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NUMERICAL STUDY OF THE TIME BEHAVIOUR OF IMPURITY CONCENTRATION IN A TOKAMAK

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Numerical Study of the Time Behaviour of Impurity Concentration in a Tokamak

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Numerical analysis has been made of the time evolution in density profiles of the impurities in a Tokamak. The diffusion and atomic processes of impurities are treated simultaneously. Two different numerical methods were used; the results are in good agreement between the two. Calculations are made in the case of a constant spatial distribution of the plasma. The impurity concentration in the plasma is revealed. The procedure may be useful for analysis of the time evolution of a Tokamak plasma in computer simulation and for analysis of the impurities by spectrum measurement.

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数値計算によるトカマク中の不純物の挙動の解析

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トカマク中での不純物の密度の空間分布の時間変化を数値計算により解析した。不純物の拡散過程と原子過程の両方を同時に正しく取り扱うことができた。数値計算は，2つの異なった方法で行い，両方の結果は非常に良い一致をみた。プラズマの密度や温度の空間分布は時間変化しない場合に限って計算を行い，不純物がプラズマ中心に集積する様子を示す。本論文の手法は，トカマク・プラズマの計算機シミュレーションによる解析や不純物の分光測定の解析などに役立つものである。

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目　次　な　し

§1. Introduction

Impurities, small amounts of multiply charged ions, play an important role in Tokamak devices. It is well known that impurities enhance the radiation losses of a plasma and that the impurity-plasma ion collisions produce an inward diffusion of the impurities into the interior of the plasma. It is considered that impurities have serious effects on the confinement and heating of a plasma. Therefore, it seems to be very important to examine the behaviour of impurities in a plasma precisely. The impurity behaviour is a very complicated process which includes interactions with a plasma, wall interactions such as sputtering or recycling as well as the diffusion and atomic processes such as ionizations or recombinations of impurities.

In the present paper, we analyze numerically the time development of density profiles of impurities in a Tokamak plasma under a rather simple boundary condition. In this problem, the diffusion of impurities across the magnetic field and atomic processes such as ionizations or recombinations should be treated simultaneously in the analysis. For this problem, Tanaka et. al.[1)] obtained an analytic solution under the assumption of the uniform plasma. Tajima et al.[2)] have given a stationary solution taking the distribution of plasma into account. However, these works neglect the term of inward diffusion of impurities. On the other hand, impurity problems are treated in one dimensional Tokamak plasma simulation codes. However, it seems that the treatments of impurities are insufficient in almost simulation codes. In reference [3], the diffusion and atomic processes are analyzed separately. However, under an actual condition, the atomic process, especially the ionization time varies widely with the impurity state, and further it depends strongly on the electron temperature. Accordingly, the characteristic time of atomic process varies on a wide range and as a matter of course it sometimes becomes comparable with diffusion time. Therefore, the atomic and diffusion terms should not be analyzed separately. Since ionization and recombination rates depend on the electron temperature and the density gradient of plasma ion causes the inward diffusion of impurities, it is important that the spatial distributions such as density or temperature are included in the analysis.

In this paper, considering the plasma distributions, we present a numerical result of the spatial and temporal development of impurities analyzing the diffusion and atomic processes simultaneously. Two different numerical methods are adopted. Although the time variation of plasma profiles is not considered in the present work, it is not difficult to remove this restriction. A simplified particle flux is employed for the diffusion term in order to obtain an essential point of impurity concentration. However, the present procedure could be easily developed for the more complex diffusion process. Recyclings or sputterings are left as future problems and the analysis is worked out under a rather simple boundary condition.

In §2, we give the model for the computation, in §3, we present two different numerical procedures and in §4, numerical results are shown. Conclusions and some problems are summarized in the last section.

§2. Model for the computation

In this section, we present a simple model for the computation of the time evolution of the impurity concentration in the Tokamak plasma. Densities of impurities averaged over the magnetic surface are governed by the following conservation equations of particle numbers;

$$\frac{\partial I_k}{\partial t} = -\frac{1}{r}\frac{\partial}{\partial r}(r\Gamma_k) + n_e(\alpha_{k-1}I_{k-1} - \alpha_k I_k) - n_e(\beta_{k-1}I_k - \beta_k I_{k+1}), \tag{1}$$

$$(k = 1, 2, \ldots, K)$$

with

$$\alpha_0 = \beta_0 = \alpha_K = \beta_K = 0 \tag{1-a}$$

In Eq. (1), I_k is the number density of the impurity with $(k-1)e$ electric charge(s), I_1 and I_K being densities of the neutral atom and fully stripped ion with $(K-1)e$ electric charge, respectively. Γ_k is the particle flux of the impurity I_k, n_e is the electron density, α_k is the collisional ionization rate coefficient at which the state with k is ionized to the state with k+1 and β_k represents the radiative recombination rate coefficient from the state k+1 to k. The first term of Eq. (1) gives the diffusion process and the second and last terms are the creation and annihilation per unit time of the impurity I_k due to the ionization and recombination process, respectively.

