IMPURITY TRANSPORT IN TOKAMAKS

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ABSTRACT

A review is given of the principle results of the neoclassical theory of impurity transport in tokamaks, emphasizing those collisionality regimes of most practical interest. Some new results are given for the case where there are several different impurity species present at the same time, with both hydrogenic and impurity ions in the Pfirsch-Schlüter regime.

The rate at which an impurity ion is transported into a plasma, and the radiation from it, are strongly dependent on the mean level of ionization $\langle Z \rangle$. An atomic physics code package, based on an "average ion" model is used to assess the validity of the "coronal equilibrium" assumption commonly made to determine $\langle Z \rangle$; coronal equilibrium is found to be a poor approximation for heavy metallic impurities in small present-day tokamaks, but its validity is much improved in larger devices, except perhaps in the edge region of the plasma. Our computations are compared with the results obtained in an impurity injection experiment in the ATC tokamak. In practice, the most appropriate impurity transport model would be a combination of neoclassical transport and anomalous diffusion, with the magnitude of the anomalous diffusion coefficient chosen to give agreement with observed hydrogenic particle confinement times. Computations of oxygen impurities in the edge region of a tokamak plasma, on the basis of this model, show that only a fraction (typically 0.2 - 0.6) of an incident flux of neutral impurities actually penetrates into the main part of the discharge.

1. INTRODUCTION

The contamination of tokamak plasmas with high-Z impurities is detrimental to their performance in a number of ways. In present-day devices, an excessive influx of light impurities, such as oxygen, can cause the shrinking of the current channel to the point at which MHD instability, or "disruption", occurs. For larger tokamak devices, the concern is more with the radiation losses arising from heavy metallic impurities. Where these are incompletely stripped (at least 3 electrons left) the radiated power has been shown to be as much as $4 \times 10^{-26} n_e n_i \text{ Watts/cm}^3$, where n_e and n_i are the electron and impurity densities per cm^3 [1]. Such losses would, for example, impose severe demands on the plasma purity required to achieve ignition in a DT device [2]. The occurrence of a high value of Z_{eff} , from either light or heavy impurities, can also have a detrimental effect on the heating of

tokamak plasmas by neutral injection. In the first place, the penetration into the plasma of neutral beams in the 100 keV range is adversely affected by their ionization by impact on the heavy impurities in the edge region of the discharges [3, 4]. Furthermore, a high value of Z_{eff} will increase the pitch-angle scattering of energetic beam ions into loss cones.

The problem of impurities in the tokamak, or any other low- β toroidal device, is aggravated by the fact that, in classical theory, high- Z ions have a tendency to diffuse inward toward the center of the plasma (more accurately, toward the maximum of the density of the hydrogenic ions). This is a consequence of the ambipolarity of the ion particle fluxes which, in turn, is a consequence of the conservation of momentum in ion-ion collisions [5]. As hydrogenic ions diffuse outward due to collisions with impurity ions, the impurity ions are transported inward, so that there is no net transport of charge.

2. NEOCLASSICAL IMPURITY TRANSPORT

2.1 Single Impurity Species.

We consider first the case where the plasma is composed of hydrogenic ions, denoted i , and a single species of Z -times ionized impurity ions, denoted I . We assume that the impurity mass greatly exceeds the hydrogen mass, i. e., $m_i \ll m_I$. In the classical or neoclassical, cases considered here the flux of the impurity ions due to collisions with the hydrogenic ions may be written in the form

$$\Gamma_I = \frac{4(2\pi)^{1/2}}{3} \frac{e^2 c^2 m_i^{1/2} \ln \Lambda}{(kT)^{3/2} B_T^2} \left[C_{11} \left(Z_i Z_I n_i \frac{\partial p_i}{\partial r} - Z_i^2 n_i \frac{\partial p_I}{\partial r} \right) + C_{12} Z_i Z_I n_i n_I \frac{\partial kT}{\partial r} \right] \quad (1)$$

where, of course, $Z_i = 1$. The radial flux of the hydrogenic ions is given by the ambipolarity condition, i. e.,

$$\begin{aligned} \Gamma_i &= -Z_I \Gamma_I / Z_i \\ &= -\frac{4(2\pi)^{1/2}}{3} \frac{e^2 c^2 m_i^{1/2} \ln \Lambda}{(kT)^{3/2} B_T^2} \cdot \\ &\quad \cdot \left[C_{11} \left(Z_i^2 n_I \frac{\partial p_i}{\partial r} - Z_i Z_I n_i \frac{\partial p_I}{\partial r} \right) + C_{12} Z_I^2 n_i n_I \frac{\partial kT}{\partial r} \right]. \end{aligned} \quad (2)$$

In the absence of a temperature gradient, it follows from Eqs. (1) and (2) that the diffusion of the impurities into the plasma, and the hydrogenic ions out of the plasma, tends to produce an equilibrium in which the impurity density is peaked at the center, according to the formula

$$n_I(r) / n_i(r)^{Z_I} = \text{const.}$$

The radial heat flux Q_i in the hydrogenic ion component may, in the cases considered here, be written in the form

$$\frac{Q_i}{kT} - \frac{5}{2} \Gamma_i = - \frac{4(2\pi)^{1/2}}{3} \frac{e^2 c^2 m_i^{1/2} \ln \Lambda}{(kT)^{3/2} B_T^2} \cdot \left[C_{21} \left(Z_I^2 n_i \frac{\partial p_i}{\partial r} - Z_i Z_I n_i \frac{\partial p_I}{\partial r} \right) + C_{22}^i Z_i^2 n_i^2 \frac{\partial kT}{\partial r} \right]. \quad (3)$$

