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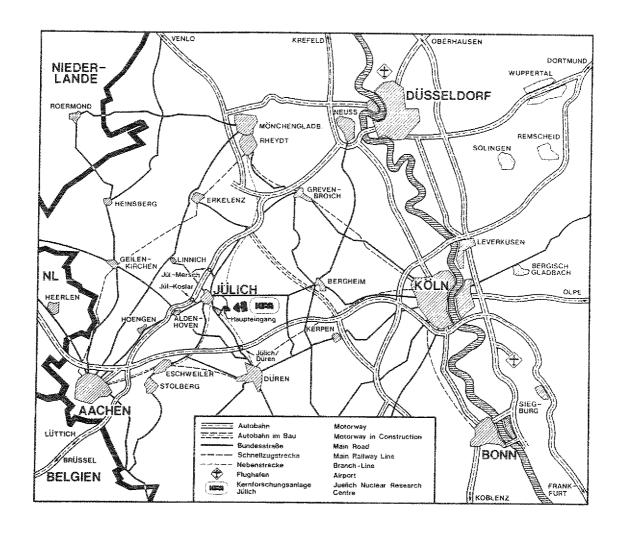
# IRON TRANSPORT IN A CONFINED HIGH-TEMPERATURE PLASMA

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# IRON TRANSPORT IN A CONFINED HIGH-TEMPERATURE PLASMA

by

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#### Abstract

The neo-classical flux,  $\Gamma_{\text{n.c}}$ , of Fe XXIII is calculated for the experimental conditions produced in PLT by using the data on the iron density profiles and the plasma parameters. The actual flux of Fe XXIII, reserved. is then evaluated from the continuity equation, by using the same data.  $\Gamma_{\text{c.e}}$  is on the average two orders of magnitude larger than  $\Gamma_{\text{n.c}}$ , the neo-classical prediction. These results are further tested by introducing the neo-classical coefficients which are multiplied by various anomaly factors into the continuity equation and solving for the density profile of Fe XXIII, using the experimental profiles of Fe XXII and Fe XXIV as given. The results of this section indicate that the first and the second terms in the neo-classical flux expression,  $\Gamma_{n,c} = -D_1(dn/dr) + D_2n$ , should be multiplied approximately by the factors (100) and (25), respectively in order to yield the experimentally observed profile of Fe XXIII. Furthermore, a sensitivity analysis is performed to investigate the dependence of the value of the flux, I on the uncertainties in the rate coefficients. This dependence is found to be quite sensitive. Uncertainties of a factor of two in these coefficients could yield radially inward or outward fluxes, which are by orders of magnitude larger than the flux computed without uncertainty factors.

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#### 1. Introduction

Impurities and their behavior in plasma confinement devices have become one of the most important research fields in fusion during the recent years. This results from their significant contribution to the radiative power losses, the electrical resistivity, other transport coefficients, the ionization rates and efficiencies of injected neutral beams. They could also be responsible for some instabilities and potentially influence the coupling of high frequency waves to the plasma. Recent spectroscopic measurements and the models applied for their interpretations have revealed a considerable amount of information on the behaviour of light impurities /1-5/. They are now developing rapidly to allow a description of the heavy impurity transport /6-11/.

Most of the published experimental results, concerning impurities have been discussed and interpreted by various groups and some tentative conclusions regarding the impurity transport mechanisms in tokamaks have been drawn. Cohen, Cecchi and Marmar /1/ have concluded that the behaviour of aluminium ions, as observed in the ATC experiments, agrees rather well with the neo-classical predictions. Similar statements have been made by Peacock et al. /5/, basing on the oxygen radiation profiles observed in DITE. On the other hand, Tazima, Nakamura and Inoue /12/ have suggested that the diffusion coefficients should be multiplied by anomaly factors on the order of 10 to explain to carbon and oxygen transport in the ST and TFR experiments, whereas Abramov /13/ reports that the neo-classical theory can account for the tungsten transport in the ISX-A device but that an anomalous diffusion term is needed to explain the majority of the impurity profiles observed in other devices.

A number of possible reasons can be invoked to explain the conflicts in these interpretations and conclusions:

a) In general, the quantitative evaluation of the density profiles from the line intensities, using some Abel inversion technique, can be subject to errors.

- b) In most of the previous works, the interpretations were based on experimental data related to light impurity ions, in particular. These ions radiate in edge regions of the plasma, since they are fully stripped in the central zones. Steep gradients, in particular of the electron temperature are superimposed on those of the impurity ion concentrations. This and the fact that the theoretical modeling, even for a pure hydrogen plasma, is poor in these regions can make it difficult to draw definite conclusions from these measurements.
- c) It must also be mentioned that the neo-classical flux expressions used in most of the previous works are incomplete, in the sense that the temperature gradients and/or the contributions of other impurity ions are ususally neglected. The comparison of flux values obtained from such incomplete expressions, with the values obtained from the continuity equation may again lead to conflicting conclusions.
- d) The calculation of impurity fluxes from the cont inuity equation may be very sensitive to the uncertainties in the rate coefficients used. Hawryluk, et.al. /17/ have illustrated theoretically that the rate coefficients provided by different authors lead to significantly different profiles of light impurities. Furthermore, the TFR group /1!/ has stated that, within an uncertainty factor of two in the ratio of the ionization to recombination rate coefficients, their experimental results on heavy impurities would agree well with the ionization-equilibrium calculations. It can therefore be presumed that the differences in the rate coefficients used by various authors may be one of the most important reasons for the differences in their interpretations, related to the impurity flux.
- e) Finally, the contributions of additional effects, of which the magnitudes could vary significantly from one experiment to another, are usually neglected in flux calculations based on the continuity equation. At least two candidates exist: inner shell excitation followed by an auto-ionization step and charge exchange reactions between the impurities and neutral

hydrogen atoms. Uchikawa et.al./14/ state that depending on the level structure and the temperature, the auto-ionization rate coefficients can be comparable to the generally accepted ionization rate coefficients. The results of Olson et.al./15 indicate that the charge exchange cross sections between impurities and neutral hydrogen atoms is on the order of 10<sup>-14</sup> cm<sup>2</sup>. This implies that for the heavy impurity ions, the charge exchange and ionization rate coefficients will be comparable when the neutral hydrogen density is equal to or larger than 10<sup>-5</sup> times the electron density. The neglect of these processes can possibly explain the diverging opinions which originated from the previous analysis.

One aim of the TEXTOR programme at Jülich is to study the release of impurities from the walls of a confinement device and their subsequent behaviour in the plasma. Before undertaking exhaustive spectroscopic observations, it appears important to make the inventory of existing data and of the state of understanding and to compare experimental results with existing theoretical models in order to decide on which points, if any, the future efforts should be concentrated.

In this work, we therefore examined the impurity transport and evaluated some of the reasons which may have led to the diverging conclusions mentioned above. For this, we have analysed an extensive set of data on the profiles of highly ionized iron impurities, which have been presented by the PLT team /7,8/. The experimental results contain practically all the information required to compute the flux of Fe XXIII in the central region using the continuity equation and to compare it with the value expected from the neo-classical model. Therefore, this particular ionization state has been chosen as the subject of interest of our work. Since we do not have access to the experiments concerned, we cannot comment on the experimental uncertainties mentioned in the first item (a) above. Due to the fact that the investigation of the behaviour of Fe XXIII requires only experimental data obtained from the near-central region, the difficulties and uncertainties in the near-wall regions mentioned in the second item (b) should be consider-

ably reduced. In order to decrease the errors in the evaluation of the neo-classical flux, mentioned in the third item (c), we have taken into consideration the temperature gradients and, as far as information was available, the expected contribution of other ionization states present at the same region. The possible contribution of experimental errors and in particular the potential role of impurities of which the density profiles are missing, are discussed. The flux of Fe XXIII,  $\Gamma_{\rm c.e}$ , is then evaluated from the continuity equation and the anomaly factors in the neo-classical transport coefficients required to yield this flux are evaluated. Finally, the errors in  $\Gamma_{\rm c.e}$ , resulting from the uncertainties present in the rate coefficients as mentioned in the last two items, are estimated and discussed.

