoms:

$$\frac{\partial f}{\partial t} + \mathbf{c} \cdot \frac{\partial f}{\partial \mathbf{r}} + \widetilde{\mathbf{F}} \cdot \frac{\partial f}{\partial \mathbf{c}} = S(f), \tag{1}$$

- the equation of the electron continuity:

$$\frac{\partial n_e}{\partial t} - \mathrm{div}\left(D_a \mathrm{grad}\, n_e - \mathbf{v}_a n_e\right) = \nu_i n_e + R_1 n_e n_a + R_2 {n_m}^2 + R_3 n_m n_e - R_4 {n_e}^2 - R_5 {n_e}^3, \tag{2}$$

- the equation of the electron heating:

$$c_p \rho_e \frac{\partial T_e}{\partial t} - \mathrm{div}\left(\lambda_e \mathrm{grad}\, T_e - \frac{5}{2} k_B n_e T_e \mathbf{v}_e\right) + \\ + \frac{3}{2} k_B \delta \nu_c n_e \left(T_e - T_a\right) = \sigma E^2 - \nu_i n_e E_I - I_1 R_3 n_m n_e, \tag{3}$$

- the equation of the metastables continuity:

$$\frac{\partial n_m}{\partial t} - \mathrm{div}\left(D_m \mathrm{grad}\, n_m\right) = R_6 n_e n_a - R_2 {n_m}^2 - R_3 n_m n_e - R_7 n_m - R_8 n_m n_a - R_9 n_m. \tag{4}$$

Here, $\mathbf{c}$ and $\mathbf{r}$ is 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, $S(f)$ is the collision integral, $\widetilde{F}$ is the reduced force which effects on neutral atoms at elastic collisions with electrons, n_e is electron density, D_a is ambipolar diffusion coefficient, ν_i is the ionization frequency, $\mathbf{v}_a$ is gas velocity, λ_e is thermal conductivity coefficient of electrons, c_p is the heat capacity of the electron gas, ν_c is elastic collision frequency of electrons and atoms, σ is plasma conductivity, $\mathbf{E}$ is electric field strength, $E = |\mathbf{E}|$, E_I is ionization potential, k_B is the Boltzmann's constant, $\delta = m_e/2m_a$, m_e, m_a are the electron and the atom masses, dV is volume element. $I_1 = 11.56$ 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 photorecombination 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.

Coefficients D_a, ν_i, λ_e are functions of the electron temperature [3, 7–9],

$$\widetilde{\mathbf{F}} = -\frac{1}{m_a}\operatorname{grad} W_T, \quad W_T = \int E_c \,\mathrm{d}V\mathrm{d}t, \quad E_c = \frac{3}{2}k_B\delta\nu_c n_e(T_e - T_a).$$

The system (1)–(4) is considered at the following initial conditions:

$$f(\mathbf{c},\mathbf{r},0) = f_0(\mathbf{c},\mathbf{r}), \quad n_e|_{\mathrm{t=0}} = n_{e_0}, \quad T_e|_{\mathrm{t=0}} = T_{e_0}, \quad n_m|_{\mathrm{t=0}} = n_{m_0}, \tag{5}$$

and the following boundary conditions:

$$n_e|_{\mathrm{inlet}} = n_{e_{\mathrm{inlet}}}, \quad n_e|_{\mathrm{outlet}} = n_e|_{\mathrm{walls}} = 0, \quad n_e|_{\mathrm{body}} = 0, \tag{6}$$

$$T_e|_{\mathrm{inlet}} = T_{e_{\mathrm{inlet}}}, \quad T_e|_{\mathrm{outlet}} = T_e|_{\mathrm{walls}} = T_{e_{\mathrm{room}}}, \quad \left.\frac{\partial T_e}{\partial \mathbf{n}}\right|_{\mathrm{body}} = 0, \tag{7}$$

$$n_m|_{\mathrm{inlet}} = n_m|_{\mathrm{outlet}} = n_e|_{\mathrm{walls}} = 0, \quad n_e|_{\mathrm{body}} = 0. \tag{8}$$

Here f_0 is Maxwell velocity distribution function. Terms of impermeability are defined for $f(\mathbf{c},\mathbf{r},t)$ on the body and walls boundary surfaces as well as soft boundary conditions [3] on the inlet and outlet borders.

Equations (1)–(4) is closed by the following relations:

$$\mathbf{v}_a(\mathbf{r},t) = \int_{-\infty}^{\infty} \mathbf{c} f(\mathbf{c},\mathbf{r},t)\,\mathrm{d}\mathbf{c}, \quad p_a = n_a k_B T_a, \quad \mathbf{v_e} = \mathbf{v}_a - (D_a/n_e)\operatorname{grad} n_e, \tag{9}$$

$$\sigma = \frac{n_e e^2 \nu_c}{m_e\left(\nu_c^2 + \omega^2\right)}, \quad T_a = \frac{m_a\overline{\mathbf{c}'^2}}{3k_B} = \frac{m_a}{3k_B}\left(\overline{\mathbf{c}^2} - \mathbf{v}_a^2\right), \quad \overline{\mathbf{c}^2} = \int_{-\infty}^{\infty} \mathbf{c}^2 f(\mathbf{c},\mathbf{r},t)\,\mathrm{d}\mathbf{c}.$$