The heat flux Q_I in the impurity component has the form

$$\frac{Q_I}{kT} - \frac{5}{2} \Gamma_I = \frac{4(2\pi)^{1/2}}{3} \frac{e^2 c^2 m_I^{1/2} \ln \Lambda}{(kT)^{3/2} B_T^2} C_{22}^I Z_I^2 n_I^2 \frac{\partial kT}{\partial r}. \quad (4)$$

In general, the heat conduction in the impurity component is small compared with the conduction in the hydrogenic component. In Eqs. (1) - (4), we have assumed that all ions have the same temperature T (a reasonable assumption in view of the strong temperature equilibration between different ions in a typical tokamak plasma).

The quantities C_{mn} appearing in Eqs. (1) - (3) depend on which of the various neo-classical regimes is applicable, i.e., they depend on

$$\nu_{i*} = \frac{4\pi^{1/2} R^{3/2} B_T n_i Z_i^4 e^4 \ln \Lambda}{3B_\theta r^{1/2} (kT)^2}, \quad (5)$$

$$\nu_{I*} = \frac{4\pi^{1/2} R^{3/2} B_T n_I Z_I^4 e^4 \ln \Lambda}{3B_\theta r^{1/2} (kT)^2}.$$

They also depend on a parameter

$$\alpha = n_I Z_I^2 / n_i Z_i^2, \quad (6)$$

that characterizes the strength of the impurity effects.

For a straight classical plasma [5], $C_{11}=1$, $C_{12}=C_{21}=-1.5$, and $C_{22}^i=1.4 + 3.2 \alpha$. Expressions have now been obtained for the quantities C_{mn} in the banana regime [6, 7, 8], the banana-plateau regimes [8], and the Pfirsch-Schlüter regime [9, 10, 11]. Care must be taken, however, in selecting the applicable regime, in view of the fact that the collisionality parameter of the impurities tends to be greater than that of the hydrogenic ions, i.e., $\nu_{*i} \ll \nu_{*I}$. For example, the theory of Ref. [8] applies only when both hydrogenic and impurity ions are in the banana or plateau regimes, i.e., when both ion species have mean free paths long compared with the connection length around the torus.

The most relevant case in practice, however, is where the impurities are in the collisional (Pfirsch-Schlüter) regime, i. e., their mean free path is short compared with the connection length. To support this assertion, we observe that present-day tokamaks have achieved values of ν_{i*} as low as 0.5, but tend to have impurity strengths α in the range 1-4. In the case of fully stripped oxygen, for example, the parameter $\nu_{I*} = \alpha Z_I^2 \nu_{i*}$ would then, typically, exceed 30. Thus, the condition $\nu_{I*} > (R/r)^{3/2}$ for the impurities to be in the Pfirsch-Schlüter regime would be satisfied over most of the plasma cross section. In future tokamaks, the main concern is not with light impurities, such as oxygen, but with heavy metallic impurities, such as iron, molybdenum, tungsten, etc., which would be stripped at least 20 times. Furthermore, even in the reactor regime, the values of ν_{i*} would not fall much below 0.1. Thus, with $\alpha \sim 1$, the parameter $\nu_{I*} = Z_I^2 \nu_{i*}$ would again, typically, greatly exceed $(R/r)^{3/2}$ over most of the plasma. Thus, the assumption that the impurities are in the Pfirsch-Schlüter regime seems to be valid in most of the cases of interest.

The "mixed collisionality" case, in which the impurities are in the Pfirsch-Schlüter regime [$\nu_{I*} > (R/r)^{3/2}$] and the hydrogenic ions are in the banana regime ($\nu_{i*} < 1$) has recently been worked out [12]. The results are rather surprising. We may note that the ambipolarity of the particle fluxes must continue to hold, despite the fact that the two ion species are in different collisionality regimes. We may note also that, in neoclassical theory, the radial flux of particles of a given species is related to the parallel component of the frictional force acting on that species arising from its parallel flow velocity relative to the other species. In the case being considered here, the strong collisional coupling of the parallel flow of the impurities to the parallel flow of the hydrogenic ions reduces the parallel component of the frictional force on the hydrogenic ions, with the result that the magnitude of the radial flux of the (banana regime) hydrogenic ions is reduced to a value characteristic of the Pfirsch-Schlüter regime. Specifically, the values of the coefficients C_{11} and C_{12}^I appearing in Eq. (1) are found to be [12]

$$C_{11} = 2 q^2 ; \quad C_{12} = -3 q^2 , \quad (7)$$

where $q = R \bar{B}_T / r \bar{B}_\theta$ is the usual tokamak "safety factor". There is no relation analogous to ambipolarity constraining the parallel heat flow. Accordingly, the radial thermal conductivity of the hydrogenic ions has the usual value characteristic of the banana regime. Specifically, the coefficients C_{21} and C_{22} appearing in Eq. (3) are found to be

$$C_{21} = C_{12}$$

$$C_{22}^I = 2 q^2 \left(\frac{R}{r} \right)^{3/2} \frac{0.48 (1 + 1.5 \alpha)}{1 + 0.36 (1 + 1.5 \alpha) \nu_{i*}} \quad (8)$$