### 2. The Experimental Data Used

The local emissivities of Fe XV, Fe XVIII, Fe XXII, Fe XXIII and Fe XXIV have been measured in a recent experiment in PLT /8/ and the corresponding density profiles have been obtained by dividing these emissivities by the separately measured electron densities and the calculated excitation rate coefficients /18, 19/. In order to evaluate the flux of a particular ion from the continuity equation, the density profiles of this ion and of its adjacent ionization states must be known. Therefore, the flux of Fe XXIII is chosen as the subject of interest for our calculations. As far as the plasma region is concerned, the calculations are limited to the  $r \leq 15$  centimeters range, although published data on the density profiles of Fe XXII, Fe XXIII and Fe XXIV extend further outwards. This restriction is due to the fact that the strong resonance line of Fe XXIII at 132.9  $^{
m o}{
m A}$ overlaps with a Fe XX resonance line at 132.86 OA. Although the transition probability corresponding to the latter is smaller, the Fe XX line may make an appreciable contribution at the edge of the Fe XXIII distribution, i.e. between r ~ 15 and 20 centimeters /18/. The density profiles of the

ionization states mentioned above are illustrated in Figure 1 for the range  $r \leq 15$  centimeters.

The plasma parameters, on the other hand, required for the flux evaluations are the electron and ion temperatures, the densities and the safety factor q. The ion temperature is estimated from the given electron temperature profile and the Doppler broadening of Fe XX and Fe XXIV lines. The plasma ion density is taken to be 15 % less than the electron density, since the total iron density in the region concerned is approximately 0.75 % of the electron density and their average contribution to the electron density is roughly 20 electrons per atom. The measured electron density and temperature profiles, the safety factor and the estimated ion temperature profile are plotted in Figure 2.

Finally, the calculated ionization rate coefficients /20, 21/ of
Fe XXII and Fe XXIII are plotted together with the radiative and dielectronic recombination rate coefficients /16/ of Fe XXIII and Fe XXIV in
Figure 3. Their radial variations can easily be obtained by using the
electron temperature profile shown in Figure 2.

## 3. The Neo-Classical Flux, Inc., of Fe XXIII

Various expressions for the neo-classical flux of impurities in To-kamaks have been derived during the past few years. Rutherford /22/ has considered the case where both the impurity and the plasmaions are in the Pfirsch-Schlüter regime and assumed that only one impurity species is present. Cohen et al. /1/ have generalized these results by considering the case of multiple-ion species but have neglected the temperature gradients. Samain and Werkoff /23/ have again considered the case of a single impurity species in the Pfirsch-Schlüter regime, whereas the plasma ions were allowed to be in any of the three regimes. The results of Engelmann and Nocentini /24/ seem to be most appropriate for this work, since they have considered

the case of multiple-ion species, all in the collision-dominated regime and taken into account the temperature gradients and the energy transfer between ions and electrons, thus offering a most general expression for this regime.

In order to check whether all the ions in the experiments concerned were in the collision-dominated regime, the following criterion /24/ is applied,

$$\omega < v^{\text{tot}} < \Omega, \\
\text{bj j}$$
(1)

where  $\omega_{\rm bj}$ ,  $v_{\rm j}^{\rm tot}$  and  $\Omega_{\rm j}$  are the bounce frequency, the total collision frequency and the cyclotron frequency of the j-th species, respectively. It is sufficient to check this criterion for the plasma ions only, since it is well known that the heavy impurity ions are always in a more collisional regime. For the given values of ion temperature, the safety factor and the 30 kGauss magnetic field, the bounce and the cyclotron frequencies for the deuterium ions are roughly 3 x 10<sup>4</sup> s<sup>-1</sup> and 2.5 x 10<sup>7</sup> s<sup>-1</sup>, respectively. The ion-electron and the ion-impurity collision frequencies for the range of interest are typically on the order of 2 x 10<sup>4</sup> s<sup>-1</sup> and 10<sup>4</sup> s<sup>-1</sup>, respectively. Considering the fact that there are six or seven impurity species in the region considered, with more or less equal contributions to the collisions with plasma ions, it can safely be stated that the criterion applies to all the ions in this case.

Therefore the following expression for the neo-classical impurity flux /24/ is adopted,

$$(\Gamma_{n,c})_{I} = \Gamma_{Ii} + \sum_{I' \neq I} \Gamma_{II'}$$
(2)

where, 
$$\Gamma_{\text{Ii}} = \frac{e_{i}}{e_{\text{I}}} q^{2} \frac{r^{2}_{\text{Li}}}{\tau_{\text{iI}}} \frac{1}{T_{i}} \left\{ \left[ c_{1}(\alpha) + \frac{1}{1 + s_{\text{ie}}^{2}} \frac{c_{2}^{2}(\alpha)}{c_{3}(\alpha)} \right] \left[ \frac{dP_{i}}{dr} - \frac{e_{i}n_{i}}{e_{\text{I}}n_{\text{I}}} \frac{dP_{\text{I}}}{dr} \right] \right\}$$

$$\begin{split} &-\frac{5}{2}\frac{1}{1+s_{ie}^{2}}\frac{c_{2}(\alpha)}{c_{3}(\alpha)}n_{i}\frac{dT_{i}}{dr}+\frac{1}{1+s_{ie}^{2}}\frac{c_{2}^{2}(\alpha)}{\alpha c_{3}(\alpha)}\sum_{I'\neq I}\alpha_{i}^{I'}\left[\frac{e_{i}n_{i}}{e_{I}n_{I}}\frac{dP_{I}}{dr}\right] \\ &-\frac{e_{i}n_{i}}{e_{I'}n_{I'}}\frac{dP_{I'}}{dr}\right], \end{split}$$

$$\Gamma_{II'} = - q^2 \frac{r_{LI}^2}{T_I} \frac{\ell_{II}^{II'}}{m_{I}^n_{I}} \left[ \frac{d^P_I}{dr} - \frac{e_{I}^n_{I}}{e_{I'}^n_{I'}} \frac{d^P_{I'}}{dr} \right],$$

 $e_i$ ,  $r_{Li}$ ,  $r_i$ ,  $r_i$ ,  $r_i$ ,  $r_i$  and  $r_i$  represent the charge, Larmor radius, temperature, pressure, density and the mass of plasma ions, respectively. When the subject "i" in these notations is replaced by I and I', then the notations refer to the impurity ion considered and to the other impurities, respectively.  $r_{iI}$  is the ion-impurity collision time given as

$$\tau_{iI} = \frac{3\sqrt{m_i} T_i^{3/2}}{4\sqrt{2\pi} \ln \lambda e_i^2 e_I^2 n_I},$$

sie is the coupling coefficient for the energy transfer between ions and electrons and

$$\alpha_{j}^{j,'} = \frac{e_{j,n_{j,'}}^{2}}{e_{j,n_{j,'}}^{2}},$$

$$\alpha = \sum_{\mathbf{I}^*} \alpha_{\mathbf{i}}^{\mathbf{I}^*} + \alpha_{\mathbf{i}}^{\mathbf{I}}.$$

 $c_{j}(\alpha)$  and  $\ell_{11}^{II}$  are given in references /22/ and /25/, and  $\ln\lambda$  is the Coulomb logarithm which roughly takes the values, 17, 14 and 11 for  $\tau_{ii}$ ,  $\tau_{iI}$  and  $\tau_{II}$ , respectively, for the range of interest.

