NEOCLASSICAL ANALYSIS OF IMPURITY TRANSPORT FOLLOWING TRANSITION TO IMPROVED PARTICLE CONFINEMENT

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ABSTRACT. Strongly peaked impurity density profiles have been observed in Alcator C after injection of frozen hydrogen pellets. Recent experiments in TEXT, ASDEX, PBX, JET and TFTR have exhibited similar impurity accumulation during regimes of improved confinement. The paper presents calculations of the neoclassically predicted equilibrium profiles of intrinsic light and heavy impurities in Alcator C and light impurities in TEXT. These calculations were performed for comparison with experimentally determined peaked profiles observed after pellet fuelling. In both machines, carbon exists in the plateau collisionality regime and its transport is dominated by collisions with the hydrogen background ions and by temperature gradient effects. In Alcator C, molybdenum is in the Pfirsch-Schlüter regime and is driven mostly by collisions with carbon inside r/a = 0.25 and by temperature gradients outside this radius. The full neoclassical multi-ion, mixed regime calculation required for the transport of carbon and molybdenum is presented. The predicted carbon profile in TEXT is in good agreement with observation; in Alcator C, less outward diffusion or an additional inward drift is required for the predicted carbon profile to agree with observation. The profile predicted for molybdenum (which may not be as close to equilibrium as carbon) is in fair agreement with observation. While the results of these studies do not support a rigorous claim of agreement with neoclassical impurity transport, the observed profiles for different regimes and experiments are consistently close to neoclassical-like peaking predictions.

1. INTRODUCTION

It is well known that transport processes in tokamaks have generally been found to be anomalous. For example, impurity profiles are typically less peaked than is predicted by neoclassical theory. However, discharges in the Alcator C tokamak with frozen fuel pellets injected into the plasma showed enhanced energy confinement [1] and strongly peaked, nearly neoclassical impurity density profiles [2]. More recent experiments on ASDEX [3-5], TEXT [6-8], JET [9] and TFTR [10] also demonstrated impurity peaking on axis following the injection of frozen hydrogen pellets or a transition to other improved confinement regimes. Similarly, Z-dependent impurity accumulation, in general agreement with estimates of neoclassical transport, has been measured during neutral beam heated H-mode discharges in PBX [11, 12]. Furthermore, peaking of heavy impurities in improved confinement modes in ASDEX has been accurately modelled using neoclassical fluxes [4], and peaking of light impurities in high density ASDEX discharges can also be explained approximately by neoclassical models [5]. In view of this, we describe calculations of the predicted equilibrium impurity profiles for both light and heavy impurities in Alcator C and for light impurities in TEXT using the neoclassical theory given by Hirshman and Sigmar [13], which has also been used in some form in TFR [14] and ASDEX [4].

The transport of ions in the source-free central region of a tokamak plasma can be described theoretically by the simple expression of particle conservation

\[ \frac{\partial n}{\partial t} + \nabla \cdot \Gamma = 0 \]  

where \( \Gamma \) is the flux of ions across the magnetic flux surfaces and \( n \) is the particle density. For the case of one impurity, the neoclassical impurity fluxes given in Ref. [13] are found in various collisionality regimes by performing the proper averaging of flux surfaces in a circular tokamak [15]. The classical flux of an impurity driven by friction against a single working main ion species is given (after Ref. [13], Eq. (5.11), but correcting for an erroneous factor of two) by

\[ \Gamma_T^C = \frac{\rho_D \nu_{D,\text{imp}}}{2Z_I} \times \left( \frac{\partial \ln P_D}{\partial r} - \frac{Z_D T_I}{Z_I T_D} \frac{\partial \ln P_I}{\partial r} - \frac{3 \partial \ln T_D}{2 \partial r} \right) \]
The banana-plateau (BP) flux is given (after Ref. [13], Eq. (7.43)) by
\[
\Gamma_{fp}^{BP} = \frac{3c^2r_D}{2e^2B_0^2R^2Z_D^2Z_I^2} \left( \frac{1}{1/K_{11}^0 + 1/K_{11}^1} \right) 
\times \left[ Z_I \left( \frac{\partial \ln P_D}{\partial r} - \frac{5 \partial \ln T_D}{2 \partial r} \right) 
- Z_D \left( \frac{\partial \ln P_I}{\partial r} - \frac{5 \partial \ln T_I}{2 \partial r} \right) 
+ \left( \frac{Z_I K_{12}^D}{K_{11}^D} - \frac{Z_D K_{12}^I}{K_{11}^I} \right) \frac{\partial \ln T_D}{\partial r} \right]
\]
(3)

for which the expressions for the viscosity matrix elements \(K_{11}^0, K_{11}^1, K_{11}^I\) and \(K_{12}^D\) are given in Appendix A.

Finally, the Pfirsch-Schluter flux is given (after Ref. [13], Eq. (6.75), but correcting for an erroneous factor of two and restoring agreement with Ref. [16]) by
\[
\Gamma_{fp}^{PS} = \frac{q^2n_D v_D^2 \nu_{DI}}{Z_I} 
\times \left[ K \left( \frac{\partial \ln n_D}{\partial r} - \frac{Z_D \partial \ln n_I}{Z_I} \right) + H \frac{\partial \ln T_D}{\partial r} \right]
\]
(4)
where (after Ref. [13], p. 1138)
\[
K = 1 - \frac{0.52\alpha}{0.59 + \alpha + 1.34g^{-2}}
\]
(5)
\[
H = -0.5 + \frac{0.29 + 0.68\alpha}{0.59 + \alpha + 1.34g^{-2}}
\]
(6)
Here, \(\alpha\) is the impurity strength parameter, \(\alpha = n_I Z_I^n D Z_B, g\) is the working ion collisionality parameter, \(g = \omega_{\text{to}} \tau_{\text{DD}} = \epsilon^{3/2} \nu.\) Regarding Eq. (4), we emphasize that the standard Pfirsch-Schluter enhancement factor 2\(q^2\) over the classical flux in Eq. (2) applies differently to the first two terms on the right hand side of Eq. (4) and to the thermal friction term \(T/T\).

