Mathematical Modeling of RF Plasma Streams at Low Pressure

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Abstract. *This article describes mathematical model of RF plasma's stream at a pressure of 13.3-133 Pa in the transition regime at Knudsen* $8\bullet10^{-3} \leq Kn \leq 7\bullet10^{-2}$ *for the neutral gas. The model based on a statistical approach of neutral component and on continuum model for the electronic and ionic components. The calculations were performed using the method of MPI for the given directions. Results of RF plasma flows simulation are presented for unperturbed flow and with presence of specimen. Simulation has an agreement with the available experimental data.*

Keywords

Parallel processing, HPC-UA, mathematical modeling, RF plasma, low pressure, plasma streams, transient mode, Monte-Carlo method, statistical modeling.

1 Introduction

The plasma radio frequency (RF) discharges at low pressure (p = 13.3-133 Pa) with the gas blow is effectively used to modify the surfaces of materials of organic and inorganic nature [1]. The plasma produced by this type of discharge, has the following properties: the degree of ionization is 10^{-4} -10^{-7}, the electron density 10^{15} – 10^{19} m^{-3}, the electron temperature is 1 - 4 eV, the temperature of the atoms and ions in a plasma clot (3 - 4)·10^3 K in the plasma jet (3.2 - 10) ·10^2.

The flow in RF plasma at low pressure is carried out in the transitional regime, for which there is no well-established models such as the Navier-Stokes equations. The main difficulty in describing the physical process of the transition flow of rarefied gas is necessary to agree the submission of a random walk of molecules in the molecular and viscous flow in the laminar regime.

2 Related works

Research in the field of plasma physics, radio frequency discharges are being extensively carried out worldwide [2 , 3]. The main groups of researchers working in the U.S. (MJKushner), Canada (M.Boulos), France (JPBoeuf), the Netherlands (Godheer), Russia (Yu.P.Rayzer) , China, South Korea. The main focus of this research is to study the properties of RF plasma in different conditions, different gases without purging gas.
In work on mathematical modeling of the plasma using different approaches depending on the kind and the plasma pressure at which the processes take place , temperature , etc. In a number of finite volume method is used to calculate the gas dynamics of the plasma stream at atmospheric pressure and flow pattern of neutral gas diluted such as a method for the direct simulation of G.Bird [3] for low blood pressure.

At the moment, there is no mathematical model of the jet stream RF low-pressure plasma in the transitional regime for carrier neutral gas in Knudsen 0.008 <Kn <0.07 at subsonic speeds in the presence of charged particles in a stream of RF plasma. Therefore, to simulate the jet stream RF low-pressure plasma requires the development of a new mathematical model. Creating a mathematical model of the gas dynamics of the RF plasma flow at low pressure will allow the study of laws of formation flow characteristics of the RF plasma to improve the treatment of organic materials and inorganic nature , which will reduce the costs of a large number of costly and time-consuming experiments.

3 Main sections

The RF plasma flow at low pressure is different from the flow of neutral gas by the presence of charged component. The interaction between charged particles in the discharge is carried out long-range Coulomb forces. In the pressure range of p = 13.3 - 133 Pa the plasma is thermal equilibrium, the thermal non-equilibrium degree $\theta = T_e / T_a = 10 - 100$, where T_e - electron temperature, T_a - the gas temperature. The analysis and evaluation of the characteristic scale of elementary processes in plasma showed that the flow of high-frequency plasma in low pressure has specific features. The Knudsen number Kn for the electron gas, $10^{-3} < Kn < 10^{-1}$, for ions gas $5 \cdot 10^{-4} < Kn < 5 \cdot 10^{-3}$, for the neutral gas $8 \cdot 10^{-3} < Kn < 7 \cdot 10^{-2}$. This means that for the electron and the neutral gas flows in a transitional regime between continuum flow and free-molecular flow, while for the ions can be considered as occurring in the regime of continuous medium due to the influence of Coulomb forces. As a result of elastic collisions of electrons with atoms and ions are heated heavy particles. The frequency of elastic collisions in which energy is exchanged between the plasma particles in the low-pressure RF discharge $v_c \backsim 10^{10} - 10^{11}$ Hz.