On the basis of the neo-classical theory, the particle flux of impurity Γ_k is obtained by Connor in the banana regime[6], by Hinton and Moore in the banana-plateau regime[7] and by Tuda and Tanaka[8] and by Rutherford[9] in the Pfirsch-Schlüter regime. Although, it is necessary to use the results of the neo-classical theory properly in each regime, in the present paper, we restrict ourselves to the case of Pfirsch-Schlüter domain in order to get the essential point of the impurity concentration. The present method of the numerical calculation would not become difficult if we considered the generalization of the particle flux Γ_k. Further we consider only impurity-plasma ion collisions in the result of Tuda and Tanaka in the Pfirsch-Schluter region[8]. Then,

$$\Gamma_k = -D_k \frac{\partial I_k}{\partial r} + W_k I_k , \qquad (2)$$

with

$$W_k = D_k \frac{k-1}{Z_i} \frac{1}{n_i} \frac{\partial n_i}{\partial r} , \qquad (2\text{-a})$$

$$D_k = (1 + 2q^2)\, \nu_k \rho_k^2 , \qquad (k \neq 1) \qquad (2\text{-b})$$

$$\rho_k^2 = \frac{m_{ki} c^2 T_i}{(k-1)^2 e^2 B_Z^2} , \qquad (k \neq 1) \qquad (2\text{-c})$$

$$\nu_k = \frac{4}{3} \frac{\sqrt{2\pi}\,(k-1)^2 Z_i^2 e^4 n_i \ell n \Lambda}{\sqrt{m_{ki}}\; T_i^{3/2}} \qquad (2\text{-d})$$

Here, Z_i, n_i, T_i, m_i are the electric charge, density, temperature and mass of the background ion, B_Z the toroidal magnetic field, $\ell n \Lambda$ the Coulomb logarithm, e the electric charge, m_k the mass of impurity I_k and m_{ki} the reduced mass of m_i and m_k. Eq. (2) is derived under the assumption that all the ions have the same temperature T_i. The dffusion coefficient for the neutral atom D_1 is different from Eq. (2-b). This is estimated simply by taking the charge exchange between the neutral atom and proton into account in the reference [1]. The first term is the usual diffusion by the density gradient of impurity itself and the second term represents the so-called inward diffusion of impurities oriented to the direction of the density gradient of background ion. Impurity ions have the tendency to accumulation in the plasma center due to this effect[4,5].

It is difficult to estimate rate coefficients for ionization and recombination α_k, β_k correctly. Here, we employ the approximate estimation given by Hinnov[10]. That is,

$$\left.\begin{aligned} \alpha_k &= 5.9 \times 10^{-8} q_k (E_k^{k+1})^{-3/2} \sqrt{x_k}\, K_1(x_k), \quad [\mathrm{cm}^3/\mathrm{sec}] \\ \beta_k &= 5.2 \times 10^{-14} \cdot k \cdot x_k^{3/2} \cdot K_1(x_k), \qquad [\mathrm{cm}^3/\mathrm{sec}] \end{aligned}\right\} \quad (3)$$

$$x_k = E_k^{k+1} \cdot \chi_H / T_e \quad , \qquad (T_e\text{: in eV unit}) \qquad (3\text{-a})$$

$$K_1(z) = \int_z^{\infty} \frac{e^{-t}}{t}\, dt \quad , \qquad (3\text{-b})$$

where q_k is the number of valance electrons in the outermost shell, E_k^{k+1} is the ionization potential in rydberg unit to ionize the state k to k+1 and χ_H = 13.6 eV. Only ground states are considered and the dielectronic recombination[11] has not been included in Eq. (3).

In the present paper, we slove Eq. (1) numerically when the particle flux and rate coefficients are given by Eqs. (2) and (3), respectively. We neglect the effect of the diffusion and atomic processes of impurities on the background plasma, assuming that the impurity density is relatively small compared with that of plasma. Further, for simplicity, we assume the spatial distributions of plasma densities $n_e(r)$, $n_i(r)$, plasma temperatures $T_e(r)$, $T_i(r)$ and toroidal and poloidal magnetic fields $B_z(r)$, $B_\theta(r)$ to be constant with time. The present procedure could be easily extended to the case when these time variations of plasma were taken into account. If we consider the effect of impurities such as diffusion, atomic process or radiation loss on the plasma ions and electrons, we must use the Tokamak plasma simulation code[12] on the basis of one-dimensional conservation equations.

§3. Method of numerical calculation

The spatial difference equation for Eq. (1) becomes

$$\frac{\partial}{\partial t} I_{j-1/2}^{k} = -\frac{2}{r_j + r_{j-1}} \cdot \frac{1}{\Delta r}\left(r_j \Gamma_j^k - r_{j-1}\Gamma_{j-1}^k\right) + n_{j-1/2}^{e}\left(\alpha_{j-1/2}^{k-1} I_{j-1/2}^{k-1} - \alpha_{j-1/2}^{k} I_{j-1/2}^{k}\right) - n_{j-1/2}^{e}\left(\beta_{j-1/2}^{k-1} I_{k-1/2}^{k} - \beta_{j-1/2}^{k} I_{j-1/2}^{k+1}\right) \qquad (4)$$

$$\Gamma_j^k = -D_j^k \frac{1}{\Delta r}(I_{J+1/2}^k - I_{j-1/2}^k) + \frac{W_j^e}{2}(I_{j+1/2}^k + I_{j-1/2}^k) . \qquad (4\text{-a})$$

The subscripts j and j-1/2 stand for values at integral and half integral mesh points, respectively. The boundary condition at r=0 is $\partial I^k/\partial r=0$, that is $I_{1/2}^k = I_{3/2}^k$. As an another boundary condition, we give impurity densities $I_{J+1/2}^k$ at the outermost mesh point (J+1/2) which lies outside the plasma boundary r=a corresponding to the mesh point J-1/2. (See Fig. 1)