Specifically, the density gradient terms are multiplied by \(2q^2 K\), but the temperature gradient term is multiplied by \(2q^2 H\), as first shown by Rutherford [16]. In these expressions, \(\Gamma_{fp}^{BP}\) is the banana-plateau flux, dominant for \(\epsilon^{3/2} \leq \epsilon^{3/2} \nu < 1\), and \(\Gamma_{fp}^{PS}\) is the Pfirsch-Schluter contribution, dominant for \(\epsilon^{3/2} \nu > 1\). The 'collisionality' \(\nu\) is defined as \(\nu = e^{3/2} / \nu_{DI}\). For example, in Alcator C, for deuterium
\[
\nu_D = \frac{16\sqrt{\pi} e^4 \ln \Lambda}{3m_D v_{TD}^3} \left[ \frac{n_D}{\sqrt{2}} + n_C Z_C^2 + n_Mo Z_Mo^2 \right]
\]
(7)
for carbon
\[
\nu_C = \frac{16\sqrt{\pi} e^4 Z_C^2 \ln \Lambda}{3m_C} \left[ \frac{n_D}{\sqrt{2}} + \frac{n_C Z_C^2}{\sqrt{2}m_C v_{TC}^3} + \frac{n_Mo Z_Mo^2}{m_Mo v_{TC}^3} \right]
\]
(8)
and for molybdenum
\[
\nu_{Mo} = \frac{16\sqrt{\pi} e^4 Z_{Mo}^2 \ln \Lambda}{3m_{Mo}} \left[ \frac{n_D}{m_D v_{TD}^3} + \frac{n_C Z_C^2}{m_C v_{TC}^3} + \frac{n_Mo Z_Mo^2}{\sqrt{2}m_{Mo} v_{TC}^3} \right]
\]
(9)
Here we use \(\tau_{ab}^{-1}\) from Appendix B, Eq. (B.30), if \(m_a < m_b\). For \(m_a = m_b\), \(\nu_{ab} = (2 - 1/2) \nu_{ab}\).

For \(m_a > m_b\), following Trubnikov [17], \(\nu_{ab} = \nu_{ab}(m_a, n_a, \ldots, n_a)\). The thermal velocity \(v_T = \sqrt{2T/m}\). Note that Eqs (2)-(4) can be written in the 'standard form' \(\Gamma_i = -D_i \partial n_i / \partial r - V_i n_i\), often used in experimental analysis, and we have introduced the subscripts \(D\) for deuterium and \(I\) for the impurity.

In Alcator C \((R_0 = 0.64 \text{ m}, a = 0.165 \text{ m})\) the main intrinsic impurities were carbon (C) and molybdenum (Mo). In the particular deuterium gas discharge considered here, the experimental conditions were (see Fig. 3 of Ref. [2])
\[
T_{Mo} = T_C = T_D = T_e = 1.6 \text{ keV at } r = 0, \text{ and } n_{Mo}(0) = 2.3 \times 10^{15} \text{ m}^{-3}, n_c(0) = 1.6 \times 10^{19} \text{ m}^{-3}, n_D(0) = n_e(0) = 5.6 \times 10^{20} \text{ m}^{-3}.
\]
Thus, recalling the impurity strength parameter \(\alpha = n_I Z_I^n D n_D, (\alpha = 3 \times 10^{-3}, \alpha_C = 0.9)\), we recall that if \(\alpha > \sqrt{m_a / m_D}\), the main ion collision friction \(R_{D} = R_{De} + R_{Dj}\) is dominated by \(R_{Dj}\), the ion-impurity friction, rather than \(R_{De}\), the ion-electron friction (see Appendix C). Thus, \(C\) is a strong impurity and Mo is a trace impurity. All nine permutations of the central collision frequencies \(\nu_{ab}\) (where \(a, b = D, C, Mo\)) are given in Table I together with the total collision frequencies and the ion thermal velocities. The relevant central values of the quantity \(\epsilon^{3/2} \nu\) are \(\epsilon^{3/2} \nu_C = 0.46\) and \(\epsilon^{3/2} \nu_{Mo} = 40\). Hence we conclude that in the central region of interest, \(C\) is mainly in the plateau regime and Mo is mainly in the Pfirsch-Schluter regime. Radial profiles of the quantity \(\epsilon^{3/2} \nu\) are shown in Fig. 1. Carbon lies in the plateau regime (between the dashed regime boundaries) from \(r = 0\) to about \(r = 10\) cm. Molybdenum, on the other hand, is in the Pfirsch-Schluter regime across the entire plasma. In principle, this multi-ion situation does not present
TABLE I. COLLISION FREQUENCIES AND THERMAL VELOCITIES

| Species | $\nu_{ab}$ (s$^{-1}$) | $\nu_{ab}$ (s$^{-1}$) | $\nu_{ab}$ (s$^{-1}$) | $\nu_{ab}^{\text{mol}}$ (s$^{-1}$) | $\nu_{T}$ (m·s$^{-1}$) |
|---------|-----------------|-----------------|-----------------|-----------------|-----------------|
| D       | $4.34 \times 10^3$ | $6.18 \times 10^3$ | $2.54 \times 10^1$ | $1.05 \times 10^4$ | $3.91 \times 10^3$ |
| C       | $3.68 \times 10^4$ | $6.43 \times 10^4$ | $3.73 \times 10^2$ | $1.55 \times 10^5$ | $1.60 \times 10^4$ |
| Mo      | $1.15 \times 10^5$ | $2.84 \times 10^5$ | $2.33 \times 10^3$ | $4.02 \times 10^5$ | $5.65 \times 10^4$ |