An order of magnitude estimate shows that  $s_{ie}^2$  is much smaller than unity and can be neglected. However, the contributions of the other impurities, in particular through the  $\Gamma$  term, are not negligible at all and  $\Pi$ can be comparable to the contributions of the plasma ions to the impurity flux, at some radial distances. This is unfortunate, since some impurity profiles are not available. The missing profiles, that would be of interest in the region concerned, are those of Fe XIX, Fe XX, Fe XXI, and Fe XXV. A rigorous discussion of the errors resulting from their omission indicates that their main contribution would be through terms involving their pressure gradients which sould be added algebraically to the components  $\Gamma_{ ext{II}}$ , since the coefficients  $c_{i}(\alpha)$  and  $\ell_{i}^{II}$  are slowly varying functions of  $\alpha$  and the summation in the component  $\Gamma_{Ti}$  is already small compared to the other terms in this component. In order to estimate the contribution of the omitted ionization states to the flux of Fe XXIII, the sum of the components  $r_{II}$ ,  $\Gamma_{\text{Ii}}$  and the total neo-classical flux,  $(\Gamma_{\text{n.c}})$ , are evaluated with the given profiles and plotted separately in Figure 4. The summation of the impurityimpurity components seems to be at most 30 % of the ion-impurity component for r < 12 centimeters. It increases rapidly up to 60 % at r = 15 centimeters, due to the steepening profile of Fe XVIII in this local region. Referring to Figure 1, it can be seen that the missing profiles are unlikely to present very steep gradients in the region of interest; it can furthermore be predicted that the contribution of Fe XXV and the total contribution of the other three missing profiles would be opposite in sign. The net error resulting from neglecting these ionization states should therefore be even smaller than 30 %. These arguments lead us to conclude that the solid curve in Figure 4 should be a fairly good approximation of the neo-classical flux of Fe XXIII.

Some general conclusions, regarding the evaluation of the neo-classical flux of impurities from experimental profiles, can also be drawn. It can be

stated that, the precision in determining the impurity profiles is not critical and knowing the density profiles of all the other impurities in the region investigated is not of vital importance, but neglecting their contributions altogether would be quite misleading, especially when the degree of accuracy aimed at is within a factor of two. On the other hand, the temperature gradients must always be taken into consideration, since they constitute the fundamental terms in the neo-classical flux expression, as can be seen from equation (2).

# 4. Computation of the Flux $\Gamma_{\text{c.e}}$ from the Continuity Equation

Provided that the relevant rate coefficients and density profiles are known, the flux  $\Gamma_{\rm I}$  of a particular ionization state I, can be computed in a straightforward fashion from the complete continuity equation

$$\frac{\partial n_{I}}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (rr_{I}) = n_{e} \left[ s_{I-1,I} n_{I-1} + \alpha_{I+1,I} n_{I+1} - (s_{I,I+1}) + \alpha_{I,I-1} n_{I-1} \right], \qquad (3)$$

where  $n_{\rm I}$  represents the density of the ionization state I,  $n_{\rm e}$  is the electron density, the letters s and  $\alpha$  represent the ionization and the recombination rate coefficients, respectively. The ionization is considered to be due to electron collisions in the ground state. Both the radiative and dielectronic recombination processes are taken into account. The adequacy, or rather inadequacy of considering only these processes will be discussed in the following sections.

Since the available density profiles were obtained in the steady state, the flux can be written from equation (3) as

$$(r_{c.e})_{I} = r^{-1} \int_{0}^{r} f_{I}(r^{\dagger}) dr^{\dagger},$$
 (4)

where,

$$f_{I}(r) = rn_{e} \left[ s_{I-1,I} n_{I-1} + \alpha_{I+1,I} n_{I+1} - (s_{I,I+1} + \alpha_{I,I-1}) n_{I} \right]$$

and the subscripts (c.e) are used for the flux to indicate that it is the flux obtained from the continuity equation, distinguishing it from the neo-classical flux,  $(\Gamma_{n,c})_{\rm I}$ . Inserting the data given in Figures 1, 2 and 3, the function  $f_{\rm I}(r)$  can be plotted for Fe XXIII and integrated graphically, as shown in Figure 5. The flux of Fe XXIII is then evaluated according to equation (4) and plotted again in the same figure. It can be seen that, on the average, this flux is approximately two orders of magnitude larger than the neo-classical flux; this suggests strongly that some anomalous mechanism should be involved.

#### 5. Determination of the Anomaly Factors

It is in principle possible to evaluate the density profile of Fe XXIII from the continuity equation, if the density profiles of the neighbouring ionization states Fe XXII and Fe XXIV have been measured, if accurate values of the rate coefficients concerned are available and if the transport mechanism and the associated anomaly factors are known. This approach allows then to select the appropriate values of transport coefficients by solving accordingly for the density profile of Fe XXIII and by comparing the result with the profile experimentally observed.

Since internal disruptive instabilities or other phenomena of strong-ly nondiffusive nature have not been explicitly reported to occur during the experiments concerned, the particle is assumed to obey phenomenologically a law similar to equation (2), the flux being given by the sum of two terms proportional to  $\mathbf{n}_{\mathrm{I}}$  and  $\mathrm{dn}_{\mathrm{I}}/\mathrm{dr}$ , respectively. Anomaly factors are therefore introduced in the conventional way /12/ by writing the flux expression in the following form,

$$(\Gamma_{n,c})_{I} = -A_{I}D_{I}(r) \frac{dn_{I}}{dr} + A_{2}D_{2}(r)n_{I}$$
, (5)

where  $A_1$  and  $A_2$  are some constant anomaly factors. Equation (2) must now be written in the above form.

Using the density profiles of the impurities, the term  $\alpha$  in equation (2) is found to be varying roughly from 3.4 to 2.4 in the region of interest. The values of the coefficients  $c_1(\alpha)$ ,  $c_2(\alpha)$  and  $c_3(\alpha)$  range from 0.39 to 0.42, from 1.05 to 0.96 and from 6.5 to 5.5 and are therefore taken as 0.4, I and 6, respectively. It is also found, using the experimental data, that the summation in the expression for  $\Gamma_{\text{I}i}$  is negligible compared to the other terms. Finally, an order of magnitude estimation concerning the  $(\ell_{11}^{\text{II'}}/m_{\text{I}}n_{\text{I}})$  terms for this case, shows that they can be approximately given by,

$$\ell_{11}^{\text{II'}}/m_{\text{I}}^{\text{n}}_{\text{I}} \approx \alpha_{\text{I}}^{\text{I'}}/\tau_{\text{II}}.$$

With these approximations, the neo-classical flux expression in equation (2) can be written in the form given in equation (5), with

$$D_{1}(r) = \frac{q^{2}}{e_{I}^{2}} \left\{ \frac{0.57 e_{i}^{2} r_{Li}^{2} n_{i}}{n_{I}^{\tau} i I} + \frac{r_{LI}^{2}}{n_{I}^{\tau} I I} \sum_{I' \neq I} e_{I'}^{2} n_{I'} \right\},$$

$$D_{2}(r) = q^{2} \left\{ \frac{e_{i}r_{Li}^{2}}{e_{I}^{n}_{I}^{T}_{iI}} \left(0.57 \frac{dn_{i}}{dr} + \frac{0.12 n_{i}}{T_{i}} \frac{dT_{i}}{dr}\right) + \frac{r_{LI}^{2}}{n_{I}^{T}_{II}} \sum_{I' \neq I} \frac{e_{I'}}{e_{I}} \right\}$$

$$\times \left[ \frac{dn_{I'}}{dr} + \left(1 - \frac{e_{I'}}{e_{T}}\right) \frac{n_{I'}}{T_{i}} \frac{dT_{i}}{dr} \right]$$

and  $A_1 = A_2 = I$ . It should be noted that the factors,  $n_I^{\tau}iI$  and  $n_I^{\tau}II$  are independent of  $n_T$ .

