

SIMULATION OF NON-UNIFORM HIGH DENSITY ELECTRONEGATIVE PLASMA FOR OPTIMIZATION OF H⁻ ION AND THEIR EXTRACTION

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Abstract

Numerical simulations of radio frequency multi-cusp volume type H⁻ ion source have been performed under non-uniform electronegative plasma equilibrium conditions in order to understand the physics of formation of various ion species (H⁺, H⁻, e⁻ etc.) and for optimization of H⁻ ion formation and extraction. Coupled momentum balance equations along with continuity equations were solved in a cylindrical geometry to obtain the density profile of various ion species. The relevant cross-section data available in the literature as a function of temperature has been used in the computation. The hydrodynamic model of plasma in equilibrium with background neutral gas has been used. Low degree of ionization ($\approx 1\%$) has been assumed. The collision less sheath formation, penetration of electric and magnetic field and power requirement to sustain the plasma has been worked out numerically. An effort has been made to give a self-consistent numerical scheme for the solution of inductively coupled plasma(ICP) in equilibrium, and the results obtained have been presented.

INTRODUCTION

In order to meet the high current requirement of H⁻ ion for spallation neutron source, which is being proposed to be developed at RRCAT, a detailed theoretical investigation of H⁻ ion source has been carried out. The fluid model has been applied by various authors, to study various aspects of ion source [1, 2, 4]. In our numerical model we have retained the inertial derivative term. The effective collision frequency of electron and RF field frequency has been computed assuming Maxwellian velocity distribution. This was crucial because the discharge is assumed to be operated at 13.56 MHz, and typical plasma parameters are such that, neither high frequency nor the dc limit will be suitable. At this frequency it is safe to assume that electron respond to RF field while ions respond to the average field.

STEADY STATE FLUID MODEL

The steady state equilibrium of different species in the RF field implies the average value of different measurable parameter over several RF cycles remain unchanged. We have numerically solved the steady state equilibrium values in cylindrical geometry for H⁺, H⁻, e⁻ species in H⁻ ion source. It is assumed that the background hydrogen molecular density to be uniform, depending only on the pressure of the plasma chamber. The particle balance equation in

the steady state for i^{th} species is:

$$\vec{\nabla} \cdot \vec{\Gamma}_i = (G - L)_i \quad (1)$$

where $\vec{\Gamma}_i$ is the flux of the i^{th} species and G and L are the gain and the loss term of the i^{th} species. It has been evaluated from the cross-section data [2]. The flux of the i^{th} species is given by $\vec{\Gamma}_i = n_i \vec{u}_i$, where n_i is the density and \vec{u}_i is the diffusion velocity. The momentum balance equation in steady state for i^{th} species is written as:

$$m_i n_i (\vec{u}_i \cdot \vec{\nabla}) \vec{u}_i = -\vec{\nabla} P_i - e n_i \vec{\nabla} \phi + e n_i \mu \vec{u}_i \times \vec{H} - f_i \vec{u}_i \quad (2)$$

Where ϕ is electric potential. For neutral species the forces due to electric and magnetic field would be absent. Here f_i is the effective coefficient of frictional force on i^{th} species assumed to be proportional to diffusion velocity. It arises due to loss of momentum in the collisions with background molecules and in the creation and destruction of the species inside the plasma. It can also be evaluated using cross-section data and collision frequencies.

Plasma equilibrium in RF field

The discharge is assumed to be created by inductive coupling of RF power through antenna coil wound over cylindrical ceramic chamber. Cylindrical co-ordinate system has been used with \hat{z} axis coinciding with the antenna axis. Due to cylindrical symmetry any variation in the $\hat{\theta}$ direction has been ignored. The z variation in the plasma has been ignored which is a good approximation if $Z \gg R$ or in the mid plane of the plasma cylinder. Hence we can write:

$$\vec{H} = H(r, t) \hat{z} \quad (3)$$

$$\vec{E} = E_r(r, t) \hat{r} + E_\theta(r, t) \hat{\theta} \quad (4)$$

$$\vec{u}_i = \tilde{u}_{ir}(r, t) \hat{r} + \tilde{u}_{i\theta}(r, t) \hat{\theta} \quad (5)$$