Note: The total collision frequency for species $a$ is $\nu_{a}^{\text{tot}} = \sum \nu_{ab}$. For the thermal velocity for each species, $\nu_{T}$, it is assumed that all temperatures are equal to the central electron temperature of 1.6 keV.

any calculational difficulties for C, since it is driven predominantly by the main deuterium ions. However, since the Mo flux is driven largely by the C ions, it is necessary to properly take into account the C ions and the existence of mixed regimes when calculating the Mo transport.

This paper is organized as follows. In Section 2 we describe the calculation of equilibrium profiles for C. In Section 3, we describe the multi-ion, mixed regime calculation for the equilibrium profile of Mo. Conclusions are given in Section 4. In the Appendices, the required details of the neoclassical calculation are summarized for completeness.

2. CARBON

The equilibrium carbon density profile can be found most simply (but not rigorously) by setting the asymptotic form of the radial plateau flux from Ref. [14] equal to zero. (The meaning of 'asymptotic' is given after Eq. (D.4) of Appendix D.) The asymptotic plateau flux has the form

$$\Gamma_p^P = 1.25 \frac{q}{R} \sqrt{m_I T_D} \frac{T_D^{3/2}}{B^2_Z e^2} \left[ \frac{\partial \ln n_D}{\partial r} - \frac{1}{Z_I} \frac{\partial \ln n_I}{\partial r} + 1.5 \frac{\partial \ln T}{\partial r} \right]$$

Then, in equilibrium,

$$\frac{\partial \ln n_D}{\partial r} - \frac{1}{Z_I} \frac{\partial \ln n_I}{\partial r} + 1.5 \frac{\partial \ln T}{\partial r} = 0$$

This has the solution

$$\frac{n_I(r)}{n_I(0)} = \left( \frac{n_D(r)}{n_D(0)} \right)^{Z_I} \left( \frac{T(r)}{T(0)} \right)$$
which is similar to the original result of Braginskij [18] and Taylor [19]. However, Taylor assumed a flat temperature profile, in which case the C profile would not derive any additional peaking from temperature gradients. Note that if C were in the Pfirsch–Schlüter regime, the result from Eq. (4) for the C profile would be

\[
\frac{n_T(r)}{n_T(0)} = \left( \frac{n_D(r)}{n_D(0)} \right)^{Z_I} \left( \frac{T(r)}{T(0)} \right)^{H_{Z_I}/K}
\]  

(13)

For the case of intermediate to low working ion collisionality (small g), in contrast to the result of Eq. (12), this would give temperature screening (i.e., a negative temperature gradient causes a flatter C profile) instead of the temperature peaking implied by Eq. (12).

As emphasized in Ref. [7], the asymptotic plateau expression is insufficient for calculating the equilibrium carbon density profiles; the collisionality-dependent expression of Eq. (3) must be used. Furthermore, even though C is in the plateau regime, the classical and Pfirsch–Schlüter fluxes from Eqs (2) and (4) contribute significantly to the total C flux.
NEOCLASSICAL ANALYSIS OF IMPURITY TRANSPORT

Figure 2(a) shows the equilibrium C profiles in Alcator C calculated in three different ways: (i) using the asymptotic banana-plateau formula of Eq. (10), (ii) using the collisionality dependent banana-plateau flux of Eq. (3), and (iii) using all three neoclassical fluxes in Eqs (2)-(4). The experimentally observed C profile in Alcator C using the nominal experimental parameters agrees best with the asymptotic plateau result; the experimental profile is more peaked than the equilibrium profile calculated using the sum of the three neoclassical fluxes. Thus, less outward diffusion or an additional inward drift is required to bring the complete neoclassical calculation into agreement with the observation. (The hollowness in the complete equilibrium profile is driven by the central proton deficit.)

The effect of experimental uncertainties was also examined by varying $T_e, T_h \text{ and } n_c$ within the error bars. The result is shown in Fig. 2(b), which indicates that significantly better agreement between the experiment and the full, more accurate, neoclassical calculation can be obtained within the uncertainties.

Good agreement between experimental carbon profiles and the full neoclassical calculation was found previously in TEXT [6]. We have performed the same calculation to provide an independent comparison with neoclassical theory. The result is shown in Fig. 3(a), which confirms the good agreement between the TEXT experimental result and the full neoclassical prediction. In TEXT, the experimental profile is broader than that predicted for both the asymptotic banana-plateau regime and the collisionality dependent banana-plateau regime. However, by varying the carbon density profile within the experimental uncertainty, near agreement with the less accurate asymptotic banana-plateau result can be obtained.

These two experimental profile uncertainty studies suggest the need for caution in claiming agreement in some cases and, also, disagreement in others.