It is assumed that the working part of the RF plasma system of low pressure is composed of a cylindrical quartz discharge chamber radius R_{rk} and length L_{rk}, connected to the vacuum chamber radius R_{vk} and length L_{vk}. The discharge is generated by the inductor and/or the outer ring electrodes, coaxial with the discharge chamber. All the boundary conditions for the plasma jet will be installed on the following areas of the vacuum chamber, designated indices: the inlet - *inlet*, outlet - *outlet*, the specimen - *body*, the remaining walls of the vacuum chamber - *walls*.
In elastic collisions electrons transfer energy to the atoms

$$E_c = \frac{3}{2} K_b \delta v_c n_e \left(T_e - T_a\right) \tag{1}$$

Specific power of the distributed heat source can be written as

$$W_T = \int E_c dVdt\,, \tag{2}$$

where $\delta = \dfrac{2m_e}{m_a}$, m_a - mass of the atom, m_e - mass of the electron, k_B - Boltzmann's constant, n_e - the concentration of electrons.
Plasma flow is different from the neutral gas flow by presence of distributed heat source by power density (1). Under the above assumptions, the gas-dynamic properties of the quasi-neutral plasma jet RF low-pressure system described by the initial-boundary value problems:
1. for the neutral gas:

$$\begin{aligned}
&\frac{\partial f}{\partial t} + \mathbf{c} \cdot \frac{\partial f}{\partial \mathbf{r}} + \tilde{\mathbf{F}} \cdot \frac{\partial f}{\partial \mathbf{c}} = S(f), \\
&\mathrm{f}(\mathbf{c}, \mathbf{r}, 0) = \mathrm{f}_0(\mathbf{c}, \mathbf{r}), \\
&\tilde{\mathbf{F}} = -(1/\mathrm{m_a})\ \mathrm{grad}\ \mathrm{W_T}
\end{aligned} \tag{3}$$

2. boundary value problem for the equation of the electron density:

$$\begin{aligned}
&\frac{\partial n_e}{\partial t} - div(D_a grad\, n_e - \mathbf{v}_a n_e) = v_i n_e, \\
&n_e\big|_{inlet} = n_{einlet}, n_e\big|_{outlet} = 0,\ n_e\big|_{walls} = 0,\ n_e\big|_{body} = 0 \\
&n_e\big|_{t=0} = n_{e0}
\end{aligned} \tag{4}$$

3. boundary value problem for the electron temperature:

$$\begin{aligned}
&c_p \rho_e \frac{\partial T_e}{\partial t} - div(\lambda_e grad\, T_e - \frac{5}{2} k_B n_e T_e \mathbf{v}_e) + \\
&\quad + \frac{3}{2} k_B \delta v_c n_e (T_e - T_a) = \sigma E^2 - v_i n_e E_I, \\
&T_e\big|_{inlet} = T_{einlet}, \quad T_e\big|_{outlet} = T_{eroom}, \quad T_e\big|_{walls} = T_{eroom}, \\
&\left.\frac{\partial T_e}{\partial \mathbf{n}}\right|_{body} = 0, \quad T_e\big|_{t=0} = T_{e0}
\end{aligned} \tag{5}$$

4. closing equations:

$$p_a = n_a k_B T_a, \quad \mathbf{v}_a(\mathbf{r},t) = \int_{-\infty}^{\infty} \mathbf{c}\, f(\mathbf{c},\mathbf{r},t)\, d\mathbf{c},$$
$$\mathbf{v}_e = \mathbf{v}_a - (D_a / n_e)\,\mathbf{grad}\, n_e. \tag{6}$$

where $f(\mathbf{c},\mathbf{r},t)$ - distribution function of particle density neutral plasma component in the phase space, **c** and **r** — vector velocities and coordinates, respectively; D_a - ambipolar diffusion coefficient, λ_e - thermal conductivity of the electron gas, ν_i - the ionization frequency, c_p - specific heat of electron gas, ν_c - frequency of elastic collisions of electrons with atoms and ions, $\tilde{\mathbf{F}}$ - reduced force acting on neutral atoms in elastic collisions with electrons , σ - conductivity of the plasma, **E** - the electric field vector, E=|**E**|, E_i - the ionization potential.