Inserting equation (5) into equation (3), the following differential equation for the density of Fe XXIII at steady state is obtained,

$$-rA_{1}D_{1}\frac{d^{2}n_{I}}{dr^{2}} + (rA_{2}D_{2} - rA_{1}\frac{dD_{1}}{dr} - A_{1}D_{1})\frac{dn_{I}}{dr}$$

$$+ \left[rA_{2}\frac{dD_{2}}{dr} + A_{2}D_{2} + rn_{e}(s_{I,I+1} + \alpha_{I,I-1})\right]n_{I} = rn_{e}(s_{I-1,I}n_{I-1} + \alpha_{I+1,I}n_{I+1}).$$

$$+ \alpha_{I+1,I}n_{I+1}$$

$$+ \alpha_{I+1,I}n_{I+1}$$

$$(6)$$

Using the available data, the coefficients of  $n_{\rm I}$ , of its derivatives and the term on the right hand side have been plotted as a function of r; the resulting curves are then approximated by polynomials in powers of r. This has allowed to transform equation (6) into the following form:

$$\frac{d^{2}n_{I}}{dr^{2}} + (\frac{A_{2}r}{75A_{I}} + r^{-1})\frac{dn_{I}}{dr} + (\frac{2A_{2} - 670 + 22r}{75A_{I}})n_{I} = \frac{10^{10}}{3A_{I}}(88 + 8.8r - 0.056 r^{3}).$$
 (7)

This equation was numerically solved for  $n_1$  using the Runge-Kutta algorithm /26/. Various sets of anomaly factors  $A_1$  and  $A_2$  have been used. The initial conditions required are taken arbitrarily as the density of Fe XXIII and its gradient at r=15 cm. The results are illustrated in Figure 6. It can be seen that the neo-classical transport coefficients are too small; if they were valid, extremely steep density gradients of Fe XXIII would be required to satisfy equation (7). A satisfactory fit results when the values  $A_1 \sim 100$  and  $A_2 \sim 25$  are used. This agrees reasonably well with the results of the previous section. However, it must be mentioned that the values of the anomaly factors depend sensitively on the initial conditions, due to the extrapolating nature of the algorithm used.

The last two possible reasons mentioned in the introduction, concerning the diverging conclusions of previous workers on impurity transport can now be investigated. For this, a sensitivity analysis is carried out: the uncertainties in the rate coefficients, the autoionization rates and the charge exchange processes between the impurities and the neutral hydrogen are discussed and their possible contributions to the value of the flux,  $\Gamma_{c,e}$ , obtained from the continuity equation are illustrated.

#### 6. Sensitivity Analysis

#### 6.1 Unvertainties in the Rate Coefficients

It is generally accepted that the uncertainties in the rate coefficients are appreciable. Hawryluk et al. /17/, comparing the results of Lotz, of Breton et al., of Burgess and of Drawin with the experimental data, have stated that the collisional ionization and recombination rate coefficients can differ within a factor of two. Similar conclusions were drawn by Post et al./16/ who have stated that the uncertainties in the rate coefficients for high Z-materials are within a factor of two, but increase as the electron temperature goes below! keV.

In order to estimate the order of magnitude of the error which can result from these uncertainties in the flux computations, we multiplied the rate coefficients  $\mathbf{s_{I-1}}$ ,  $\alpha_{I+1,I}$ ,  $\beta_{I,I+1}$  and  $\alpha_{I,I-1}$  in equation (4) by the constants  $(1+\delta_1)$ ,  $(1+\delta_2)$ ,  $(1+\delta_3)$  and  $(1+\delta_4)$ , respectively. The values of  $\delta_1$  to  $\delta_4$  are restricted to the range from -0.5 to 1, corresponding to the extreme cases for an uncertainty factor of two. The modification of the results by these factors is of course the largest when  $\delta_1$  and  $\delta_2$  have the same sign and when both  $\delta_3$  and  $\delta_4$  have the other sign. Such cases are illustrated in Figure 7 by the fluxes  $\Gamma_1$ ,  $\Gamma_2$ ,  $\Gamma_3$  and  $\Gamma_5$  where errors of a factor of either two or 10 % have been assumed. The original flux, computed

without the uncertainties, is also represented in the same Figure by  $\Gamma_{\rm x}$ . The curves  $\Gamma_1$  and  $\Gamma_3$ , corresponding to uncertainty factors of two, indicate the maximum and minimum possible values which the flux can take at any point, respectively, within the assumed error bracket. It can be seen from the curves  $\Gamma_2$  and  $\Gamma_5$  that the fluxes computed assuming errors in the rate coefficients as small as 10 % can already be larger by an order of magnitude than the original flux and can even have different signs. This is particularly true in the domain for r between 10 and 15 centimeters.

To assess the influence of such errors on the evaluation of anomaly factors, we have repeated the procedure of section 5 after introducing uncertainty factors of  $\pm$  5 % only, into the rate coefficients. To determine the maximum modification of the anomaly factors, which could result from such a small error, the rate coefficients on the left and right hand sides of equation (6) have been multiplied by 1.05 and 0.95, respectively. The results, illustrated in Figure 8, indicate that this minor change in the assumed  $\alpha$ 's and S's results in an increase of the derived anomaly factors by approximately an order of magnitude.

In order to explain the particularly strong dependence of the computed flux on the uncertainties in rate coefficients, the sums of the first and the last two pairs of integrals in equation (4) (i.e. in the case when all the  $\delta$ 's are equal to zero) are plotted separately in Figure 9. The flux is equal to the difference between these two curves. It can be visualized that the flux term is approximately an order of magnitude smaller than each of these two terms taken independently. It becomes even smaller in the region for r between 10 and 15 centimeters. A deviation as small as 10 % in the rate coefficients can therefore change the difference between these two curves drastically and/or even reverse its sign. The curves  $\Gamma_1$ ,  $\Gamma_2$ ,  $\Gamma_3$  and  $\Gamma_5$  in Figure 7, for instance, have been drawn by choosing the signs of the individual errors as to maximize the resulting uncertainties in the flux and in the anomaly factors.

The flux corresponding to a different, "systematic" type of uncertainty, whereby both of the recombination rate coefficients are increased by a factor of two, leaving the ionization rate coefficients unchanged, has also been computed from equation (4). This flux is plotted in Figure 7 as  $\Gamma_4$  and when compared with the curves  $\Gamma_1$  and  $\Gamma_3$  indicates that, as expected, the contribution of the uncertainties in this case is much smaller. Unfortunately, there is no clear argument to justify such a particular trend in the uncertainties in rate coefficients. Nevertheless, the curve  $\Gamma_4$  can be used in estimating the influence of such effects as autoionization and charge exchange processes with neutral hydrogen.

#### 6.2 The Autoionization Rates

The autoionization rate coefficient is given as /14/

$$\Delta s_z = 3.2 \times 10^{-6} \text{ f w}_z^{-1} \text{ T}_e^{-1/2} \exp(-\text{w}_z/\text{T}_e) \text{ cm}^3 \text{s}^{-1}$$
 (8)

where f is the oscillator strength,  $w_z$  is an estimate of the excitation energy of the autoionizing level and  $T_e$  is the electron temperature in eV. These rate coefficients are needed to be known for Fe XXII and Fe XXIII, since the ionization rates of only these two states are involved in our computations. Following Uchikawa et al. /14/, it can be seen that  $2.4~w_z < T_z~(T_z~being~the~ionization~potential)$  for both of these states and equation (8) can therefore be written as

$$\Delta s_z = 0.86 \times 10^{-10} T_e^{-1/2} \exp(-I_z/T_e) \text{ cm}^3 \text{s}^{-1}$$
 (9)

These rate coefficients are plotted in Figure 10 for the states Fe XXII and Fe XXIII, indicating that their contributions to the total ionization rate coefficients will be on the order of 4 %. Furthermore, these contributions correspond to the case of systematic uncertainties, since they in-

crease both of the ionization rate coefficients in equation (2) simultaneous—
ly. According to the results of the section 6.1, the contribution of such
a small, "systematic" uncertainty can easily be ignored in the flux computations, in particular, as long as uncertainties of a factor of two
exist in the rate coefficients.