3. MOLYBDENUM

The Mo impurity in Alcator C cannot be simply treated with the expressions (2)-(4) valid for one impurity frictioning on the main ion, because the Mo transport is dominated by effects from C [2] — another impurity. In their review of neoclassical impurity transport, Hirshman and Sigmar include a rigorous expression including multi-ion effects (Ref. [13], Eq. 6.129). When this expression is applied to Mo, we obtain the flux

$$Z_{Mo} \Gamma_{Mo}^{T_{Mo}} = \left( \frac{2c^2 Tq^2}{e^2 B_T^2} \right) \times \left[ \frac{L_1 \partial \ln p_I}{Z_I \partial r} + \frac{L_2 \partial \ln p_I}{Z_I \partial r} + \frac{L_3 \partial \ln T}{Z_I \partial r} + \frac{L_{11}^{TD} \partial \ln p_D}{Z_D \partial r} + \frac{L_{11}^{TT} \partial \ln p_T}{Z_T \partial r} + \frac{L_{11}^{TT} \partial \ln T}{Z_D \partial r} \right]$$

(14)

The $L$ coefficients are given in terms of the plasma parameters in Appendix B. The subscript $I$ represents the dominant impurity (C), and the subscript $T$ represents the trace impurity (Mo). All ion temperatures have been assumed to be the same.

Setting the radial trace impurity flux, $\Gamma_{Mo}^{T_{Mo}}$, to zero gives

$$\frac{L_{11}^{TT} \partial \ln n_T}{Z_T \partial r} + \left( \frac{L_1 + L_2}{Z_I} \right) \frac{\partial \ln n_I}{\partial r} + \left( \frac{L_1 + L_2 + L_3}{Z_I} \right) \frac{\partial \ln n_D}{\partial r} + \frac{L_{11}^{TT} \partial \ln T}{Z_D \partial r} = 0$$

(15)

Now the Mo density equilibrium profile is readily obtained in terms of the equilibrium C density, the deuterium density and the temperature profiles:

$$n_T(r) = n_T(0) \times \exp \left\{ - \int_0^r \frac{Z_T}{L_{11}^{TT}} \left( \frac{L_1 + L_2}{Z_I} \right) \frac{\partial \ln n_I}{\partial r} + \left( \frac{L_1 + L_2 + L_3}{Z_I} \right) \frac{\partial \ln n_D}{\partial r} \right\} \frac{\partial \ln T}{Z_D \partial r} + \frac{L_{11}^{TT} \partial \ln n_D}{Z_D \partial r} \right\} \, dr \right\}$$

(16)

Therefore, once the profile of the C density is known, this can be integrated numerically to obtain the Mo density profile.

To put this in a simpler form, similar to Eq. (12), we invoke the conditions predicted by Eq. (11) (and observed experimentally): $\partial \ln n_T/\partial r \ll \partial \ln n_C/\partial r$ and $\partial \ln n_T/\partial r \ll \partial \ln n_C/\partial r$. Then, Eq. (15) becomes

$$\frac{\partial \ln n_T}{\partial r} = - \frac{Z_T}{Z_I} \left( \frac{L_1 + L_2}{L_{11}^{TT}} \right) \frac{\partial \ln n_I}{\partial r}$$

(17)
which, using Eq. (12), has as an approximate solution

\[
\frac{n_T(r)}{n_T(0)} = \left( \frac{n_f(r)}{n_f(0)} \right)^{\lambda(r)Z_T/Z_f} = \left( \frac{n_D(r)}{n_D(0)} \right)^{\lambda(r)Z_T} \left( \frac{T(r)}{T(0)} \right)^{1.5\lambda(r)Z_T} \quad (18)
\]

Note from Eq. (18) that the Mo peaking is driven by the C profile, which is itself peaked. In this expression, \( \lambda(r) = -(L_1 + L_2)/L_{1f}^T \), and is a slowly varying positive quantity of order one. Figure 4 shows the accurate value of \( \lambda(r) \), calculated from the coefficients in Appendix B and from the plasma parameters of Ref. [2]. It is important to note here that in Ref. [2] the more rigorous form of Eq. (16), including the deuterium density gradient and the temperature gradient terms was used to predict the Mo profile for comparison with the experimental value.

![Graph](image)

**FIG. 4.** The quantity \( \lambda(r) = -(L_1 + L_2)/L_{1f}^T \) (see Eq. (18)) for the parameters measured in a particular Alcator C discharge with deuterium gas, \( B_T = 9.75 \, T \) and \( I_p = 520 \, kA \) (see Ref. [2]).

### 4. CONCLUSIONS

The neoclassical theory for impurity transport predicts equilibrium density profiles that are more peaked than the electron density profile. In the case of mildly collisional carbon, in the plateau regime, the asymptotic plateau prediction is given by Eq. (12). For carbon in Alcator C, this relation gives excellent agreement with the experimental observations [2]. However, the standard neoclassical theory using the collisionality dependent banana-plateau flux and including the classical and the Pfirsch–Schluter flux contributions (Eqs. (2)–(4)) predicts a C profile broader than that observed experimentally. In TEXT, the profile from the full neoclassical prediction agrees well with the measured profile. This difference between TEXT and Alcator C may be caused by a modification of the Pfirsch–Schluter contribution to the C flux due to a poloidal impurity density variation (up-down) in the outer region, which reduces transport in the collisional regime [20]. Note from Fig. 2 that it is precisely the Pfirsch–Schluter contribution which is responsible for significant broadening of the C profile. This asymmetry effect was not included in the analysis presented here. Neither was a more recent suggestion [21] of collisional cold ion inward convection producing a low energy deviation from the ion Maxwellian distribution. Also not included was the C-O^8+ interaction, for lack of data on oxygen. Furthermore, we note that the parameter \( \sqrt{m_p/m_e} = 0.41 \), which is used as a standard expansion parameter in the collision operator calculation, is not small. In TEXT, where the working gas was hydrogen, \( \sqrt{m_p/m_e} = 0.29 \), providing a better expansion.