The coefficient C_{22}^I appearing in Eq. (4) is the same as in the Pfirsch-Schlüter regime [9]; in any case, the heat conduction in the impurity component is very small compared with

that in the hydrogen. In the expression for C_{22}^1 given in Eq. (8), we have extended the result of Ref. [12] to include the case where the hydrogenic ions are in the plateau, rather than banana, regime; hence the term containing ν_{i*} in the denominator. In the mixed collisionality case considered here, the conduction term in the radial heat flux exceeds the convection term by a factor of order $(R/r)^{3/2}$. Thus, the direction of the radial flux of the hydrogen ions has little effect on the direction of the heat flux, which is predominantly outward. The result that $C_{12} = -3C_{11}/2$ in this mixed collisionality regime implies that a strong ion temperature gradient, in the usual direction, may produce an outward flow of the impurity ions. This phenomenon has been termed "temperature gradient screening" of the impurities from the center of the plasma.

Since these rather simple expressions apply over a wide range of parameters, and over most of the discharge cross section, they may be used with some reliability in tokamak simulation codes [13]. The most important exception might be the cold edge region of the plasma, where the hydrogenic ions would tend to be in the Pfirsch-Schlüter regime, in which case the theory of Ref. [9] would apply.

2.2 Several Impurity Species.

There is considerable practical interest in the case where there are several different impurities present in the plasma at the same time. Commonly, tokamak discharges are contaminated both by light impurities, such as oxygen and carbon, and by heavy metallic impurities, such as iron, molybdenum, tungsten, etc. Although the heavy impurities are present in much smaller quantities, they reach higher Z values, with the result that both impurity species can have values $\alpha \geq 1$. Thus, one important case would be where there are three ion species: hydrogenic ions, light impurities, and heavy impurities. A second important case of this type is where there are several different ionization levels of the same impurity simultaneously present at the same place in the plasma. Although the multiple-ion-species plasma has been considered in the cases where all ions are in the banana [7, 8] or banana/plateau regimes [8], the more relevant Pfirsch-Schlüter regime has not been considered.

A treatment of the multiple-ion species-plasma has recently been completed for the case where all ions, hydrogenic and impurity, are in the Pfirsch-Schlüter regime [14]. This calculation is somewhat more complicated than the case discussed in Sec. 2.1 in which the hydrogenic ions are taken to be in the banana regime, since it involves a Chapman-Enskog type of evaluation of the ion distribution functions needed to compute the various parallel frictional forces that arise as a consequence of the different parallel flow velocities of the different ions. Only the results will be given here; the reader is referred to Ref. [14] for the details of the calculation.

We consider first the case of a mixture of hydrogen ions, light impurities denoted I1, and heavy impurities denoted I2, in the limit $m_i \ll m_{I1} \ll m_{I2}$. The results are as

follows. The flux of hydrogenic ions is given by a sum of two expressions like Eq. (2), one from each of the two impurity species, with the quantities C_{11} and C_{12} in each expression given by $C_{11} = C_{11}^i$ and $C_{12} = C_{12}^i$, where

$$C_{11}^i = 2q^2 C_1^*(\alpha); \quad C_{12}^i = -2q^2 C_2^*(\alpha), \quad (9)$$

with

$$C_1^*(\alpha) \equiv 0.48 + \frac{0.31}{0.59 + \alpha}; \quad C_2^*(\alpha) \equiv 0.31 + \frac{0.41}{0.59 + \alpha}; \quad (10)$$

$$\alpha = (n_{11} Z_{11}^2 + n_{12} Z_{12}^2) / n_i Z_i^2.$$

The flux of the light impurity ions is given by a sum of two terms, one arising from collisions with the hydrogenic ions, and the other from collisions with the heavy impurities. The term from collisions with the hydrogenic ions is an expression like Eq. (1), with $C_{11} = C_{12}^i$ and $C_{12} = C_{12}^i$. The term from collisions with the heavy impurities may be obtained by treating the light impurity in the same manner as the hydrogenic ions, thus obtaining an expression like Eq. (2), in which we make the replacements $i \rightarrow 11$ and $I \rightarrow 12$ in the various densities, masses, and Z-values. The applicable quantities C_{11} and C_{12} are given by $C_{11} = C_{11}^I$ and $C_{12} = C_{12}^I$, where

$$C_{11}^I = 2q^2 C_1^*(\beta), \quad C_{12}^I = -2q^2 C_2^*(\beta), \quad (11)$$

with

$$\beta = n_{12} Z_{12}^2 / n_{11} Z_{11}^2. \quad (12)$$

The flux of the heavy impurity ions is given by a sum of two terms, one arising from collisions with the hydrogenic ions, and the other from collisions with the light impurities. The term from collisions with the hydrogenic ions is an expression like Eq. (1), with $C_{11} = C_{12}^i$ and $C_{12} = C_{12}^i$. The term from collisions with the light impurities is also an expression like Eq. (1), in which we make the replacements $i \rightarrow 11$ and $I \rightarrow 12$, with $C_{11} = C_{11}^I$ and $C_{12} = C_{12}^I$. In case of a single impurity species, these results agree with those of Ref. [9].