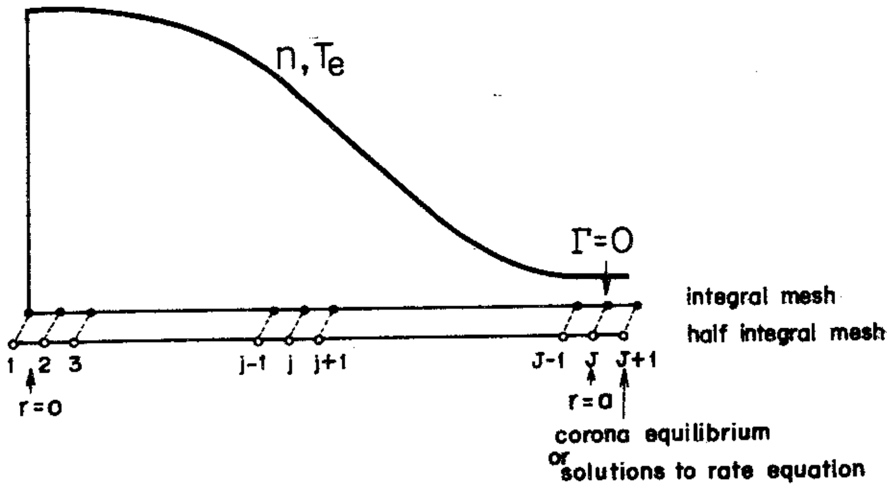

Fig.1 Diagram for numerical calculation

At the moderate electron temperature at the plasma periphery the low-Z particles such as I^1, I^2, ..., I^ℓ may already disappear by ionizations. Then, Eq. (4) hold for

$$j = 2, 3, \ldots, J,$$
$$k = \ell+1, \ell+2, \ldots, K . \qquad (\ell \geq 0)$$

If we replace $I_{j-1/2}^k$ by y_i, where $i = (k-1)(J-1) + j-1$, Eq. (4) becomes

$$\frac{\partial \vec{y}}{\partial t} = A\vec{y} + \vec{b} \quad . \qquad (5)$$

Here, $\vec{y}$ is a vector with components y_1, y_2, ..., y_N ($N = (K-\ell)(J-1)$), A is an N×N matrix and b is an N-components vector which is the boundary value at J+1/2. In general, b is a function of time.

We consider a simple boundary condition to solve Eq. (4). Neutral atoms of impurities, emitted from the wall and/or limiter by the bombardment of plasma particles and hot neutrals, are ionized quickly to produce the first few ionization degrees, then the impurities get distributed around the plasma periphery in a layer with a depth of the order of neutral atom mean free path (a few centimeters). In this layer, the ionization times are shorter than the particle confinement time only up to a limiting ionization degree[13]. We consider the following conditions;

i) The total particle flux of impurities vanishes at the plasma surface, that is,

$$\Gamma_J = \sum_{k=+1}^{K} \Gamma_J^k = 0 \tag{6}$$

ii) The corona equilibrium is established at J+1/2.

$$I_{J+1/2}^{\ell+\kappa} = \gamma_{\ell+\kappa} I_{J+1/2}^{\ell+\kappa}, \tag{7}$$

$$\gamma_{\ell+\kappa} = \frac{\alpha_{J+1/2}^{\ell+\kappa-1}}{\beta_{J+1/2}^{\ell+\kappa-1}} \frac{\beta_{J+1/2}^{\ell+\kappa-2}}{\beta_{J+1/2}^{\ell+\kappa-2}} \cdots \frac{\alpha_{J+1/2}^{\ell+1}}{\beta_{J+1/2}^{\ell+1}} \tag{7-a}$$

$$(\gamma_{\ell+1} = 1)$$

$$\kappa = 1, 2, \ldots, K-\ell. \qquad (\ell \geq 0)$$

The condition i) means that the total amount of impurities does not change with time inside the plasma. The second condition ii) is based on the consideration mentioned above. However, it takes long time to reach the corona equilibrium (Fig. 2) which is assumed only for simplicity. It would be better that we solve the rate equation at J+1/2. Under the conditions i) and ii), from Eq. (5) and (6),

$$I_{J+1/2}^{\ell+1} = -\sum_{\kappa=1}^{K-\ell} \left(\frac{D_J^{\ell+\kappa}}{\Delta r} + \frac{W_J^{\ell+\kappa}}{2}\right) I_{J-1/2}^{\ell+\kappa} \Big/ \sum_{\kappa=1}^{K-\ell} \left(-\frac{D_J^{\ell+\kappa}}{\Delta r} + \frac{W_J^{\ell+\kappa}}{2}\right) \gamma_{\ell+\kappa} \tag{8}$$

$I^{\ell+\kappa}_{J+1/2}$ ($\kappa \geq 2$) are determined by Eq. (7). Thus, the boundary values $I^{\ell+\kappa}_{J+1/2}$ are represented by a linear combination of unknown variables $I^{\ell+\kappa}_{J-1/2}$. Eq. (5) becomes to the following form;

$$\frac{\partial \vec{y}}{\partial t} = A'\vec{y} \quad . \tag{9}$$

Numerical calculations of Eq. (9) are performed by the following two different ways; 1) Hamming's predictor-corrector method[14), 2) solve the eigenvalue equation $\lambda\xi = A'\vec{\xi}$ of Eq. (9). In the latter case, we transform A' to a Hessenberg's form by the method of Gaussian elimination[15) and get eigenvalues λ_m ($m = 1, 2, \ldots, N$) by the double QR method[16). We write eigen vectors $\vec{\xi}_m$ in the form;

$$\vec{\xi}_m = e^{\lambda_m t}\,\vec{x}_m \quad . \tag{10}$$

We seak $\vec{x}_m$ by the inverse iteration method[17). If eigenvalues and eigenvectors of the system were found the solution could be written as

$$y_n = \sum_{m=1}^{N} c_m x_m^{(n)}\, e^{\lambda_m t} \tag{11}$$

$$(n=1,\ 2,\ \ldots,\ N)$$

whole $x_m^{(n)}$'s are elements of the vector $\vec{x}_m$. The initial condition gives the coefficients c_m's. We obtain c_m's solving the system of linear equations by getting the inverse matrix[18).