For highly collisional Mo, in the trace impurity limit and in the Pfirsch–Schluter regime, an exact form for the profiles is given by Eq. (16), and a simplified prediction is given by Eq. (18), with \( \lambda(r) \) shown in Fig. 4. Note that the exponent in Eq. (18), \( \lambda(r)Z_T/Z_{Te} \), is smaller than one would estimate from the simpler cases considered in Refs [18] and [19]. The predicted Mo profile is more peaked than the observed one. However, Mo is further from equilibrium than C. If the time dependence were taken into account, the predicted profile would be broader, because Mo would still be peaking. Moreover, since Mo is a trace impurity \( \alpha_{Mo} = 3 \times 10^{-3} < \sqrt{m_p/m_d} \), the ambipolar constraint between the Mo flux and the electron flux may further broaden the predicted profiles (see Appendix C).

In conclusion, the present treatment does not constitute a full proof of neoclassical impurity transport since this would also require demonstrating that the experimental time-scale to reach accumulation equilibrium agrees with time dependent neoclassical modelling (which has not been pursued here). Furthermore, it would require correct scaling with global plasma parameters for which no data exist.
NEOCLASSICAL ANALYSIS OF IMPURITY TRANSPORT

(Neoclassical scaling of the particle confinement time has been observed in the TJ-1 tokamak [22] but was not systematically tested in Ref. [2].) However, the experimentally observed tendency of the peaking of the C and Mo equilibrium profiles to agree with the detailed facets of equilibrium neoclassical theory appears to be suggestive of neoclassical particle transport after pellet injection.

Appendix A

NEOCLASSICAL VISCOSITY COEFFICIENTS

A rational approximation to calculate the viscosity matrix elements from those in the different collisionality regimes is given in Ref. [13]. For species \( a \) (from Ref. [13], Eq. (4.75)),

\[
K_{ij}^a = \frac{K_{ij}^a}{(1 + K_{ij}^a B/K_{ij}^a B^P)(1 + K_{ij}^a P/K_{ij}^a P^P)}
\]  
(A.1)

In the plateau regime (from Ref. [13], Eq. (4.65)),

\[
K_{ij}^a P^P = \frac{P_a \sqrt{\pi}}{3 \omega_{Ta}} \Gamma(i + j + 1)
\]  
(A.2)

where the transit frequency \( \omega_{Ta} = \frac{v_{Ta}}{\rho_a} \), and \( v_{Ta} = \sqrt{2T_a/m_a} \). In the Pfirsch-Schlüter regime (from Ref. [13], Eq. (4.31)),

\[
K_{ij}^a P = P_a \tau_{Ta} \kappa_{ij}^a
\]  
(A.3)

In this expression (from Ref. [13], Eqs (4.32)-(4.40)),

\[
\kappa_{11}^a = \frac{q_{11}^a}{Q_a}
\]  
(A.4)

\[
\kappa_{12}^a = \frac{7/2}{(q_{11}^a + q_{01}^a)} Q_a = \kappa_{21}^a
\]  
(A.5)

\[
\kappa_{22}^a = \frac{49/4}{(q_{11}^a + q_{01}^a + 2q_{00}^a)} Q_a
\]  
(A.6)

In these equations,

\[
Q_a = (2/5)(q_{00}^a q_{11}^a - q_{01}^a q_{01}^a)
\]  
(A.7)

The \( q^{ij} \) and \( r^{ij} \) elements are given by

\[
q_{aa}^{00} = (3 + 5z_{aa}^2)(1 + z_{aa}^2)^{-3/2}
\]  
(A.9)

\[
q_{aa}^{01} = (3/2)(3 + 7z_{aa}^2)(1 + z_{aa}^2)^{-5/2}
\]  
(A.10)

\[
q_{aa}^{11} = \frac{35z_{aa}^6}{(1 + z_{aa}^2)^{7/2}}
\]  
(A.11)

\[
r_{aa}^{00} = 1/\sqrt{2}
\]  
(A.12)

\[
r_{aa}^{01} = 3/2\sqrt{2}
\]  
(A.13)

\[
r_{aa}^{11} = 15/4\sqrt{2}
\]  
(A.14)

The quantity \( z_{ab} \) represents the ratio of thermal velocities, \( z_{ab} = v_{Ta}/v_{Db} \).

In the banana regime (from Ref. [13], Eq. (4.61)),

\[
K_{ij}^a B = \frac{f_1 n_a m_a}{2 \rho_a R^2 B^2} \left\{ x_{a}^{2(i+j-2)} \nu_D \tau_{Ta} \right\}
\]  
(A.15)

where \( f_1 = 1 - f_c = \sqrt{2}e \) is the fraction of trapped particles.