The results for the heat fluxes are as follows. The heat flux in the hydrogenic ions is given by an expression like Eq. (3) in which there are two pairs of pressure-gradient "convection" terms, one from each of the two impurity species, with the quantity C_{21} in each expression given by $C_{21} = C_{12}^i = -2q^2 C_2^*(\alpha)$. There is a single temperature gradient "conduction" term, with

$$C_{22}^i = 2q^2 C_3^*(\alpha) \quad (13)$$

where

$$C_3^* (\alpha) \equiv 1.13 + 0.50 \alpha + \frac{0.55 \alpha}{0.59 + \alpha} \quad (14)$$

In the limit $\alpha \rightarrow 0$, these results reduce to the usual factor $1.6 q^2$ for the enhancement of ion thermal conduction in the Pfirsch-Schlüter regime. The heat flux in the light impurity ions has a single pair of pressure-gradient "convection" terms, arising from collisions with the heavy impurities; these terms can be obtained from an expression like Eq. (3), in which we make the replacements $i \rightarrow 11$, and $I \rightarrow 12$, with $C_{21} = C_{12}^I = -2q^2 C_2^* (\beta)$. Again, there is a single temperature gradient "conduction" term, like the term in Eq. (4), with $I \rightarrow 11$ and

$$C_{22}^{11} = 2q^2 C_3^* (\beta) \quad (15)$$

For the heat flux in the heavy impurities, we obtain an expression exactly like Eq. (4), with $I \rightarrow 12$ and

$$C_{22}^{12} = 2.26 q^2 \quad (16)$$

In the usual case where $\alpha \sim 1$ and $\beta \sim 1$, the heat flux in the impurity components tends to be smaller than that in the hydrogenic component by a factor of order $n_1 m_1^{1/2} / n_i m_i^{1/2}$.

It is of interest to examine the practical consequences of these results to the evaluation of the rate at which a heavy impurity (12) diffuses through a plasma that is a mixture of hydrogen (i), and light impurities (11). The flux of heavy impurities is given by

$$\begin{aligned} \Gamma_{12} = & \frac{8 (2\pi)^{1/2} e^2 c^2 m_i^{1/2} q^2 \ln \Lambda}{3 (kT)^{3/2} B_T^2} \cdot \left\{ \left[C_1^* (\alpha) \left(Z_{12} n_{12} \frac{\partial p_i}{\partial r} - n_i \frac{\partial p_{12}}{\partial r} \right) - C_2^* (\alpha) Z_{12} n_i n_{12} \frac{\partial kT}{\partial r} \right] \right. \\ & + \left(\frac{m_{11}}{m_i} \right)^{1/2} \left[C_1^* (\beta) \left(Z_{11} Z_{12} n_{12} \frac{\partial p_{11}}{\partial r} - Z_{11}^2 n_{11} \frac{\partial p_{12}}{\partial r} \right) \right. \\ & \left. \left. - C_2^* (\beta) Z_{11} Z_{12} n_{11} n_{12} \frac{\partial kT}{\partial r} \right] \right\} \quad (17) \end{aligned}$$

If temperature gradients are neglected, and the light impurities are considered to be uniformly mixed with the hydrogenic ions, there are two inward convection terms, in $\partial n_i / \partial r$ and $\partial n_{11} / \partial r$, and two diffusion terms in $\partial n_{12} / \partial r$. The inward convection arising from collisions with the light impurities dominates over that due to collisions with the hydrogen by a factor $C_1^* (\beta) n_{11} Z_{11} m_{11}^{1/2} / C_1^* (\alpha) n_i m_i^{1/2}$. For a hydrogen plasma containing about 5% of 6-times ionized oxygen impurities, and very small quantities of the heavy

impurity, this factor is about 2.1 ; thus, a pulse of heavy impurities is convected into the plasma about 2 times as fast as in a pure hydrogen plasma. The diffusion of the heavy impurities due to the light impurities dominates over that due to the hydrogen by a factor $C_1^*(\beta) n_{II} Z_{II}^2 m_{II}^{1/2} / C_1^*(\alpha) n_i m_i^{1/2}$. For the case specified above, this factor is about 15; thus, the diffusion, or spreading out, of a pulse of heavy impurities is very much increased by the presence of light impurities. Both of these results seem to have been confirmed in an experiment on impurity injection into the ATC tokamak [15].

It is also of interest to examine the possibility of the "screening" out of the heavy impurities by means of an ion temperature gradient (in the usual direction). We note that $C_2^*(\alpha) \leq C_1^*(\alpha)$ for all α (equality occurring only in the limiting case $\alpha \rightarrow 0$). Thus, in the terms in Eq. (17) for the heavy impurity flux Γ_{I2} arising from collisions with the hydrogenic ions, the temperature gradient term implicit in $\partial p_i / \partial r$ exceeds the explicit temperature gradient term, resulting in a net inward transport of impurities due to temperature gradients. The same is, in general, true for the term in Eq. (17), arising from collisions with the light impurities. In this case, however, if $\beta \rightarrow 0$ (very small density of heavy impurities), we have $C_1^*(\beta) = C_2^*(\beta) = 1$ so that the dominant temperature gradient terms cancel, leaving a residual term from $\partial p_{I2} / \partial r$ giving rise to outward transport. For $\alpha \sim 1$, however, this term is smaller than the net inward transport from collisions with the hydrogenic ions, by a factor $(n_{II} Z_{II}^2 / n_i Z_{I2}) (m_{II} / m_i)^{1/2} \sim 0.5$. It follows that the "screening" of heavy impurities by means of ion temperature gradients is, in general, quite ineffective in the edge region of the plasma, where the hydrogenic ions are in the Pfirsch-Schlüter regime.