$$n_i = n_i(r, t) \quad (6)$$

Where \vec{u}_i and n_i are the velocity and density of the i^{th} species respectively. The presence of Magnetic field in the ICP cannot be ignored altogether. Neglecting screening effect, it can be shown that the $\frac{F_{mag}}{F_{elec}} \approx \frac{R(Plasma\ Radius)w(rad/sec)}{V_i(Thermal\ velocity)}$ where w is RF frequency. Typically for H⁻ ion source the, electron temperature is 5 eV and the ion temperature is ≈ 0.5 eV. Hence magnetic field has been ignored in the momentum balance of heavy ions while it has been considered in the momentum balance of electron. From the $\hat{\theta}$ component of the momentum balance of electron, writing $E_\theta(r, t) =$

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$\text{Re}[\tilde{E}_\theta(r)e^{i\omega t}]$, $H(r, t) = \text{Re}[\tilde{H}(r, t)e^{i\omega t}]$ and $\tilde{u}_{e\theta}(r, t) = \text{Re}[u_{e\theta}e^{i\omega t}]$, and after neglecting u_r/r in comparison with ν_{ef} we get:

$$u_{e\theta} = \frac{-e(\tilde{E}_\theta - u_{er}\mu\tilde{B})}{m_e(\nu_{ef} + i\omega_{ef})} \quad (7)$$

Define $f_e = m_e n_e \nu_{ef}$. Here ν_{ef} is the effective collision frequency and the ω_{ef} is the effective RF frequency. They have been evaluated over the Maxwellian energy distribution $f(\varepsilon)$ as:

$$\frac{1}{\nu_{ef} + j\omega_{ef}} = \int_0^\infty \frac{\varepsilon^{3/2}}{v_e(\varepsilon) + j\omega} \frac{df}{d\varepsilon} d\varepsilon \quad (8)$$

In the steady state equilibrium condition we are only concerned with the radial variation of the density and the diffusion velocity of the electron, averaged over several RF cycle. This, along with the assumption of isothermal plasma, the \hat{r} component of momentum balance gives:

$$u_r(r) \frac{du_r(r)}{dr} = -\frac{e}{m_e} E_r(r) - \frac{eT_e}{n_e(r)m_e} \frac{dn_e(r)}{dr} - \nu_{ef} u_e(r) \quad (9)$$

where $E(r) = \langle E(r, t) \rangle_t$, $n_e(r) = \langle n_e(r, t) \rangle_t$ and $u_e(r) = \langle \tilde{u}_e(r, t) \rangle_t$. Similarly the momentum balance for positive ions in isothermal plasma equilibrium condition is written as:

$$u_+(r) \frac{du_+(r)}{dr} = \frac{e}{m_+} E_r(r) - \frac{eT_+}{n_+(r)m_+} \frac{dn_+(r)}{dr} - \nu_{+f} u_+(r) \quad (10)$$

here the ν_{+f} is the effective collision frequency defined for positive ions in terms of frictional force ($f_+ \approx \nu_n n_{++} + \langle \sigma v \rangle_{iz} n_e n_{H_2} + \langle \sigma v \rangle_{mn} n_H - n_{H^+}$). The $\langle \sigma v \rangle$ are different reaction rates, which has been obtained from reference [2]. The continuity equation for the positive ion:

$$\frac{1}{r} \frac{d(r u_+ n_+)}{dr} = (G - L)_+ \quad (11)$$

where $(G - L)_+ \approx \langle \sigma v \rangle_{iz} n_e n_{H_2} - \langle \sigma v \rangle_{mn} n_H - n_{H^+}$. Thus to close the equation (10) and (11) for H^+ species we assume H^- and e^- are in Boltzmann equilibrium with electric potential i.e. $n_- = n_{-(r=0)} e^{\phi/T_-}$ and $n_e = n_{e(r=0)} e^{\phi/T_e}$. And quasi neutrality condition $n_+ = n_e + n_-$ to be valid. The modified Bohm velocity ($u_B = \sqrt{\frac{eT_e}{m_+} \left(\frac{1+\alpha_s}{1+\gamma-\alpha_s} + \frac{1}{\gamma_+} \right)}$), determines the diffusion velocity of the positive ion at the sheath edge. Here $\gamma_+ = \frac{T_e}{T_+}$, $\gamma_- = \frac{T_e}{T_-}$ and $\alpha_s = \frac{n_{s-}}{n_{se}}$, where n_{s-} and n_{se} are the H^- density to electron density at the sheath edge. The extracted H^- current to electron current ratio can be related in a simple way using thermal flux model as $\frac{I_-}{I_e} = \frac{n_-}{n_e} \sqrt{\frac{T_- m_e}{T_e m_-}}$.

Sheath formation

A simplistic picture of collisionless sheath has been worked out. With the assumption that H^- to electron density ratio is very small, and by balancing flux and energy

we get [4]:

$$\frac{1}{r} \frac{d^2(r\phi)}{dr^2} = \frac{en_{se}}{\varepsilon_0} \left(e^{(\phi/T_e)} - \frac{1}{\sqrt{1-\phi/\varepsilon_s}} \right) \quad (12)$$

With the knowledge of n_{se} and $\frac{d\phi}{dr}$ at the beginning of the sheath, above equation has been numerically solved for ϕ .

RF Power coupling

With the plasma parameter close to high density discharge, we can ignore the capacitive coupling of RF power to the plasma. The Power is transferred from RF electric field to the plasma electron, which essentially carry the RF discharge current. The presence of magnetic field and non uniformity in the plasma density renders the Maxwells equation analytically non-solvable. We resort to numerical solution. Since plasma frequency (ω_{pe}) \gg RF frequency, it can be safely assumed that the displacement current is negligible compared to conduction current. Hence from Maxwells equation

$$\frac{d\tilde{H}_z}{dr} = -\frac{\omega_{pe}^2 \varepsilon_0}{\nu_{ef} + j\omega_{ef}} \tilde{E}_\theta + \frac{\omega_{pe}^2 \varepsilon_0 u_r \mu \tilde{H}_z}{\nu_{ef} + j\omega_{ef}} \quad (13)$$

$$\frac{1}{r} \frac{d(r\tilde{E}_\theta)}{dr} = -j\mu\omega \tilde{H}_z \quad (14)$$

Using above two equations, we can solve for \tilde{E}_θ and \tilde{H} with boundary condition, $E_\theta(r=0) = 0$ and $H(r=R) = H_0 \approx NI_{RF}$. Where N is the number of turn of RF antenna per unit length and I_{RF} is the RF current. Using complex Poynting theorem, the time average power flowing into the plasma chamber can be calculated.

IMPLEMENTED NUMERICAL SCHEME

The radius of the plasma chamber has been discretized in equal intervals. The j is the index, which runs from 0 to n , and n can be varied to increase the accuracy of the solution. At $r=0$, we assumed the value of n_i and u_i be known for all species. With this convention the continuity equation and the momentum balance for n_i gives respectively.

$$n_j u_j = \Gamma_j = \frac{r_{j-2} \Gamma_{j-2} + (G-L)_{j-1} r_{j-1} 2\Delta r}{r_j} \quad (15)$$

$$\frac{u_j - u_{j-1}}{\Delta r} + \frac{e}{mn_j u_j} T \frac{n_j - n_{j-1}}{\Delta r} + \frac{e}{mu_j} \frac{\phi_j - \phi_{j-1}}{\Delta r} + \nu_{efj} = 0 \quad (16)$$

Using (16) and (17) to eliminate u_i and solving for ϕ_j :

$$\phi_j = \phi_{j-1} - \left[\frac{1}{n_j^2} \left(\frac{m+\Gamma_i^2+f_j\Delta r\Gamma_i}{e} \right) - \frac{1}{n_j} \left(T_i n_{j-1} + \frac{m+u_{j-1}\Gamma_i}{e} \right) + T_i \right] \quad (17)$$

Now substituting the values of ϕ_j in the charge balance equation one can iteratively solve for n_j . Special care

should be taken at $j = 1$. Momentum balance gives $n_1 = n_0$ for all species and the continuity equation gives $n_i u_i = (G - L)_i \Delta r / 2$. Using this scheme, we compute the value of n and u as a function of r and stop when $u =$ Bohm velocity. We use particle and energy balance as check on the accuracy of the solution [1, 3]. If above criteria are not satisfied within the set accuracy limit, then program will adjust the parameter T_e and $n_e(r = 0)$ in such a way that it leads closer to the real solution. The integral involved in computing energy balance has been calculated numerically.