If the boundary condition is arbitray, we must solve Eq. (5). The solution to Eq. (5), satisfying the initial condition $\vec{y}(t=0) = \eta$, is given by

$$y(t) = y_h(t) + \Phi(t)\int_0^t \Phi^{-1}(s)\vec{b}(s)ds \ , \tag{12}$$

where $\vec{y}_h(t)$ is the solution to $\partial\vec{y}/\partial t = A\vec{y}$, satisfying the same condition $\vec{y}_h(t=0) = \eta$ and Φ is a basic matrix of A.

§4. Numerical examples

First, we solve the rate equation which is given from Eq. (1) by neglecting the diffusion term. This equation is

$$\frac{\partial I_k}{\partial t} = n_e(\alpha_{k-1}I_{k-1} - \alpha_k I_k) - n_e(\beta_{k-1}I_k - \beta_k I_{k+1}) \tag{13}$$

$$k = 1,\ 2,\ \ldots,\ K$$

The stationary solution to Eq. (13) gives the corona equilibrium. As described in §3, Eq. (13) is solved both by the method of Hamming's predictor-corrector and by solving the eigenvalue equation. These two different numerical procedures have given the same result. The numerical result is shown in Fig. 2 for oxygen impurities. At $t = 0$, the density of OI (oxygen neutral atom) is $10^{10}/\mathrm{cm}^3$ and others are zero. The curves show the time development of the density of oxygen in each ionization state.

Two different approaches to the numerical calculation have also yielded a fairly good agreement for Eq. (1). Fig. 3 shows the result for oxygen impurities ($K = 9$). We have assumed that OI and OII have already ionized to vanish until they reached the plasma boundary ($\ell = 2$). The numbers of mesh points are 20 ($J = 19$). Fig. 3-(a) shows the distributions of plasma density $n(= n_e = n_i)$, electron and ion temperature T_e, T_i, current density J_z and safety factor q. It is assumed that these do not change during the time development of impurities. In Fig. 3-a, we have given the distributions approximated to the result measured in the impurity experiment of JFT-2 Tokamak[19]. Fig. 3-(b) shows the initial distribution of oxygens which is given properly on the assumption that the impurities with low-Z charges are distributed around the plasma periphery at the early phase of the discharge. At the plasma boundary (the outermost mesh point), the corona equilibrium is given. Fig. 3-(c), (d), (e) and (f) show the distribution at 10^{-4} sec, 10^{-3} sec, 10^{-2} sec and 0.6 sec, respectively. Impurity ions of low-Z are lost successively with time and accordingly, high-Z impurities appear and diffuse toward the plasma center. At 0.6 sec, Fig. 3-(f), a steady state is completely established. At the steady state low-Z ions have disappeared, and OVII, OVIII and OIX have accumulated in the plasma center. The peaking is shaper as Z increases.

The computations were performed by using FACOM 230/60 of the data processing center in JAERI.

§5. Conclusions and summary

Exact numerical computations have been performed for Eq. (1), which is frequently met in the Tokamak simulation code or in the spectrum measurement. Although, we have solved Eq. (1) under several assumption considered. We can easily include the banana and platean region, the effect of temperature gradient and impurity-impurity collisons on the particle flux Γ_k in the neo-classical theory. As a boundary condition, the solution to rate equation is preferable than the corona equilibrium. For heavy elements (F_e, M_o etc.), it is necessary to consider the sputtering and recycling instead of the first boundary condition given by Eq. (6). The initial condition given here is rather unsatisfactory. It is one of the way that we give an initial condition by solving the Boltzman transport equation for the neutral atom of impurity considering charge exchanges as well as ionizations and recombinations. Considering these, we should develop the computer code to treat the time variation of plasma distribution. A numerical analysis of the spectrum measurement of carbon and oxygen impurities in JFT-2 Tokamak[19] is now being performed by extending the present method. A further investigation of the effect of Tokamak impurity will be expected by using the Tokamak computer code with the impurity routine based on the present procedure.