No.	Process	Reaction	Coefficient
R1	impact ionization	$Ar + e \rightarrow Ar^{+} + 2e$	BOLSIG+
R2	Penning ionization	$Ar^{*} + Ar^{*} \rightarrow Ar + Ar^{+} + e$	6.2×10^{-16}
R3	step ionization	$Ar^{*} + e \rightarrow Ar^{+} + 2e$	$2 \times 10^{-11} e^{-25524.4/T_e}$
R4	photorecombination	$Ar^{+} + e \rightarrow Ar + h\nu$	$2.7 \times 10^{-19} (T_e/11602)^{-3/4}$
R5	triple recombination	$Ar^{+} + 2e \rightarrow Ar + e$	$8.75 \times 10^{-39} (T_e/11602)^{-9/2}$
R6	metastables excitation	$Ar + e \rightarrow Ar^{*} + e$	$10^{-9} (T_e/11602) e^{-134583/T_e}$
R7	radiative recombination	$Ar^{*} \rightarrow Ar + h\nu$	2.5×10^{-11}
R8	collisional quenching	$Ar^{*} + Ar \rightarrow 2Ar$	3×10^{-21}
R9	electron deexcitation	$Ar^{*} + e \rightarrow Ar + e$	10^{-11}

Table 1: Rate coefficients for metastables.

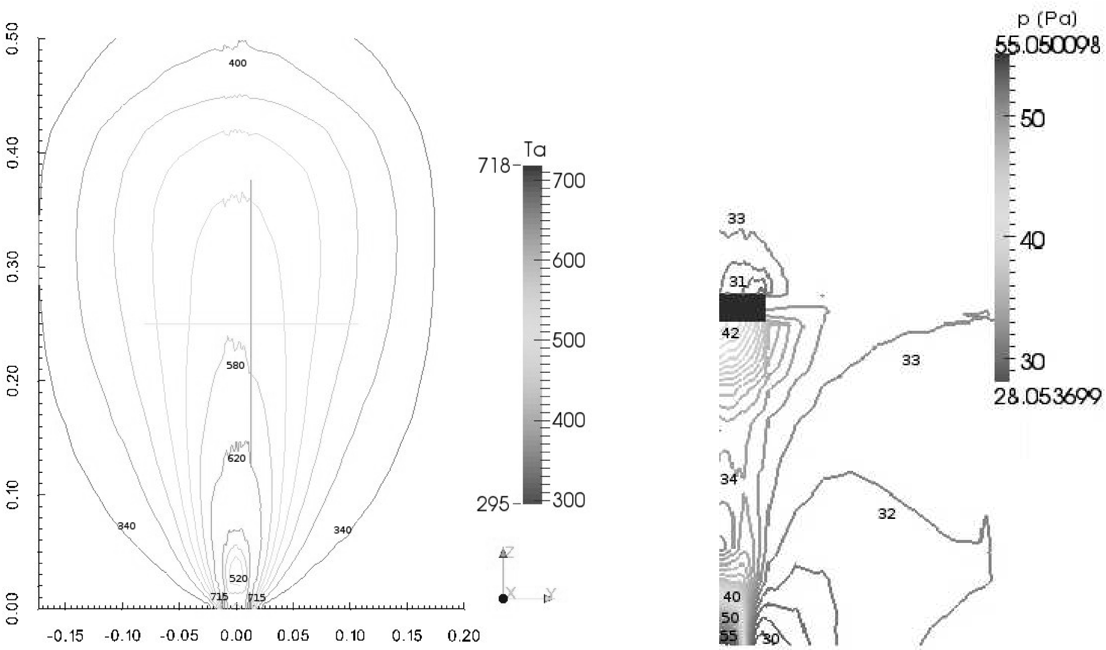
Rate coefficients are described in table 1 [8, 10, 10–15].

For constructing numerical method Bird's method is modified to take into account the distributed heat source density W_T. A three-step iterative process is constructed to solve the problem (1)–(9). On the first step a solution of (1) is found by Bird's DSMC method [16] to determine v_a and T_a. Then these values is used to solve problems (2), (5), (6) till setuped accuracy. After it on third step solving (2), (5), (7) and (2), (5), (6) problems. Further, solutions of these problems n_e and T_e are used to solve the equation 1 taking into account the distributed heat source power density W_T. The process is repeated until the maximum of successive approximation ratios becomes less than the specified tolerance. The software package for calculating of low pressure rf plasma flow is developed by using OpenFOAM [17] environment on Linux OS.