Also note that \( \nu_D^a = \Sigma_a \nu_D^a \) is the deflection frequency, and the curly brackets represent integration over the distribution function, which may be evaluated for a Maxwellian as follows (from Ref. [13], Eqs (4.62)-(4.64)):

\[
\left\{ \nu_D^{ab} \right\} \tau_{Ta} = (1 + z_{ab}^2)^{1/2} + z_{ab}^2 \ln \left[ \frac{z_{ab}}{1 + (1 + z_{ab}^2)^{1/2}} \right]
\]  
(A.16)

\[
\left\{ z_{ab}^2 \nu_D^{ab} \right\} \tau_{Ta} = (1 + z_{ab}^2)^{-1/2}
\]  
(A.17)

\[
\left\{ z_{ab}^4 \nu_D^{ab} \right\} \tau_{Ta} = \frac{2(1 + (5/4)z_{ab}^2)}{(1 + z_{ab}^2)^{3/2}}
\]  
(A.18)

Appendix B

NEOCLASSICAL COEFFICIENTS

The coefficients for Eq. (14) are summarized (from Ref. [13], p. 1148) as follows:

\[
L_1 = -\frac{m_1 m_I}{\tau_{IT}} (d_0 + 0.236d_3)
\]

\[
-\frac{m_Dn_D}{\tau_{DT}} \left[ 1 - C_1(D_TI, 0) \right]
\]  
(B.1)
\[ L_2 = \frac{m_1 n_I}{\tau_{TI}} (0.236 d_3) \]  
\[ L_3 = \frac{m_1 n_I}{\tau_{TI}} d_3 \]  
\[ L_{TT}^{II} = \frac{m_1 n_I}{\tau_{TI}} d_0 + \frac{m_D n_D}{\tau_{TD}} \]  
\[ L_{TD}^{II} = \frac{m_D n_D}{\tau_{TD}} C_1(\bar{Z}_{DI}, 0) \]  
\[ L_{TD}^{ID} = \frac{m_D n_D}{\tau_{TD}} C_2(\bar{Z}_{DI}, 0) \]

where the collision times \( \tau_{ab} \) are defined below.

The variables labelled \( d \) are:

\[ d_0 = -\left( \frac{m_T}{m_I} \right)^{1/2} \left[ \frac{\dot{M}^{01} - \dot{M}^{01} \dot{M}^{10}}{\dot{M}^{11}} \right] \]  
\[ d_1 = 0.88 \left( \frac{m_T}{m_I} \right)^{1/2} \left[ \frac{\dot{N}^{01} - \dot{M}^{01} \dot{N}^{11}}{\dot{M}^{11}} \right] - \frac{4}{15} \left( \dot{N}^{02} - \frac{\dot{M}^{01} \dot{N}^{12}}{\dot{M}^{11}} \right) \]  
\[ d_2 = \frac{\dot{M}^{01}}{\dot{M}^{11}} \]  
\[ d_3 = \frac{1}{0.885} \left[ \left( \frac{Z_I^2}{Z_T^2} \right) d_2 - d_1 \right] \]

Here, the coefficients \( C_1, C_2 \) as functions of two arbitrary variables \( \alpha \) and \( \beta \) are

\[ C_1(\alpha, \beta) = 1 - \frac{0.52 \alpha}{0.59 + \alpha + 1.34 \beta^2} \]  
\[ C_2(\alpha, \beta) = 1.5 - \frac{0.29 + 1.20 \alpha}{0.59 + \alpha + 1.34 \beta^2} \]

We also have defined

\[ \bar{Z}_{DI} = \frac{n_I Z_I^2}{n_D} \]  
\[ \beta = \omega_{TD} \tau_{TD} \]

where \( \omega_{TD} \) is the transit frequency of \( D \),

\[ \dot{M}^{ij} = M_{TI}^{ij} - \frac{M_{TI}^{2j} M_{TI}^{2j}}{M_{TI}^{2j}} \]  
\[ \dot{N}^{ij} = N_{TI}^{ij} - \frac{N_{TI}^{2j} N_{TI}^{2j}}{M_{TI}^{2j}} \]

For arbitrary species indices \( a \) and \( b \), we have

\[ M_{ab}^{00} = - \left( 1 + \frac{m_a}{m_b} \right) (1 + x_{ab}^2)^{-3/2} = -N_{ab}^{00} \]  
\[ M_{ab}^{01} = M_{ab}^{10} = -\frac{3}{2} \left( 1 + \frac{m_a}{m_b} \right) (1 + x_{ab}^2)^{-5/2} \]  
\[ M_{ab}^{11} = -\left( \frac{13}{4} + 4 x_{ab}^2 + \frac{15}{2} x_{ab}^4 \right) (1 + x_{ab}^2)^{-5/2} \]  
\[ N_{ab}^{11} = \frac{27}{4} x_{ab}^2 (1 + x_{ab}^2)^{-5/2} \]  
\[ N_{ab}^{02} = -\frac{15}{8} \left( 1 + \frac{m_a}{m_b} \right) (1 + x_{ab}^2)^{-7/2} = -x_{ab} N_{ba}^{02} \]  
\[ N_{ab}^{12} = -\left( \frac{69}{16} + 6 x_{ab}^2 + \frac{63}{4} x_{ab}^4 \right) (1 + x_{ab}^2)^{-7/2} \]  
\[ M_{ab}^{22} = -\left( \frac{443}{64} + 17 x_{ab}^2 + (459/8) x_{ab}^4 + 28 x_{ab}^6 + (175/8) x_{ab}^8 \right) (1 + x_{ab}^2)^{9/2} \]  
\[ N_{ab}^{22} = \frac{2625}{64} x_{ab}^4 (1 + x_{ab}^2)^{9/2} \]  
\[ x_{ab} = \frac{v_T b}{v_T a} \]

where \( v_T a = \sqrt{2 T/m_a} \). It is important to note that

\[ M_{ab}^{00} + N_{ab}^{00} = 0 \]  
\[ M_{ab}^{ij} = M_{ab}^{ji} \]  
\[ \frac{N_{ab}^{ii}}{T_a v_T a} = \frac{N_{ba}^{ii}}{T_b v_T b} \]

and the collision time is taken from Braginskij to be

\[ \tau_{ab} = \left( \frac{3 \sqrt{\pi}}{4 \pi} \right) \frac{m_a^2 v_T a^3}{4 \pi n_a e_a^2 e_b^2 \ln \Lambda} \]  
\[ m_a < m_b \]
Appendix C