RESULT AND DISCUSSION

From Figure 1, it is evident that the different species shows maxima at the center of the chamber. This is because the loss due to diffusion is minimum in the central region. The density of the charged species changes sharply

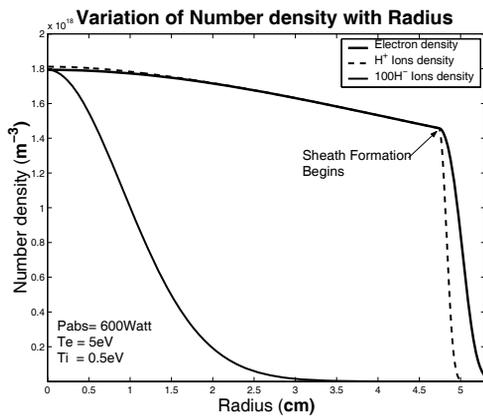


Figure 1: Density Profile of Different species

at the onset of the sheath formation. It is also clear that the density of the H^- ion become insignificant in the sheath region. Hence in the sheath region, the ion flux is essentially balanced by the electron flux and the quasi-neutrality is no longer valid. Within the plasma region, the H^- ion

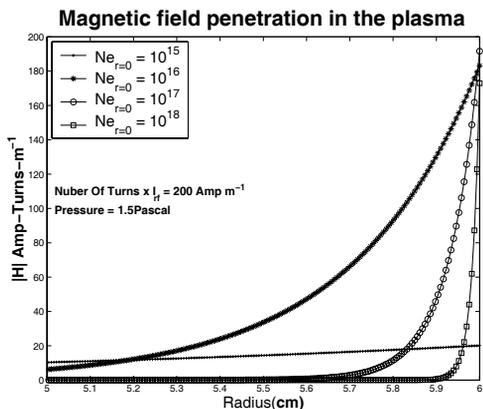


Figure 2: Profile of Magnetic field inside the plasma.

density decreases sharply towards the presheath edge, this

is possibly because electron and H^+ gain enough energy due to acceleration in the presheath potential, that it strips out an extra electron attached to the H^- ion. For computing penetration of electric and magnetic field in the plasma, the product of number of turns of RF antenna and RF current ($N \times I_{RF}$) is taken as input to the program. From the Figure 2 and Figure 3, it is clear that as the density of electron decreases the electric and magnetic field penetrates to a greater depth inside the plasma. The electric field decreases sharply for the low electron density. Thus there is crossover of electric field when we go from low electron density to high electron density. Such result has also been reported by experimental measurement [5]. The overall nu-

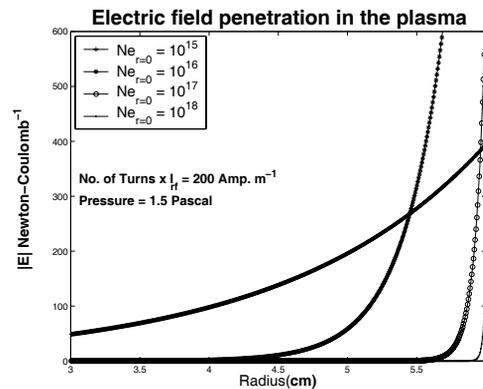


Figure 3: Profile of electric field inside the plasma.

merical scheme seems quite suitable for the simulation of the steady state equilibrium plasma of H^- ion source and are improved over uniform density model [3]. The other qualitative features are in good agreement with the experimental results of RF driven H^- ion source. In future work the sheath formation will be more accurately worked out considering collisional process. Further surface effect will be taken into account appropriately.

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