The second case considered in Ref. [14] is the case of several different ionization levels of the same impurity. The particle fluxes due to collisions between the hydrogenic ions and the impurities are, not surprisingly, given by expressions similar to those obtained above. The impurity fluxes due to collisions between different ionization levels are, in general, more complicated expressions, for which reference must be made to [14]. For parameters of practical interest, however, the flux of impurities of one ionization level I1 due to collisions with another level I2 is given approximately by the expression

$$\Gamma_{I1} = \frac{8\pi^{1/2} e^2 c^2 m_I^{1/2} q^2 \ln \Lambda}{3 (kT)^{3/2} B_T^2} \left[\left(Z_{II} Z_{I2} n_{II} \frac{\partial p_{I2}}{\partial r} - Z_{I2}^2 n_{I2} \frac{\partial p_{I1}}{\partial r} \right) - 0.56 Z_{I2} (Z_{I1} - Z_{I2}) n_{I1} n_{I2} \frac{\partial kT}{\partial r} \right] \quad (18)$$

Summing over the different ionization levels I1 and I2, we find that the principle effect of these terms is to cause a transport of the higher Z impurities toward the peak of the density of the lower Z impurity, and a somewhat larger transport of the lower Z impurities in the opposite direction. The heat flux in the impurity component I1 is given

approximately by the expression

$$\frac{Q_{11}}{kT} - \frac{5}{2} \Gamma_{11} = - \frac{8\pi^{1/2} e^2 c^2 m_I^{1/2} q^2 \ln \Lambda}{3 (kT)^{3/2} B_T^2} \left[0.56 \left(Z_{11} Z_{12} n_{11} \frac{\partial p_{12}}{\partial r} \right. \right. \\ \left. \left. - Z_{12}^2 n_{12} \frac{\partial p_{11}}{\partial r} \right) + \left(1.6 n_{11} Z_{Z1}^2 + 2.4 n_{12} Z_{12}^2 \right) n_{11} \frac{\partial T}{\partial r} \right] \quad (19)$$

3. CORONAL AND NON-CORONAL MODELS

Tokamak simulation codes [13] commonly use the coronal equilibrium model (collisional ionization balanced by radiative and dielectronic recombination) to determine the mean local Z of a given species of impurity, and the local radiated power. How valid is this model?

To investigate this question, we have used an atomic-physics computer-code package known as XSNQ [16]. The XSNQ code is based on an "average ion" model, in which the populations in the various levels are determined by solving rate equations using general analytic expressions for the transition rate coefficients. The transition processes included in the model are collisional ionization, radiative recombination, collisional excitation and de-excitation, radiative de-excitation, and dielectronic recombination. Emission processes include free-free, free-bound, and bound-bound ($\Delta n = 0$ and $\Delta n \neq 0$ transitions). Fuller details of this model may be found in Refs. [16] and [17]. As a first case to investigate, we have considered an experiment on impurity transport that was performed on the ATC tokamak [15].

In the ATC experiment, short bursts of aluminum atoms were injected into the discharge, with an energy of about 3 eV, and the various ionization levels were followed spectroscopically. Each ionization level was found to occur only in one particular cylindrical shell of the plasma and the various levels appeared sequentially in time, as the pulse penetrated into the discharge. From these measurements, it was possible to deduce the velocity with which the aluminum ions moved through the plasma. It was found that this velocity could be closely approximated by the formula $v = 2.1 - 0.2 x$ cm/msec, where x is the penetration distance into the discharge in cm. (Measurements were made only over the outer 7 cm, with the limiter at $a = 15$ cm.) Using this velocity, and the following approximations for the experimental electron density and temperature profiles:

$$n_e(r) = 2.5 \times 10^{13} \left(1 - \frac{r^2}{a^2}\right) \text{ cm}^{-3}; \quad T_e(r) = 1.4 \left(1 - \frac{r^2}{a^2}\right)^3 \text{ keV},$$

we can calculate the time-dependent electron density and temperature seen by the moving aluminum pulse. This is used as input to the XSNQ code.

The results are shown in Fig. 1. As a check on the pulse velocity employed, Fig. 1(a) shows the calculated densities of various aluminum ionization levels as functions of time, together with the times at which the intensity from each level was at its peak in the experiment. Figures 1(b) and (c) illustrate the differences between the coronal and the non-coronal models, by showing the mean Z and total aluminum radiation as functions of time. (In the code, the coronal results are produced by letting the atomic processes reach steady state at each time, before proceeding with the next time step.) As is to be expected, the aluminum reaches higher Z values (in particular, the helium-like level) earlier in the coronal model than in the non-coronal model. Figure 1(c) shows that this results in a marked disparity between the two calculations for the total radiation.