Finding RF electromagnetic field in an inhomogeneous medium with a conductivity is a separate task, since it reduces to the calculation of the 12 first order differential equations in 3-dimensional space. This problem in its entirety is far from being resolved, so in this paper module of tension $E(x,y,z)$ on the right side of (5) can be approximated from experimental data. To solve the system (3) - (6) suggests the following numerical method. The method is based on a two-step iterative process, which consists of the following steps:

- The choice of initial approximation: The initial approximation is chosen by solving the system (2) for the neutral gas by the method of direct statistical modeling (DSMC) of G.Berd [4]. As a result, we calculate the concentration field of neutral atoms n_a, temperature T_a and velocities $\mathbf{v_a}$ in the jet without the presence of charged particles in a stream;
- The first step: Solving systems (4) - (5) for the electron temperature T_e and electron density n_e by the finite volume method (FVM). After we calculate the concentration field for a charged plasma component n_e, temperature T_e, and velocity $\mathbf{v_e}$;
- The second step: Solving system (3) for the neutral component of the plasma, taking into account the distributed heat source power density (2) with the calculated values of the first stage of n_e, T_e and $\mathbf{v_e}$.

The steps are repeated until convergence.

The program for flow calculation of the neutral and charged components of RF plasma at low pressure developed on the basis of the package OpenFOAM, which includes a libraries of DSMC (Direct simulation Monte-Carlo) and FVM. Parallelization technology for calculations is MPI.

The calculation was performed for the model of the vacuum chamber of radius R = 0.2 m, the radius of the inlet r = 0.012 m and a length of the camera L = 0.5 m. Cylindrical specimen has a size R_b = 0.03 m, L_b = 0.02 m and is located in the center of the stream at a distance L_{tb} = 0.2 m from the inlet. The specimen position is perpendicular to the sample stream. Through the inlet of the vacuum chamber is flowing stream of the plasma working gas (argon) with the inlet pressure in the range of P_{inlet} = 35 - 185 Pa, the temperature T_{inlet} = 400 - 600 K and the electron temperature T_e = 2 - 4 eV. The gas consumption $G \backsim$ 0.12 - 0.24 g/s. The degree of ionization in the chamber $\delta_n = 10^{-4}$, the initial chamber pressure P_0 = 3.5 - 18.5 Pa.

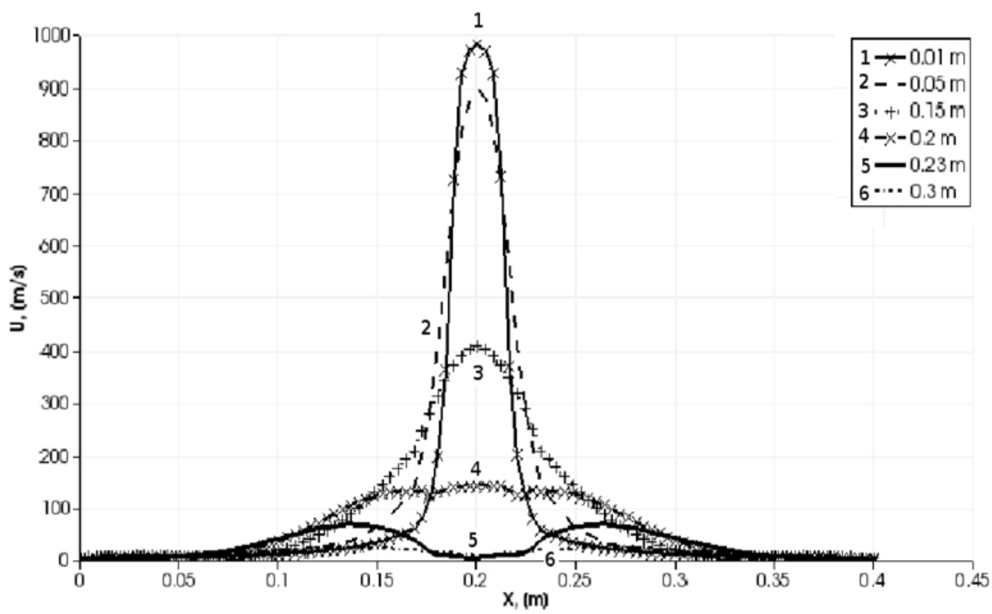

Fig. 1. The distribution of pressure and temperature in the cross section of undisturbed flow depending of distance from the inlet.