## 6.3 The Charge Exchange Between Impurities and Ho

According to the predictions of Olson et al. /15/, the cross sections for charge exchange between atomic hydrogen and heavy, highly stripped ions are expected to be on the order of  $10^{-14}$  cm<sup>2</sup>, implying rate coefficients on the order of  $2 \times 10^{-6}$  cm<sup>3</sup>s<sup>-1</sup>. These rates would already be comparable to the rates used in our computations, when the neutral hydrogen density is five orders of magnitude smaller than the electron density. Therefore, it is difficult to evaluate their contributions, unless the neutral hydrogen density is accurately known. Various authors have attempted to determine this quantity and estimated its near-core value to be of the order of  $10^8$  cm<sup>-3</sup>. If this is the case, these rates would be comparable to the radiative or dielectronic recombination rates in most of the experiments, as well as in the experiment considered in this work.

This process, on the other hand, corresponds again to the case of "systematic" uncertainties, since it can be taken into account by increasing the recombination rate coefficients in both the source and sink terms by certain amounts. The curve  $\Gamma_4$  in Figure 7 simulates therefore roughly the flux corresponding to this case, showing that the error to be anticipated in the flux computations due to the exclusion of this process is unlikely to be the dominant one. Nevertheless, a rigorous computation should be carried out in the future, when the neutral hydrogen density is more accurately known.

#### 7. DISCUSSION OF THE RESULTS AND CONCLUSION

In this work, we have evaluated the flux of Fe XXIII in PLT experiments from the neo-classical theory and the continuity equation separately, mainly to examine the sources of differences in the conclusions of previous workers concerning the impurity transport. The neo-classical flux has been found to be one to two orders of magnitude smaller than the flux obtained from the continuity equation, when the rate coefficients for ionization and recombination given in the literature /16, 20, 21/ are used. This suggests strongly that some anomalous mechanism is involved. The first and second terms in the neo-classical flux expression,  $P_{n,c} = -D_1(dn/dr) + D_2n$ , had to be multiplied by anomaly factors of 100 and 25, respectively, to yield the flux evaluated from the continuity equation. The possible sources of error in these results have been investigated in order to decide on which points, if any, the future efforts for determining the impurity transport mechanisms from such experimental data should be concentrated. Since we had no access to the experiments concerned, the experimental data has been assumed to be accurate and only the errors in their interpretation have been considered.

In evaluating the neo-classical flux, the temperature gradients and the effects of three other ionization states of iron have been taken into consideration. A possible source of error would be the contribution of the four other states and the impurities of other elements in the region concerned, of which the density profiles are not available. A rough estimation of the missing profiles and of their contributions have indicated that neither the uncertainties in the impurity profiles, nor the lack of data on some of them are critical for the evaluation of the neo-classical flux, as long as the degree of accuracy aimed at is within a factor of two. However, neglecting the contributions of the temperature gradients and of the other impurities altogether, would have led to much larger errors. Therefore as long as

these effects are taken into consideration, the errors in the neo-classical flux evaluations are not likely to be the sources of differences in the interpretations of various authors, concerning the impurity transport.

In evaluating the flux from the continuity equation, it has been found that the error which results from neglecting autoionization phenomenon is negligible here. The charge exchange between the impurities and neutral hydrogen on the other hand, can modify the recombination rates significantly. It is however unlikely to affect the conclusions regarding impurity transport, since it increases a source and a sink term simultaneously. The fundamental sources of error in this case, are the uncertainties in the ionization and recombination rate coefficients. It has been shown that, a deviation as small as 10 % in these coefficients can lead to flux values which are by an order of magnitude larger than the originally computed flux, or which can even have the opposite sign. The resulting uncertainty in the value of the flux is largest when these deviations have different signs in the source and sink terms, respectively. The dependence of derived flux on the rate coefficients is particularly strong in the near-core regions, where the flux is much smaller than each of the ionization and recombination rates.

These arguments suggest that even small differences in the rate coefficients used by various authors might be the main reason for the differences
in their conclusions. A higher degree of accuracy in calculating or measuring
the cross sections involved is obviously required for the interpretation of
such experimental data. This is therefore one of the points on which the
future effort should be concentrated. Furthermore, several suggestions for
the future experiments can be deduced from the results obtained in this
work: It would be advisable to measure the impurity density profiles in a
region which is neither too near the core, nor too near the wall. In the
near-core regions, the flux is very small and its evaluation is therefore
sensitively dependent on the rate coefficients. On the other hand, the near-

wall regions involve uncertainties, which have already been discussed in the introduction. Secondly, if measurements are made on iron or similar elements, the peak electron temperature should be increased to achieve 1 keV or more in this optimum region of steeper gradients. This results from the fact that the uncertainties in the rate coefficients and the abundance of neutral hydrogen, which also contributes to the error through the charge exchange processes, increase when the temperature is lower than 1 keV. Finally, different substances, of which a fraction can exist in the fully stripped state in such an optimum region, may be better candidates for future experiments, since the accuracy in the rate coefficients of the three highest ionization states would then be expected to be greater.

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#### References

- /1/ S.A.Cohen, J.L. Cecchi and E.S. Marmar, Phys. Rev. Lett. <u>35</u>, p. 1507 (1975)
- /2/ TFR Group, Phys. Rev. Lett. 36, p. 1306 (1976)
- /3/ TFR Group, Nucl. Fusion 17, p. 1297 (1977)
- /4/ M. Shiho et al., Nucl. Fusion 18, p. 1705 (1978)
- /5/ N.J. Peacock et al., Nucl. Fusion Spec. Suppl. 1, p. 303 (1979)
- /6/ S. Suckewer and E. Hinnov, Phys. Rev. Lett. 41, p. 756 (1978)
- /7/ H. Eubank et al., Phys. Rev. Lett. 43, p. 270 (1979)
- /8/ S. Suckewer and E. Hinnov, Phys. Rev. A 20, p. 578 (1979)
- /9/ S. Suckewer et al., Phys. Rev. A 22, p. 725 (1980)
- /10/ U. Feldman et al., J. Appl. Phys. <u>51</u>, p. 190 (1980)
- /11/ TFR Group, Plasma Physics 22, p. 851 (1980)
- /12/ T. Tazima, Y. Nakamura and K. Inoue, Nucl. Fusion 17, p. 419 (1977)
- /13/ V.A. Abramov, Nucl. Fusion 20, p. 225 (1980)
- /14/ S. Uchikawa, H.R. Griem and D. Düchs, Garching Report IPP 6/199, p. 4 (1980)
- /15/ R.E. Olson et al., Phys. Rev. Lett. 41, p. 163 (1978)
- /16/ D.E. Post et al., Atomic Data and Nuclear Tables 20, p. 397 (1977)
- /17/ R.J. Hawryluk, S. Suckewer and S.P. Hirshman, Nucl. Fusion 19, p. 607
- /18/ E. Hinnov, Proc, NATO Advanced Study Institute, Bonas, France (August 1979), Eds. M.R.C. McDowell and A. Ferendeci (Plenum Press, 1980)
- /19/ A. Merts et al., Report at Workshop on Atomic Processes in Controlled
  Thermonuclear Fusion Research, Los Alamos (1978)
- /20/ L.B. Golden and D.H. Sampson, J. Phys. B 10, p. 2229 (1977)
- /21/ D.L. Moores, J. Phys. B 11, p. 1403 (1978)
- /22/ P.H. Rutherford, Phys. Fluids 17, p. 1782 (1974)

- /23/ A. Samain, F. Werkoff, Nucl. Fusion 17, p. 53 (1977)
- /24/ F. Engelmann, A. Nocentini, Nucl. Fusion 17, p. 995 (1977)
- /25/ S.P. Hirshman, Phys. Fluids 20, p. 589 (1977)
- /26/ M. Abramowitz and I.A. Stegun, Handbook of Mathematical Functions,
  Dover Publications, Inc., New York, p. 897 (1965)