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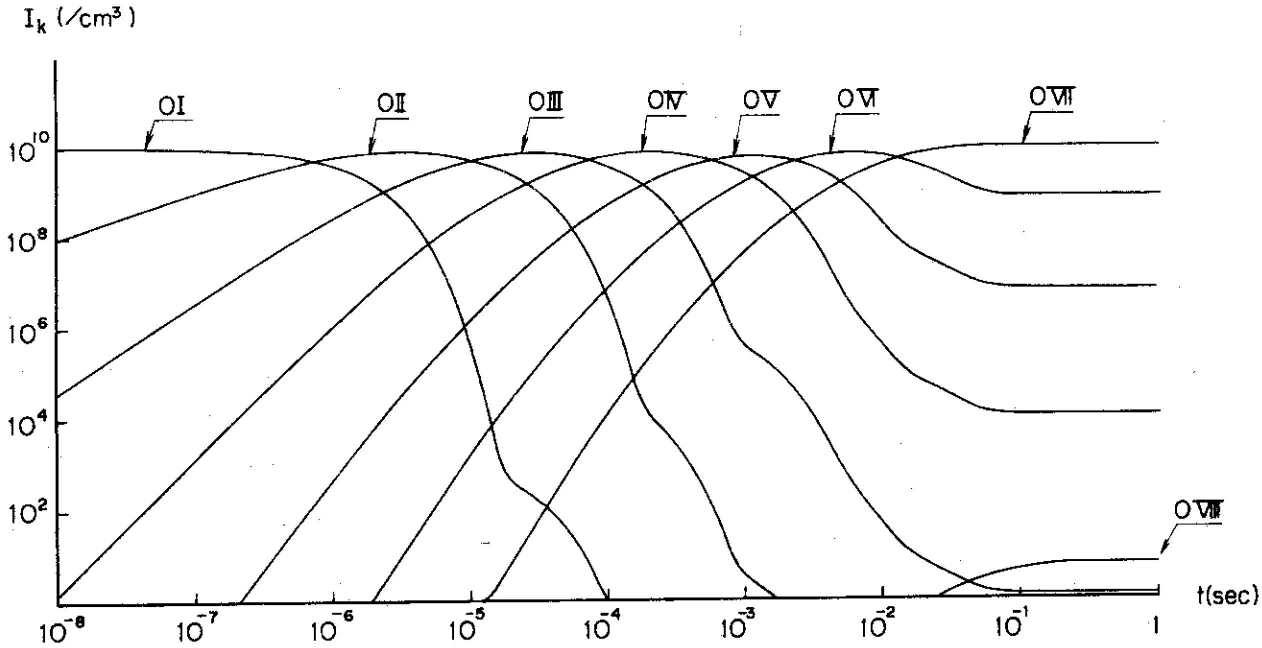

Fig. 2-(a) Te = 30 eV

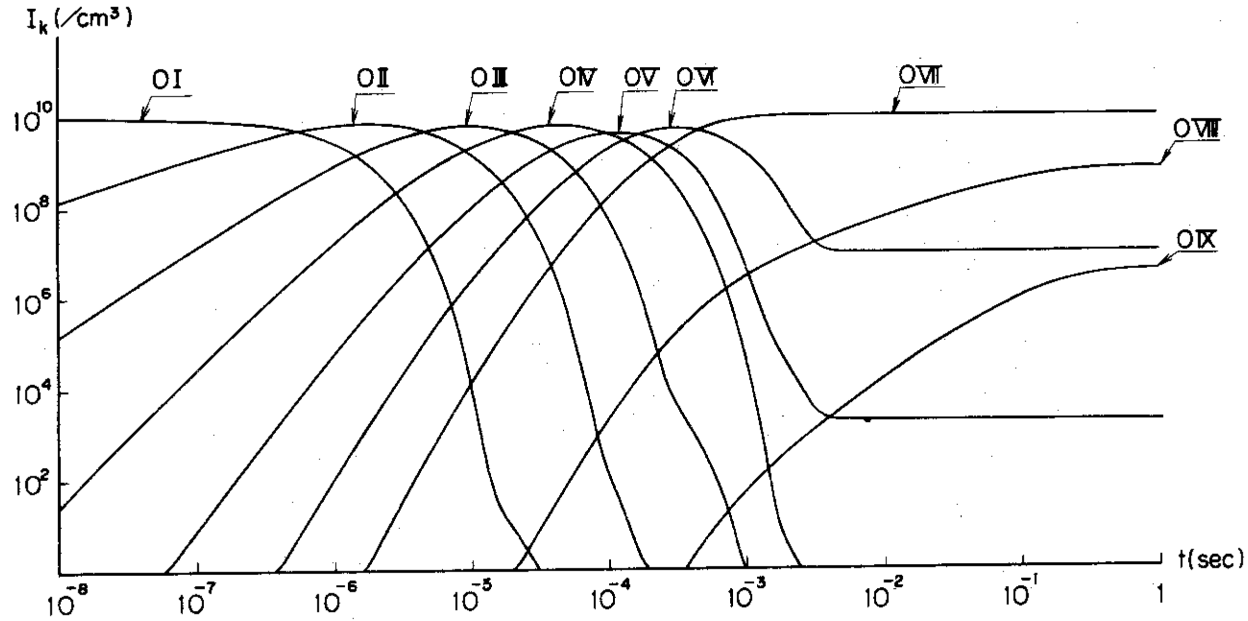

Fig. 2-(b) Te =100 eV

Fig. 2 Solutions to rate equation given by Eq. (13) for oxygen impurities. At t=0, the density of OI is $10^{10}/cm^3$ and others are zero.