AMBIPOLAR DIFFUSION FOR A TWO-ION SPECIES PLASMA

Taking the toroidal momentum balance, the radial particle flux $\Gamma_a$ follows from

$$0 = eZ_a B_p + R_a; \quad R_a = \sum_{b \neq a} R_{ab}$$

(C.1)

where the collisional friction is

$$R_{ab} = -m_an_a\nu_{ab}(v_a - v_b)$$

(C.2)

and (see Appendix B, Eq. (B.30))

$$\nu_{ab} \sim Z_a^2 n_b/(m_a^{3/2})$$

(C.3)

and $v_a \sim v_{Ta} \rho_a/r_n$. Here, $r_n$ is the radial scale length defined as $\langle n/(\partial n/\partial r) \rangle$, and $\rho_a$ is the poloidal gyroradius of species $a$, which can be $e$, $D$, $C$ or $Mo$ in the case at hand. From Eqs (C.1) and (C.2) and $R_a = -R_{oa}$ follows the collisional transport ambipolarity condition

$$Z_{Mo} \Gamma_{Mo} = \Gamma_e - (\Gamma_D + Z_C \Gamma_C)$$

(C.4)

Defining the impurity strength parameter,

$$\alpha_j = n_j Z_j^2/nD; \quad j = C, Mo$$

(C.5)

and using the scaling expression (C.3) in Eq. (C.2), one finds in general $R_{D}/R_{DI} \sim \sqrt{m_e/m_D/\alpha_D}$. Then, $R_{DP}/R_{DP} \sim \sqrt{m_e/m_D/\alpha_D} \ll 1$, but $R_{DP}/R_{Mo} \sim \sqrt{m_e/m_D/\alpha_Mo} \gg 1$, $R_{DMo}/R_{DC} = \alpha_{Mo}/\alpha_C \ll 1$, and $R_{CMo}/R_{DC}$ is entirely negligible (recalling $\alpha_C \sim 1$ and $\alpha_Mo \sim 3 \times 10^{-5}$). From Eqs (C.1), (C.2) and (C.3), the deuterium flux scales as

$$\Gamma_D \sim R_{DC} \left(1 + \frac{\sqrt{m_e/m_D}}{\alpha_C} + \frac{\alpha_{Mo}}{\alpha_C}\right)$$

(C.6a)

and the carbon flux scales as

$$-Z_C \Gamma_C \sim R_{DC} \left(1 + \frac{\sqrt{m_e/m_D}}{\alpha_C}\right)$$

(C.6b)

Therefore, to zeroth order in $\sqrt{m_e/m_D}$,

$$\Gamma_D^{(0)} + Z_C \Gamma_C^{(0)} = 0$$

(C.7a)

and for our case of $\alpha_{Mo}/\alpha_C < \sqrt{m_e/m_D}$,

$$\Gamma_Mo^{(0)} = 0$$

(C.7b)

This result is indeed borne out from Eq. (14) (or Eq. (4)) for Mo if one notices that $\nu_{Mo} \propto \alpha_{Mo}$ and is therefore of first order.

To obtain the first order flux $\Gamma_D^{(1)}$ the neoclassical electron flux must be retained, which scales as

$$\Gamma_e \sim R_{DC} \frac{\sqrt{m_e/m_D}}{\alpha_C} \left(1 + \alpha_C + \alpha_{Mo}\right)$$

(C.8)

and is thus of first order in $\sqrt{m_e/m_D}$. Thus, from Eq. (C.4),

$$Z_{Mo} \Gamma_Mo^{(1)} = \Gamma_e^{(0)} + Z_{Mo} \Gamma_{Mo}^{(0)}$$

(from Eq. (14))

(C.9)

where the last term derives from the Mo–D and Mo–C friction, including the thermal friction proportional to $T'/T$. For $\Gamma_e^{(0)}$, we can take the usual electron banana regime expression

$$\Gamma_e^{(0)} = -D_e^{BP} n_e \left(\frac{n_s'}{n_s} \left(1 + \alpha \right) + \frac{n_i'}{n_i} + \frac{\alpha n_s'}{Z n_s}ight)$$

$$+ k_{BP} \frac{T'}{T} + \Gamma_e^{(Ware)}$$

(C.10)

We note that this is radially outward even when the ions have satisfied Eq. (C.7a). This outward flow will retard the Mo peaking. The Ware flux is inward. In Eq. (C.9), $\Gamma_{Mo}$ (from Eq. (14)) is also inward. Thus, the overall rate of inward Mo transport will be affected by the detailed balance of the terms in $\Gamma_e^{(0)}$. The exact equilibrium condition follows from setting the right hand side of Eq. (C.9) equal to zero, with $\Gamma_e^{(0)}$ from Eq. (C.10). This will lead to a dependence of the Mo equilibrium profile on the ratio of the electron diffusion coefficient $D_e^{BP}$ in Eq. (C.10) and the diffusion coefficients contained in Eq. (14).