#### Figure Captions

- Fig. 1 The iron density profiles for various ionization states.
- Fig. 2 The plasma parameters.
- Fig. 3 The ionization and recombination rate coefficients for the ionization states concerned.
- Fig. 4 The neo-classical flux,  $(\Gamma_{\rm n.c})_{\rm I}$ , of Fe XXIII.  $\Gamma_{\rm Ii} \ \ {\rm and} \ \ \Sigma \ \ \Gamma_{\rm Ii'}, \ {\rm are \ the \ contributions \ of \ the \ plasma}$  ions and Fe XVIII, Fe XXII, Fe XXIV, respectively.
- Fig. 5 The flux,  $\Gamma_{\rm c.e}$ , of Fe XXIII, derived from the continuity equation and the related computational functions.
- Fig. 6 The density profiles of Fe XXIII, corresponding to various anomaly factors.
- Fig. 7 The dependence of the value of the flux,  $\Gamma_{c.e}$ , on the uncertainty factors.
- Fig. 8 The density profiles of Fe XXIII for various anomaly factors with 5 % uncertainty in the rate coefficients, i.e.  $\delta_1 = \delta_2 = -0.05, \ \delta_3 = \delta_4 = 0.05.$
- Fig. 9 The functions  $f_1$ ,  $f_2$  and the flux  $\Gamma_{c.e}$ , where  $f_1 f_2 = \Gamma_{c.e}$ .
- Fig. 10 The ionization and autoionization rate coefficients for the ionization states concerned.