3 CALCULATIONS OF CHARACTERISTICS OF LOW PRESSURE RF PLASMA FLOW

The gas-dynamic characteristics of low pressure rf plasma undisturbed flow as well as stream with overflowing sample in the vacuum chamber of $R_{\mathrm{vk}} = 0.2$ m, $L_{\mathrm{vk}} = 0.5$ m and $R_{\mathrm{rk}} = 0.012$ m, on the center of the base plate is carried out. A cylindrical sample of radius $R_b = 0.03$ m and a height $L_b = 0.02$ m located in the plasma jet at a distance $L_{\mathrm{tb}} = 0.02$ m. Flow input parameters are the following: the plasma forming gas is argon, gas flow rate $G = 0.02$–0.24 g/s, pressure $P_{\mathrm{inlet}} = 3.5$–135 Pa, the temperature $T_{\mathrm{inlet}} = 400$–600 K, the degree of ionization $\delta_i = 10^{-4}$. The initial pressure in the vacuum chamber $P_0 = 0.35$–13.5 Pa.

Results of plasma flow calculations for electrons and metastables density, distributions of electron temperature, neutral component velocity, pressure and temperature at a prescribed electric field are obtained.



(*a*) (*b*)

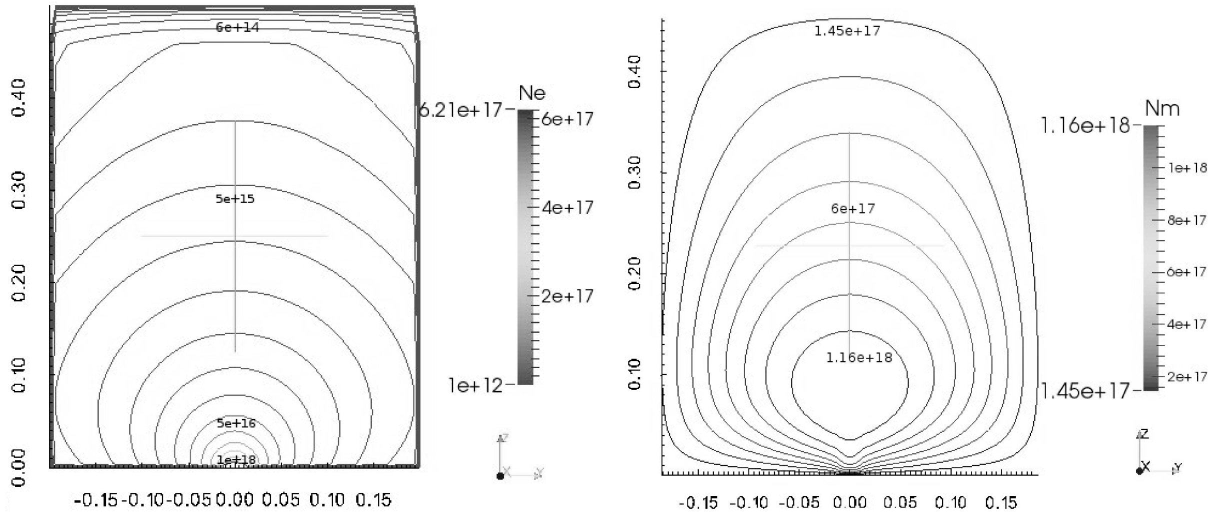
Figure 2: (*a*) Isolines of neutral gas temperature T in free stream, and (*b*) isolines of pressure p for the flow with sample.

The effect of an overheating up of a plasma stream on the periphery of a stream is found and described with comparing with experiment in work [18]. The overheating gas in the mixing zone of the plasma stream and stationary gas in the vacuum chamber is observed in the vicinity of the inlet, figure 2(*a*).

When placed the sample in a jet, the pressure at the distance $0.05 - 0.15$ m from the inlet firstly falls, then near the sample is increasing, which is due with deceleration of flow, figure 2(*b*). A region of low pressure is created behind the sample, and then it aligned, as in the model without a sample.

The calculations showed that the electron density n_e decreases along the jet from 10^{18} to 10^{14}, which corresponds to the experimental data [1], figure 3(*a*). The profiles n_e in the radial distribution are bell-shaped and the distribution is aligned to the end of the jet.

Metastables distribution along jet is not steady. The maximum value is 1.3×10^{18} m^{-3} on distance 0.08 m from inlet, after it metastables profile steadly goes down, figure 3(*b*). In radial cross-section profile of metastables density has a bell-shaped form in all cross-sections. The presence of a peak in the distribution of metastable particles is due to the predominance of the



(*a*) (*b*)

Figure 3: (*a*) Isolines of electron density n_e in free stream, and (*b*) isolines of metastables n_m in free stream.

process of excitation of metastable particles at the beginning of the jet and the predominance of blanking over excitation by downstream.

4 CONCLUSIONS

The mathematical model of the rf plasma flow at a pressure of 0.15–150 Pa with metastable atoms is developed. Results of plasma flow calculations for electrons and metastables density, distributions of electron temperature, neutral component velocity, pressure and temperature at a prescribed electric field are presented. It is established that the distribution of electrons density falls steady along jet, density of metastables has a maximum. Density value of metastables is comparable with electrons density. Along the jet electron temperature is distributed almost uniformly through the chamber and sharply decreases at the walls of the vacuum chamber. The uniformity of the distribution of T_e is related to the effective heat transfer in the electron gas. It is described pressure distribution for flow with sample in the stream.

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