The velocity with which the aluminum ions are observed to move through the plasma agrees quite well with the neoclassical model. The neoclassical impurity convection velocity for an ion of charge Z due to collision with hydrogenic ions of density n_H and oxygen ions of density n_O and charge Z_O is given by Eq. (17), namely

$$v_r = \frac{8(2\pi)^{1/2}}{3} \frac{e^2 c^2 m_H^{1/2} q^2 \ln \Lambda}{(kT_i)^{1/2} B_T^2} \left[C_1^* \left(\frac{n_O Z_O^2}{n_H} \right) Z \frac{\partial n_H}{\partial r} + \left(\frac{m_O}{m_H} \right)^{1/2} Z_O Z \frac{\partial n_O}{\partial r} \right]. \quad (20)$$

Using the experimental parameters, and the non-coronal model for Z , we find that the neoclassical velocity due to collisions with the hydrogen alone is a factor 2-3 lower than the observed velocity. This discrepancy can probably be explained in terms of the effect of the oxygen impurities. Equation (20) would qualitatively support such an explanation, although a quantitative analysis is difficult in view of the experimental uncertainties in the profiles of the oxygen ion densities.

It is of interest to determine whether the validity of the coronal model is improved in a larger tokamak, such as the PLT. Using the coronal model for Z , and the following approximations for the PLT parameters:

$$\begin{aligned} n_e(r) &= 5 \times 10^{13} \left(1 - \frac{r^3}{a^3}\right) \text{ cm}^{-3}; & T_e(r) &= 2 \left(1 - \frac{r^2}{a^2}\right) \text{ keV}; \\ T_i(r) &= \left(1 - \frac{r^2}{a^2}\right) \text{ keV}; & q(r) &= 1 + 2 \frac{r^2}{a^2}; & B &= 35 \text{ kG}; \end{aligned}$$

we estimate the neoclassical convection velocity for an iron impurity to be about 0.5 cm/msec in the edge region, dropping to about 0.1 cm/msec at 15 cm into the plasma. [These estimates are based on a factor 3 enhancement of the value given by Eq. (20) for a pure hydrogen plasma.] We have considered the case of iron and molybdenum impurities in PLT using, for simplicity, a constant velocity in this range. The results are shown in Fig. 2. In the case of iron, we notice that discrepancies between the two models for the radiation occur whenever the coronal model gives complete stripping of a given shell

while the non-coronal model gives only partial stripping. On the whole, however, the results indicate that the coronal model should be a much better approximation in PLT-sized plasmas, due to the slower rate of impurity transport. The discrepancy between the coronal and non-coronal models is significant only in the extreme edge region of the discharge.

4. DIFFUSION OF IMPURITIES IN THE EDGE REGION

It would be a consequence of a purely classical, or neoclassical, transport model that all impurities would be retained permanently in a tokamak plasma. This is because the outward diffusion term is always smaller than the inward convection term. In practice, tokamak discharges are usually subjected to an influx of impurities at the edge, either due to the sputtering of heavy metallic impurities off the wall and limiter, or due to the desorption of non-hydrogen gas, such as oxygen, from the walls. In these circumstances, neoclassical theory would predict a continual build up of the impurity content of the plasma.

In the experiments, there is substantial evidence that the impurity content does not actually increase significantly in time, but rather that the impurities are lost from the plasma edge at about the same rate as the hydrogenic component. In this context, the initial results from the T-10 and PLT devices with currents in the 400-500 kA range are also encouraging. The discharge voltage, temperature, and therefore presumably Z_{eff} , are reported to hold approximately constant for the entire discharge time of about 500 msec. In these experiments, however, the dominant impurities, as far as contributions to Z_{eff} are concerned, are the lighter lower-Z elements especially oxygen.

To account for these observations, a model has been proposed [18] in which the neoclassical transport model for the impurities is supplemented by an anomalous diffusion term. On theoretical grounds, there are sound reasons for assuming that the same anomalous diffusion coefficient should apply equally to all ions, both hydrogenic and impurity. All ions would respond in a similar manner to drift wave turbulence, for example. On this basis, the magnitude of the anomalous diffusion coefficient to be applied to the impurities can be chosen so as to give agreement with the observed confinement times of the hydrogenic ions.

In this section, we examine the consequences of such a model in more detail. Specifically, we investigate the case of an influx of oxygen impurities into the edge region of a tokamak plasma. The influx is composed of neutral oxygen. Ionization and recombination of the various oxygen ions, inward convection, and outward diffusion, are all computed self-consistently. Since we are interested only in the edge region of the plasma, we employ a slab geometry, rather than a cylindrical one. Transport processes will take place on a rather short time scale in this narrow edge region. Moreover, ionization and recombination also occur rapidly for typical tokamak parameters. Accordingly, we may assume the edge region to be in steady state. We neglect the effects of temperature gradients on impurity transport, and we assume that all ions, hydrogenic and impurity, are in the Pfirsch-

Schlüter regime.