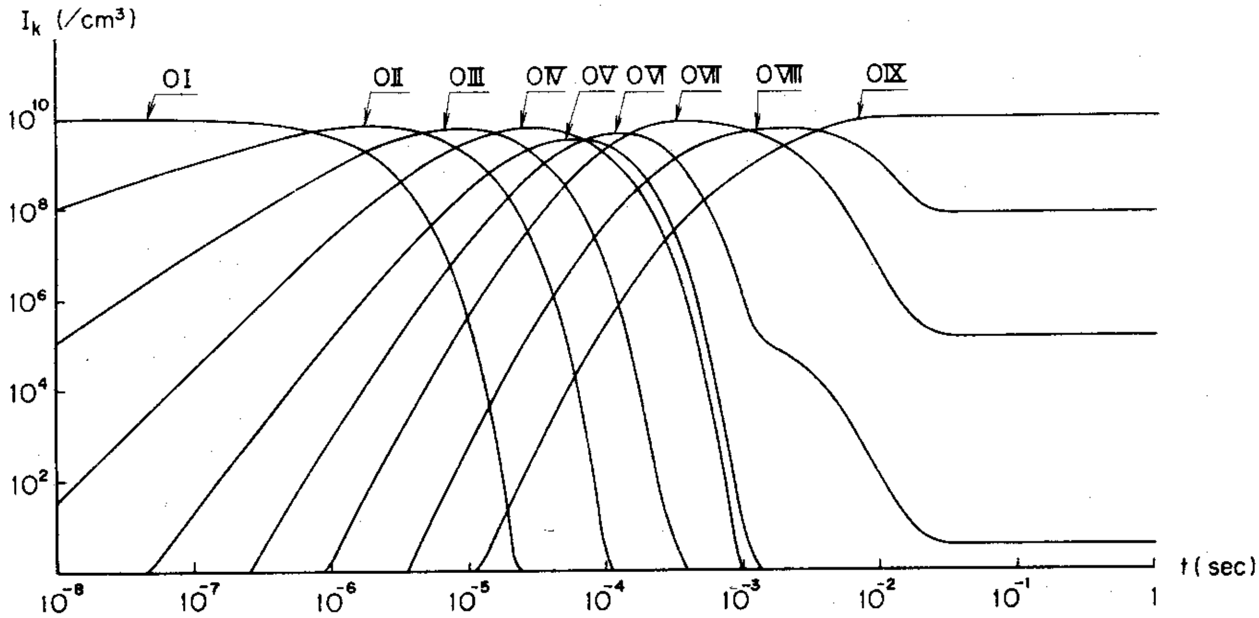

Fig. 2-(c) Te = 1000 eV

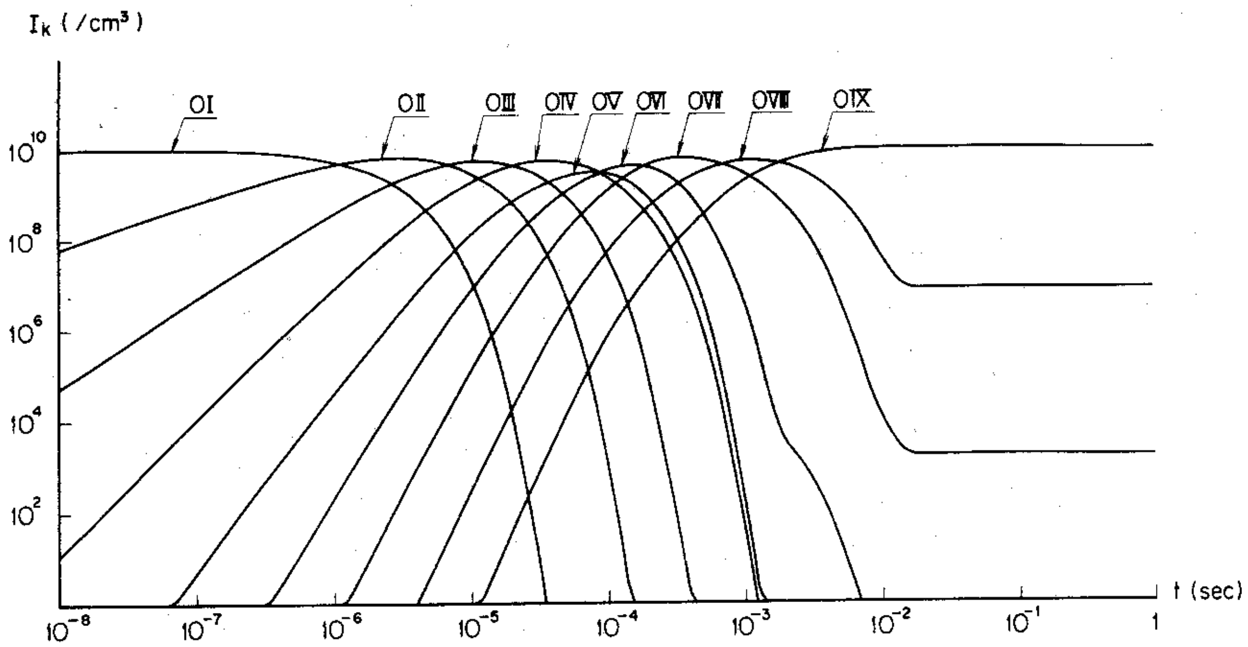

Fig. 2-(d) Te = 5000 eV

Fig. 2 (continued)

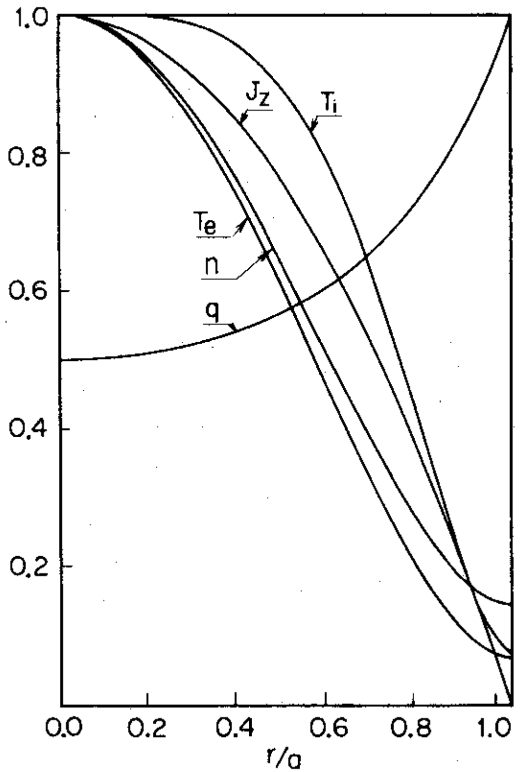

Fig. 3-(a) radial profiles of n, Te, Ti, J_z, q.
maximum : n = 1.4×10^{13}/cm^3, Te = 300.0 eV
T_i = 200.0 eV, q = 4.46