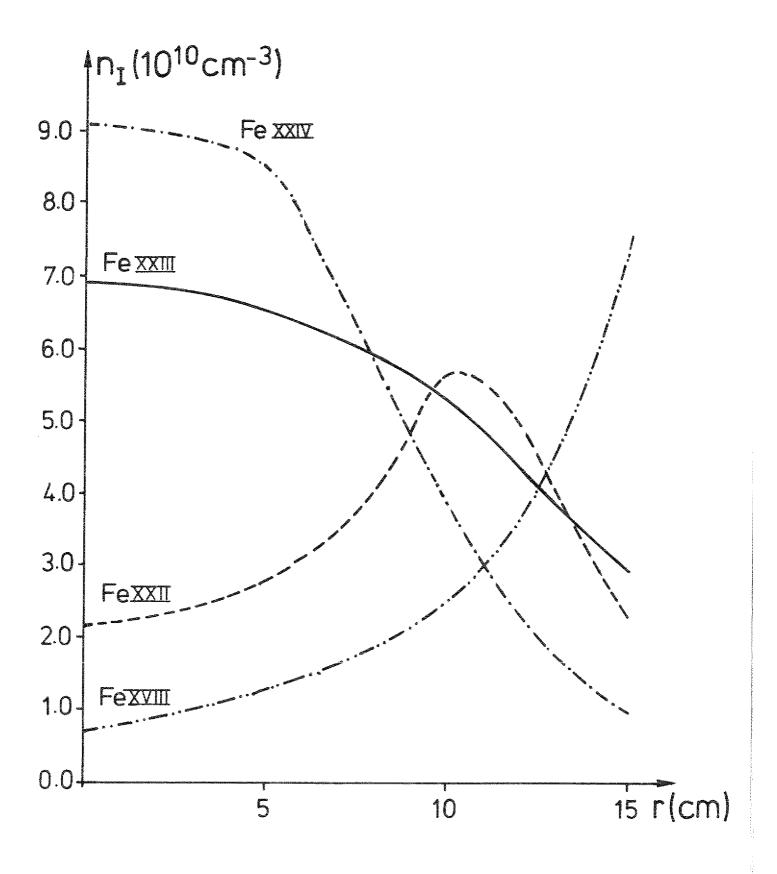


Fig. 1

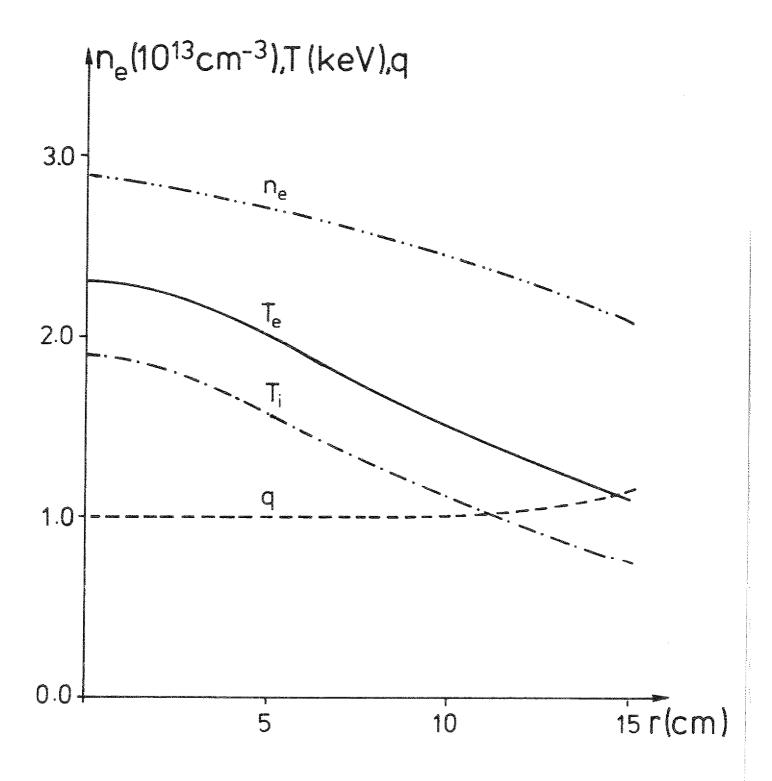


Fig. 2

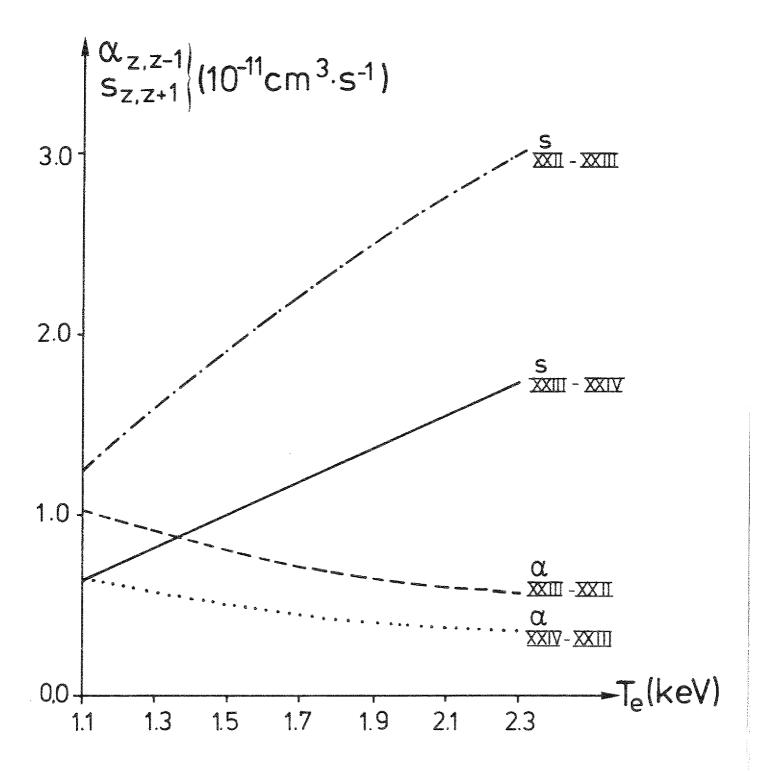


Fig. 3

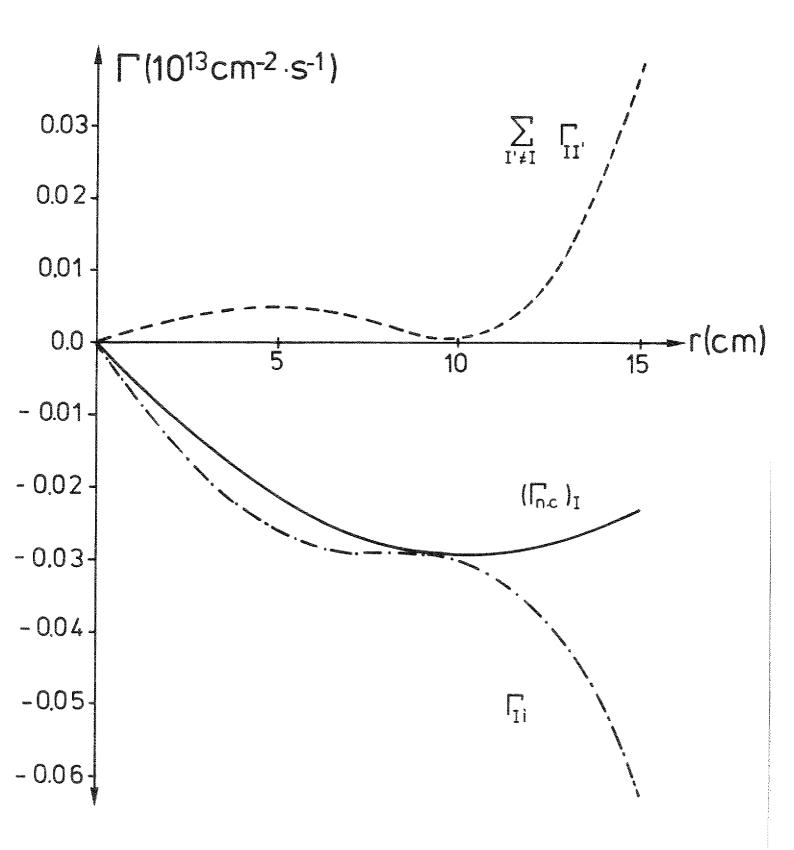


Fig. 4

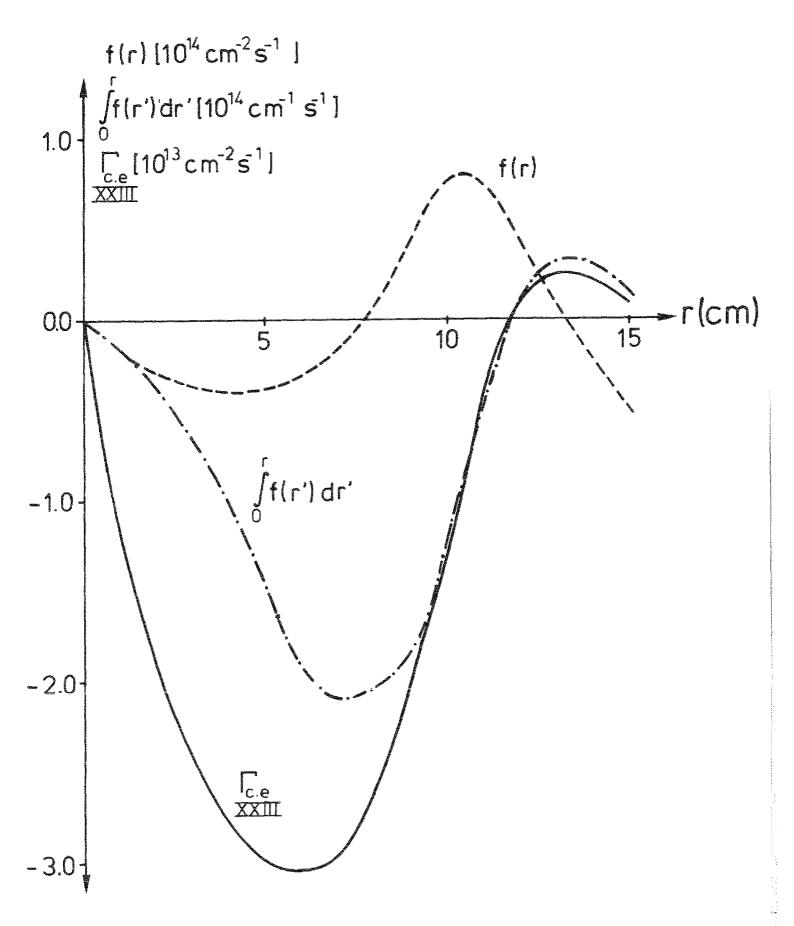
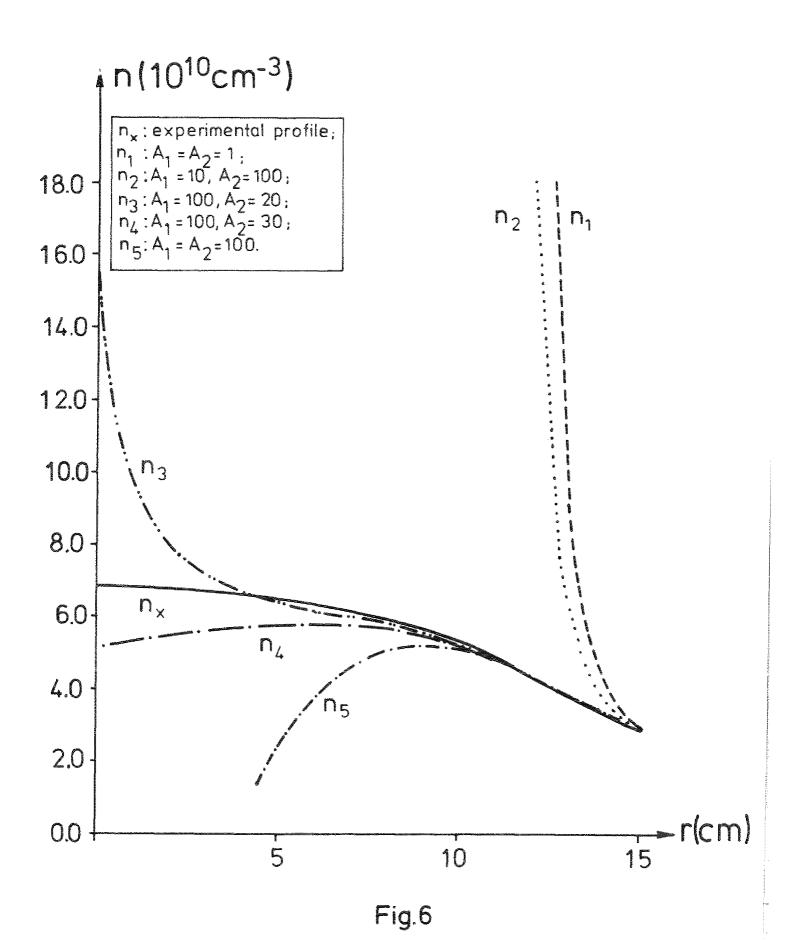