With these assumptions, and making use of the preceding theory, the equations for the densities n_{Oj} of the various ionization levels of oxygen are:

$$\begin{aligned}
 0 = \frac{\partial}{\partial x} \left[D \frac{\partial n_{Oj}}{\partial x} - C_{OH} \left(Z_j n_{Oj} \frac{\partial n_H}{\partial x} - n_H \frac{\partial n_{Oj}}{\partial x} \right) \right. \\
 \left. - C_{OO} \sum_{k \neq j} \left(Z_j Z_k n_{Oj} \frac{\partial n_{Ok}}{\partial x} - Z_k^2 n_{Ok} \frac{\partial n_{Oj}}{\partial x} \right) \right] \\
 + n_e (S_{j-1} n_{O, j-1} - S_j n_{Oj}) \\
 + n_e [(\alpha_{j+1} + \gamma_{j+1} n_e) n_{O, j+1} - (\alpha_j + \gamma_j n_e) n_{Oj}] ,
 \end{aligned} \tag{21}$$

where

$$C_{OH} = \frac{8(2\pi)^{1/2}}{3} \frac{e^2 c^2 m_H^{1/2} q^2 \ln \Lambda}{(kT_i)^{1/2} B_T^2} C_1^*(\alpha) , \tag{22}$$

$$C_{OO} = \frac{8\pi^{1/2}}{3} \frac{e^2 c^2 m_O^{1/2} q^2 \ln \Lambda}{(kT_i)^{1/2} B_T^2} \tag{23}$$

$$\alpha = \frac{1}{n_H} \sum_j Z_j^2 n_{Oj} .$$

Here, n_{Oj} is the density of j -times ionized oxygen; n_e and n_H are the electron and proton densities; S_j is the coefficient of ionization from the level j to the level $j+1$ taken from Ref. [19]; α_j and γ_j are the coefficients of radiative and collisional recombination from the level j to the level $j-1$ taken from Ref. [20]; the suffix 0 refers to the neutral atoms; and D is the anomalous diffusion coefficient. We include only the first 6 oxygen ionization levels in our computations, since the helium-like state is not, typically, reached in the edge region of a tokamak. Accordingly, we solve Eq. (21) only for $j=1-6$, and set $S_6 = 0$. We also neglect recombination to the neutral state, setting $\alpha_1 = \gamma_1 = 0$. In this approximation, the density n_{O0} of neutral oxygen arises entirely from the influx at the edge for a prescribed influx Γ_0 of neutral oxygen atoms each having a velocity v_0 , the neutral density within the plasma is given by

$$n_{O0}(x) = \frac{\Gamma_0}{v_0} \exp \left(- \frac{1}{v_0} \int_0^x S_0 n_e dx \right) ,$$

where the edge of the plasma is at $x = 0$.

The equation for the hydrogen density n_H is

$$0 = \frac{\partial}{\partial x} \left[D \frac{\partial n_H}{\partial x} + C_{OH} \sum_j \left(Z_j^2 n_{Oj} \frac{\partial n_H}{\partial x} - Z_j n_H \frac{\partial n_{Oj}}{\partial x} \right) \right] + S_H n_e n_{H0} \quad (24)$$

where n_{H0} is the hydrogen neutral density and S_H is the hydrogen ionization coefficient. The electron density is given by

$$n_e = n_H + \sum_j Z_j n_{Oj}.$$

The first problem that we have considered is: given a flux Γ_0 of neutral oxygen from the wall, what is the flux Γ_1 of oxygen ions that penetrate into the main part of the plasma? We have considered the edge 5 cm of a plasma of PLT parameters, i.e., the region $0 < x < x_1$ where $x_1 = 5$ cm. Rather than solve Eq. (24), we have taken a fixed profile for the hydrogen density of the form

$$n_H(x) = n_H^{\max} \left[1 - \left(1 - \frac{x}{a} \right)^4 \right] \quad 0 < x < x_1,$$

where $a = 40$ cm is the plasma radius, and $n_H^{\max}$ is the central plasma density, for which we have taken the two values $3 \cdot 10^{13} \text{ cm}^{-3}$ and $6 \cdot 10^{13} \text{ cm}^{-3}$. In evaluating C_{OH} and C_{OO} , we have taken $B_T = 30$ kG and $q = 5$. We have also taken fixed profiles for the temperatures, consistent with typical PLT results, namely

$$T_e(x) = T_i(x) = 1 + 100 \frac{x}{x_1} \text{ (eV)} \quad 0 < x < x_1.$$

The boundary conditions at $x=0$ are that the densities of all the oxygen ionization levels $j=1-6$ should vanish. The appropriate boundary conditions at $x=x_1$ are less obvious. Since we want to determine the proportion of the neutral influx that penetrates as ionized oxygen into the main part of the plasma, we want a condition that there be no diffusion back out from the main part of the plasma. Accordingly, we impose the conditions $\partial n_{Oj}/\partial x = 0$ at $x=x_1$, for $j=1-6$. With these boundary conditions our calculation determines the total flux of oxygen ions across $x=x_1$, and we denote this flux Γ_1 .