The calculations for the undisturbed flow of RF plasma at low pressure and specimen circumfluence for neutral component and for charged component are presented (Figs 1,2). Fig. 1. show that with presence of specimen, speed decreases when the gas flow is approaching to the body and around the body speed becomes more than in the stream's collision with specimen plane (lines 4 and 5), that correspond to the experimental pattern of the gas flow. Fig. 2 show the profile of the electron density n_e in the longitudinal section of the unperturbed flow. As can be seen, the electron density decreases along the stream from 10^{18} to 10^{14} 1/m^3. Calculations showed that the settling time to steady state flow at these conditions amounted to about 10^{-2} s.

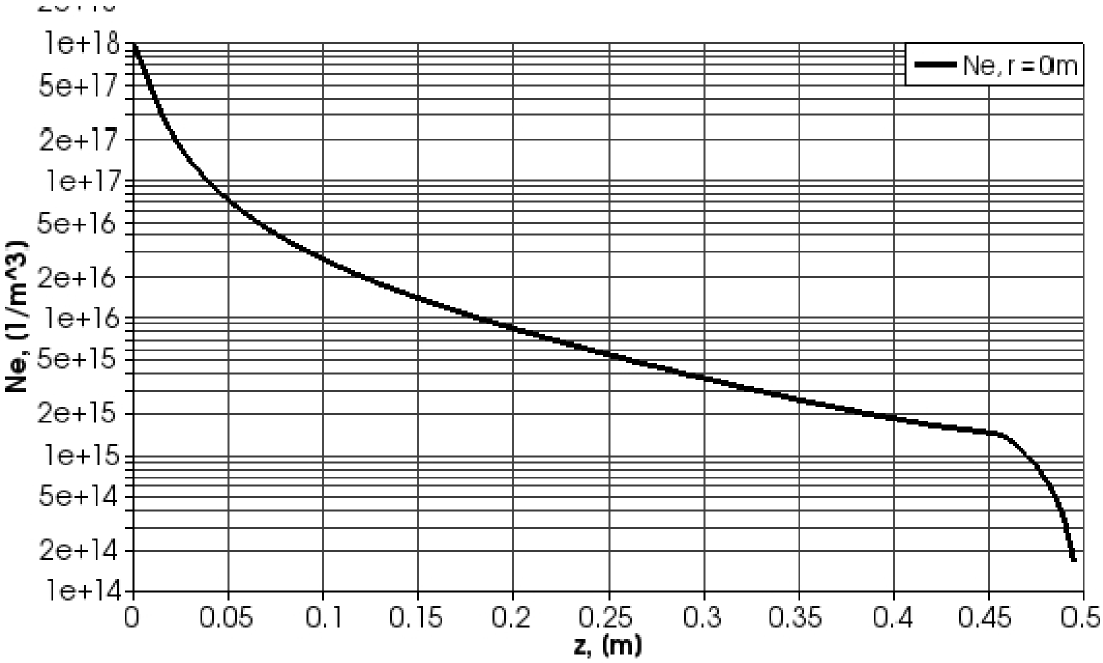

Fig. 2. The electron density n_e in longitudinal sectional undisturbed stream (in the middle of the stream).

4 Conclusion

The mathematical model of flow of RF plasma at low pressure are constructed. The results of calculations is in satisfactory agreement with experimental data.

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References

[1] Abdullin I.Sh., Zheltukhin V.S., Sagbiev I.R., Shaekhov M.F. Modification of nano-layers in RF plasma in low pressure. *Kazan*, 356 p., 2007.

[2] Yu.P.Rayzer, M.N.Shneyder, N.A.Yatsenko. High-frequency capacitive discharge: physics, engineering, applications. *Moscow: Publishing House of the Mosk.fiz.-technical. Inst, Science, FIZMATLIT,* 320 p., 1995.

[3] I.Sh.Abdullin, V.S. Zheltukhin. Mathematical modeling of the processing of solids in the high-low pressure plasma. Encyclopedia. Ser. "Encyclopedia of low temperature. plasma. "- Ser. B. "Ref. adj., databases and data banks. "- Themes. Volume XI-5. "J. Appl. Chem. plasma ". - *Moscow: Janus-K,* p. 502 - 532, 2006.

[4] Bird G.A. Molecular Gas Dynamics and the Direct Simulation of Gas Flows. *Oxford University Press*, 1994.- 476 p.