In all of the above, the turbulent driven fluxes $\Gamma_j^t$ (which for the typical low frequency turbulence in tokamaks have also been shown to be intrinsically ambipolar by themselves, i.e. $\Sigma_j \epsilon_{ij} \bar{e}_{ij} = 0$) have been assumed to be decoupled from the collisionally driven fluxes of Eq. (C.1). This may be justified for the typically observed low saturation amplitudes $\bar{e}_{ij}/T_e \geq 10^{-2}$ in the plasma core. There is no turbulent theory which gives the net fluctuation driven contribution including impurities to the right hand side of Eq. (C.9).
Appendix D

OUTLINE OF CALCULATION OF FLUXES IN TRANSITIONAL COLLISIONALITY REGIMES

It is shown in Ref. [13] that, in general, all three regime contributions to the flux \( T_j = \langle n_j \nu_j \cdot \nabla \psi \rangle \), driven by the friction \( \vec{R}_j \), must be kept. From toroidal momentum balance the (contravariant) flux \( \Gamma_j = \langle n_j \vec{v}_j \cdot \nabla \psi \rangle \) is given by

\[
e_j \Gamma_j = \left( \langle R \vec{e}_\phi \cdot \left( \frac{\vec{B}}{B} + \vec{R}_{\perp j} \right) \right)
\]

\[
= F \frac{\langle R|| B \rangle}{B^2} \left( 1 - \frac{B^2}{B^2} \right) + F \frac{\langle R\| B \rangle}{B^2} + \langle R \vec{e}_\phi \cdot \vec{R}_{\perp j} \rangle
\]

\[
\equiv e_j^{PS} \Gamma_j + e_j^{BP} \Gamma_j + e_j^{CL} \Gamma_j
\]

where \( F = RB_\phi \). (Note that each piece is individually ambipolar, which may be useful to know in mixed collisionality regimes.) From parallel momentum balance, to lowest order in \( \rho_{pol}/\tau_n \),

\[
0 = -\left( \vec{B} \cdot \nabla \cdot \frac{\vec{v}_j}{\tau_j} \right) + (BR||)
\]

which can be used to write

\[
e_j^{BP} \Gamma_j = F \frac{\langle \vec{B} \cdot \nabla \cdot \frac{\vec{v}_j}{\tau_j} \rangle}{B^2}
\]

It was shown (see Ref. [13]) that \( \langle \vec{B} \cdot \nabla \cdot \frac{\vec{v}_j}{\tau_j} \rangle \) rises in the banana regime, peaks in the plateau regime and evanesces in the Pfirsch-Schluter regime (where \( \tau_j \) is collisionally isotropized, but we note [20] that \( \tau_j \) can have contributions from collisions between unlike species).

In an impure plasma the Pfirsch-Schluter flux (first term on the right in Eq. (D.1)) is evidently driven by the poloidal variation of \( R||/B \), which can be shown [20] to scale with the parameter

\[
\Delta \equiv \left( \rho_{pol}/\tau_n \right) Z^2 \frac{\nu_{ii}}{\omega_{ti}}
\]

which is large in the Pfirsch-Schluter regime and evanesces into the BP regime (where the long mean free path suppresses poloidal variations). The classical flux \( \Gamma^{CL} \) will also contribute near the plasma centre where \( 2q^2 - 1 \) (particularly if \( q_0 < 1 \)). Thus, for each species \( j \) the full expression for the flux becomes (see Eqs (D.1), (D.2)):

\[
\Gamma_j = - \sum_s D_{js} \frac{\partial n_j}{\partial r} - n_j V_{js}, \quad s = PS, BP, CL
\]

i.e. \( s \) denotes the collisionality regime. \( V_{js} \) is of the form

\[
K_{js} \frac{1}{e_h n_k} + H_{js} \frac{T'}{T}, \quad \text{with} \quad k \neq j
\]

\( D_{js}, K_{js} \) and \( H_{js} \) are functions of \( \varepsilon, \nu_j \) and \( \alpha_j = n Z^2_j/n_D \), describing the transitions. Equation (3) and Appendix A show an example of these three \( \nu_j \) dependent coefficients for \( s = BP \). Thus we can define the asymptotic form of the flux \( \Gamma_j \) in Eq. (D.3) as the expression which remains when (i) taking only the dominant \( \Gamma \) contribution for the index \( s \) (i.e. \( s = \text{plateau for carbon} \)) and (ii) taking the appropriate asymptotic limit for \( \nu_j \) in the coefficients \( D_j, H_j \) and \( K_j \).

Therefore, Eq. (10) is clearly most valid in 'asymptotic' regimes away from transition boundaries, and Fig. 1 gives only a first guideline for the appropriate regimes. In connection with this general remark, we would like to mention some specific errors in Ref. [13], Eqs (5.11) and (6.75). Defining \( u_j^2 = 2T/m \) in Eq. (5.11), \( D \) should be divided by 2. In Eq. (6.75), \( e_H \) and \( e_7 \) should be replaced by \( Z_H \) and \( Z_7 \) respectively, and, because of an error similar to that in Eq. (5.11), \( D \) should be divided by 2.

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1126

NUCLEAR FUSION, Vol.30, No.6 (1990)
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NEOCLASSICAL ANALYSIS OF IMPURITY TRANSPORT

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