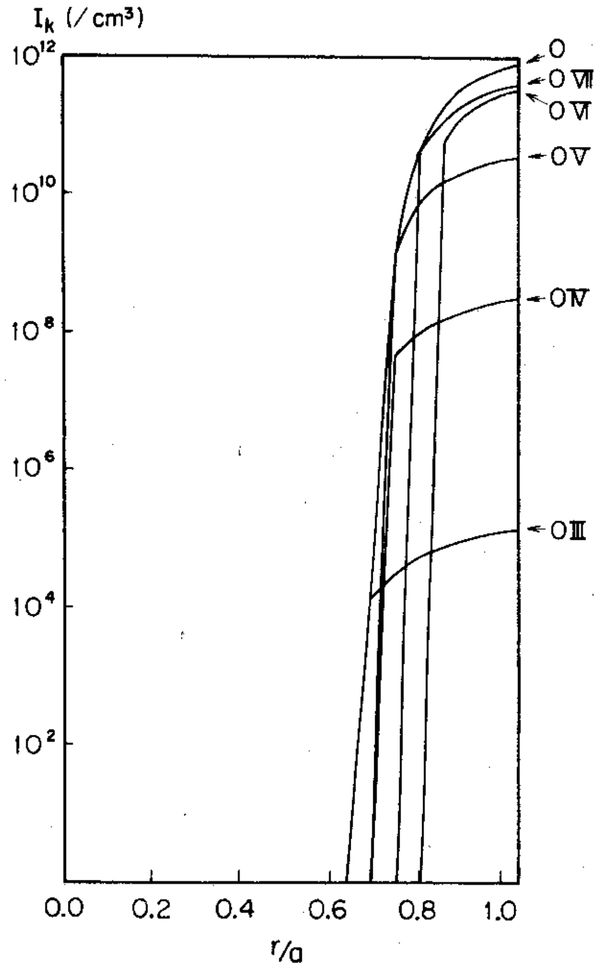

Fig. 3-(b) initial condition for oxygen impurity

Fig. 3 Time development of the densities of oxygen impurities. The plasma distribution given by Fig. 3-(a) is fixed throughout the computation. Fig. 3-(b) is the initial distribution given here and others, the solution to Eq. (1), show the impurity concentration.