Fig. 5



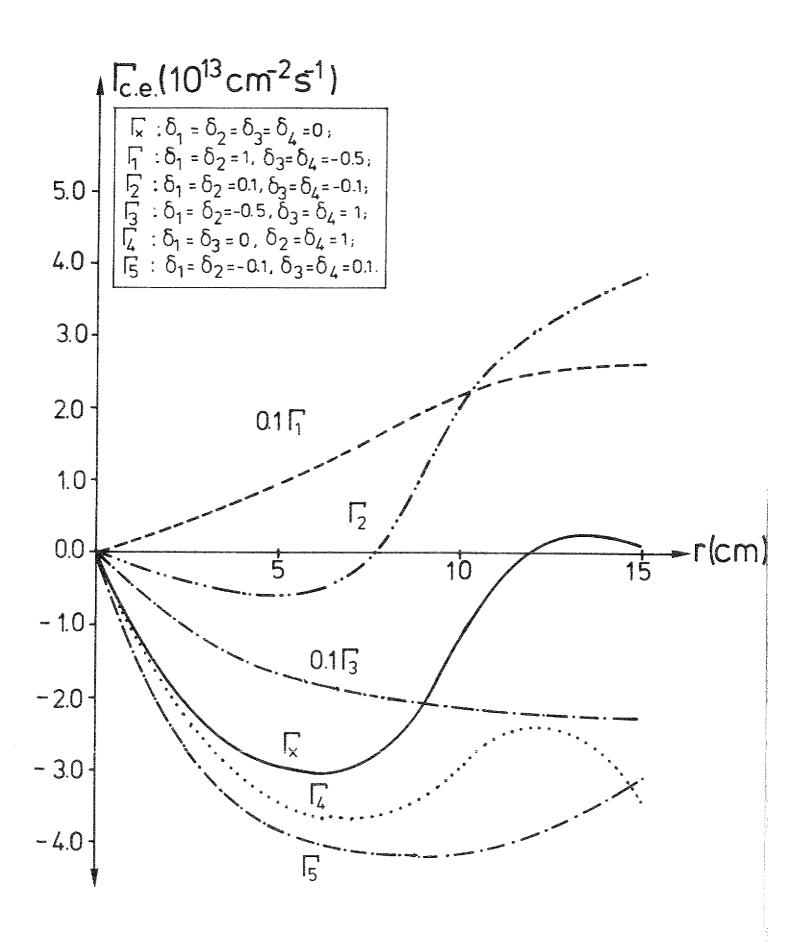


Fig. 7

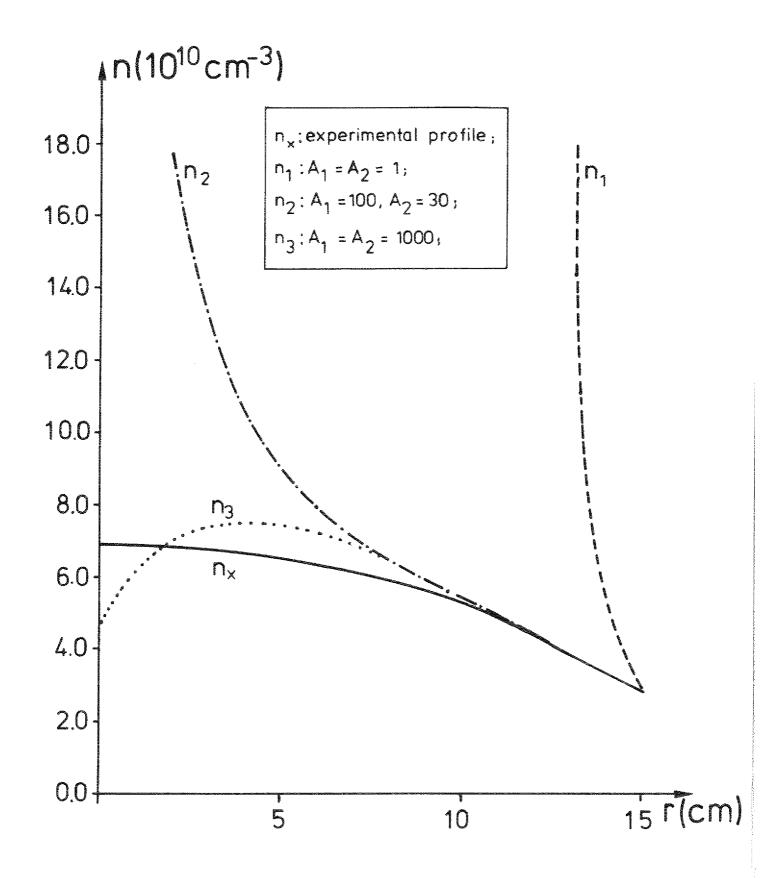
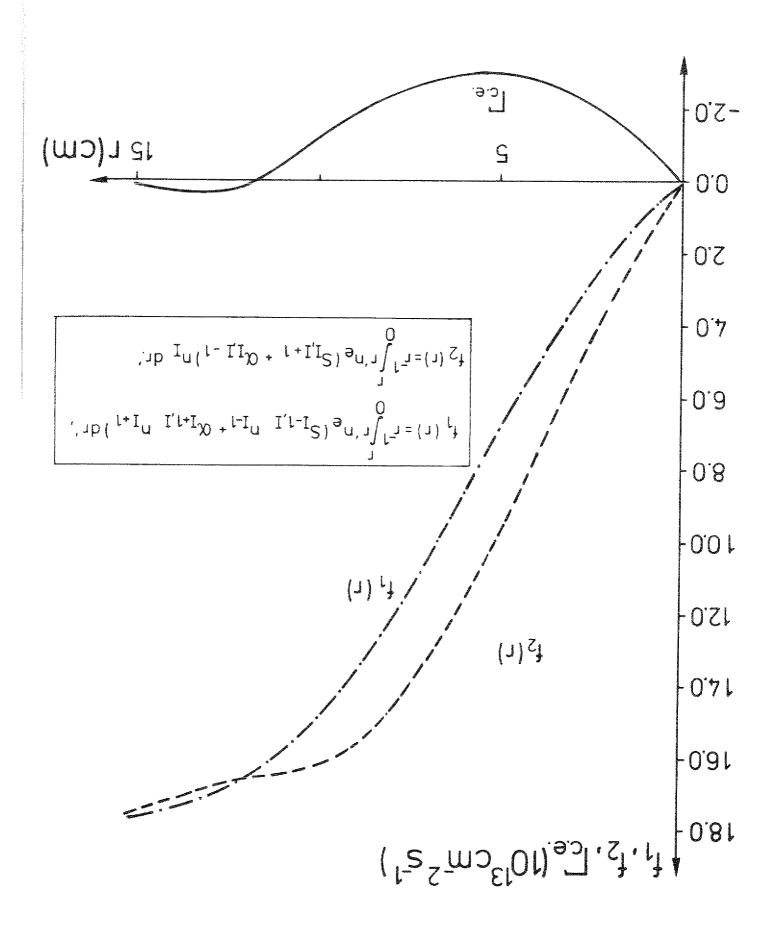


Fig. 8



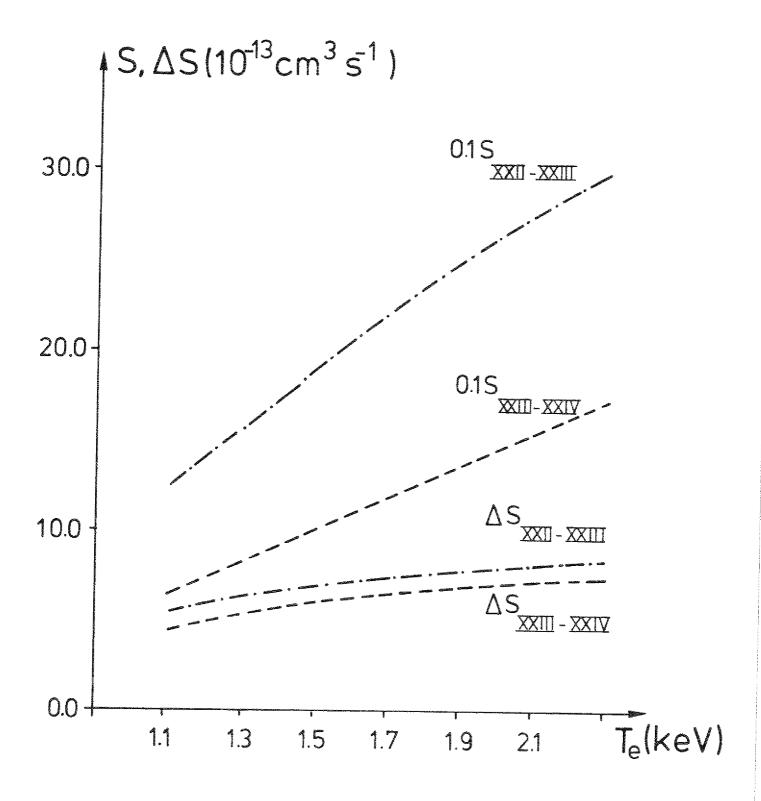


Fig.10