We have integrated Eqs (21) for a range of values of the anomalous diffusion coefficient D , the neutral oxygen influx Γ_0 , and the velocity of the incoming neutrals (the latter expressed in terms of an energy $kT_0 = m_O v_0^2/2$). The results are given in Fig. 3. In Fig. 3 (a), we show the density profiles of the various oxygen ionization levels in one particular case. In Fig. 3 (b), we show how the ratio of the fluxes Γ_1/Γ_0 depends on the various parameters. We see that the strongest dependence is on the magnitude of D . For the largest value of D ($\sim 4 \text{ cm}^2/\text{msec}$), the fraction of the neutral influx that penetrates into the main plasma is, typically, only 20%. This fraction is somewhat larger at the

higher hydrogen density, due to the increased rate of neoclassical inward convection. The dependence on the energy of the oxygen neutrals is not very pronounced, over a fairly wide range $0.05 < T_0 < 0.5$ eV. The decrease of the ratio Γ_1/Γ_0 with increasing oxygen density (increasing Γ_0) appears to be due partly to the decrease in the value of C_{OH} with increasing α , and partly due to increased electron density arising from the ionization of the oxygen, resulting in reduced penetration of the oxygen neutrals. The terms in Eq. (21) arising from oxygen-oxygen collisions seem to contribute moderately to the inward convection of the oxygen ions; for example, eliminating them by setting $C_{OO} = 0$ has the effect of reducing Γ_1/Γ_0 from 0.29 to 0.23 in case (iv) of Fig. 3(b) with $D=2$.

The second problem that we have considered is: what is the influx Γ_0 of neutral oxygen required to maintain, in steady state, a certain peak oxygen density $n_O^{\max}$ in the main part of the plasma. In this problem, the outflux of oxygen ions to the wall must, of course, exactly balance the neutral influx Γ_0 . The calculation is again done in a slab $0 < x < x_1$. The width x_1 of the slab is chosen so as to encompass the entire region penetrated by hydrogen neutrals: specifically, $x_1 = 20$ cm. To obtain a realistic profile for the density of the hydrogen ions, we have, in this case, included Eq. (24) in the set of equations that are integrated. The boundary conditions are $n_{II} = 0$ at $x = 0$, and $\partial n_H / \partial x = 0$ at $x = x_1$. The neutral hydrogen density n_{H0} is computed by the simple method proposed in Ref. [21], namely a diffusion equation

$$0 = \frac{\partial}{\partial x} \left(\frac{kT_i}{n_H m_H \langle \sigma v \rangle_{cx}} \frac{\partial n_{H0}}{\partial x} \right) - S_H n_e n_{H0} \quad (25)$$

where $\langle \sigma v \rangle_{cx}$ is the rate coefficient for charge exchange. This method is valid when the neutral mean free path for charge exchange is short compared with the plasma size, as is true for the fairly high density discharges considered here. The neutral hydrogen influx at $x=0$ is adjusted so as to give a value $n_H^{\max} = n_H(x_1) \approx 4 \cdot 10^{13} \text{ cm}^{-3}$. Since $\partial n_H / \partial x = \partial n_{Oj} / \partial x = 0$ at $x = x_1$, there is no flux of either hydrogen or oxygen into the main part of the plasma ($x_1 < x$). Thus, within our model, the main part of the plasma could be of arbitrary extent, containing uniform densities $n_H^{\max}$ and $n_O^{\max}$ of hydrogen and oxygen, respectively. The temperature profile is $T(x) = 1 + 400 x/x_1$ (eV).

The results of this calculation are given in Fig. 4, which shows the values of $n_O^{\max}$ for various values of Γ_0 and D . We see that the neutral influx Γ_0 required to maintain a given density $n_O^{\max}$ is a very strong function of D . In other words, within the range $D \sim 1 - 4 \text{ cm}^2/\text{msec}$, the oxygen confinement time decreases very sharply with increasing D .

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Fig. 1. Comparison of coronal and non-coronal (XSNQ) models for the aluminum injection experiment in the ATC tokamak. In (a), we show the calculated populations of the various aluminum ionization levels as functions of time, on the basis of the non-coronal model, and we indicate the times at which each level was at its peak in the experiment. In (b) and (c) we show the differences between the coronal and non-coronal models for the mean Z and the total aluminum radiation, respectively, as functions of time as the aluminum pulse penetrates into the plasma. In (b), we also show the electron density and temperature seen by the moving aluminum. PPPL 762257.

Fig. 2. Comparison of coronal and non-coronal models for iron and molybdenum impurities penetrating with velocity v_r into a plasma with PLT parameters. In (a) and (b), we show the mean Z and total radiation, respectively, for iron as functions of time. In (c), we show the same quantities for molybdenum. PPPL 762258.

Fig. 3. Diffusion of oxygen impurities through the edge region of a tokamak with PLT parameters. In (a), we show the density profiles of the various ionization levels for an influx $\Gamma_0 = 2.5 \times 10^{12} \text{ cm}^{-2} \text{ msec}^{-1}$ of neutral oxygen with energy $T_0 = 0.5 \text{ eV}$, an anomalous diffusion coefficient $D = 2 \text{ cm}^2/\text{msec}$, and a central hydrogen density $n_H^{\text{max}} = 3 \times 10^{13} \text{ cm}^{-3}$. In (b), we show the fraction Γ_1/Γ_0 of the neutral influx that penetrates into the main part of the plasma as a function of D , for various values of Γ_0 , T_0 , and n_H^{max} . PPPL 762256.

Fig. 4. Oxygen impurities in a tokamak with PLT parameters; steady state. We show the central oxygen density $n_O^{\max}$ that can be maintained in steady state by various values of the neutral influx Γ_0 , as a function of the anomalous diffusion coefficient D . PPPL 762255.