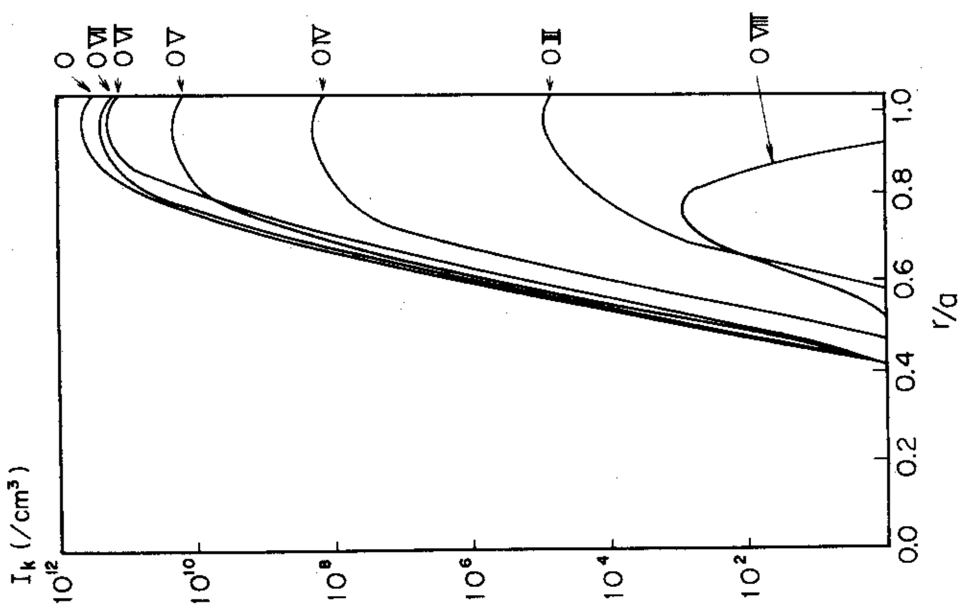

Fig. 3-(c) $t = 10^{-4}$ sec

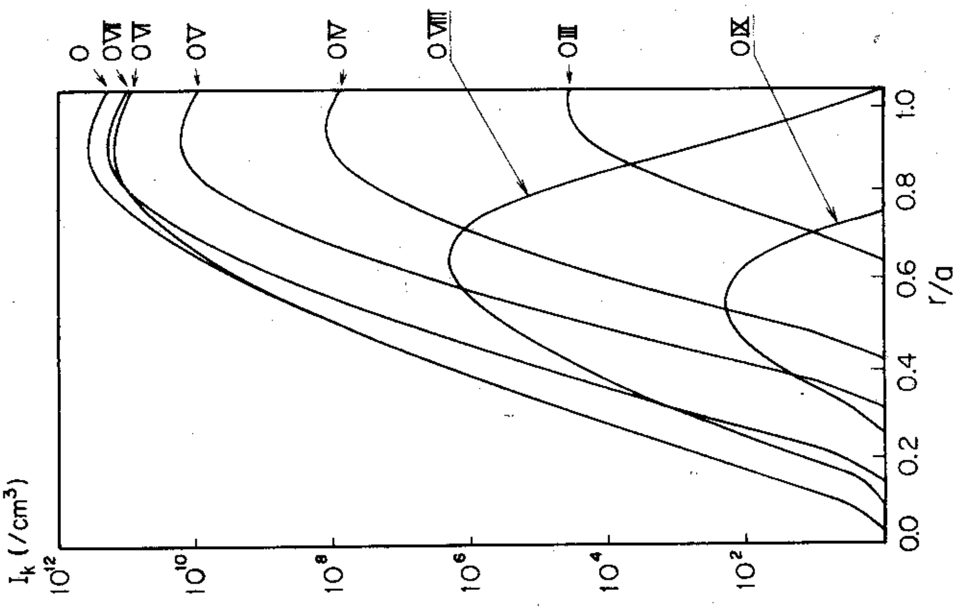

Fig. 3-(d) $t = 10^{-3}$ sec

Fig. 3 (continued)

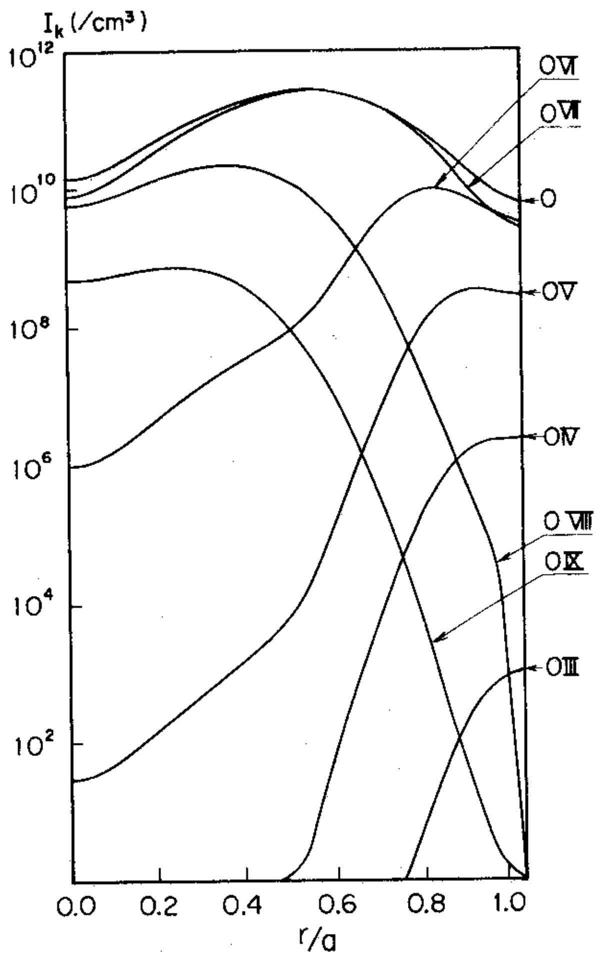

Fig. 3 – (e) $t = 10^{-2}$ sec

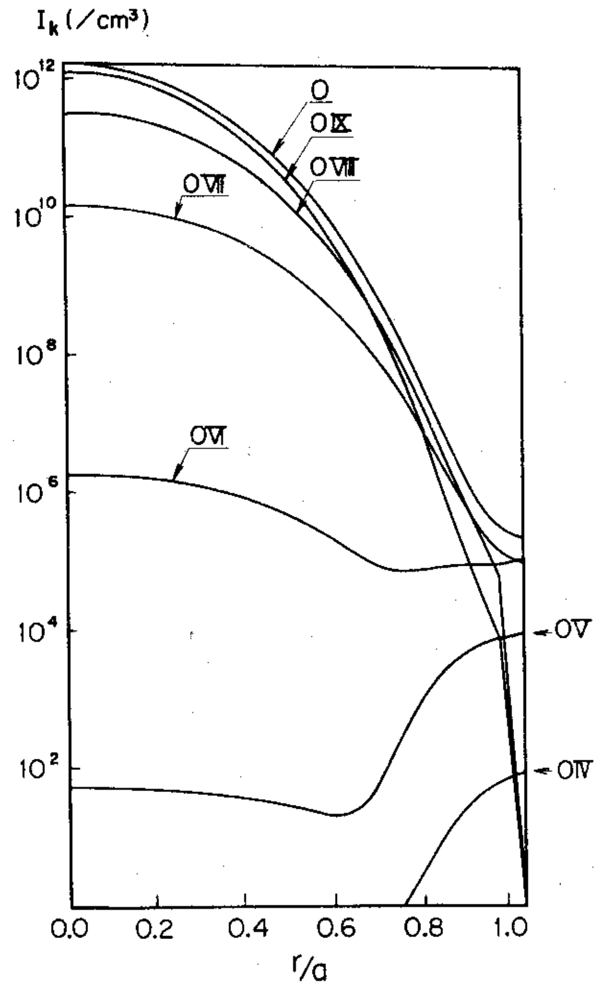

Fig. 3-(f) $t = 0.6$ sec (stationary state)

Fig. 3 (continued)