ORNL/TM-8341
Dist. Category UC-20 g

Contract No. W-7405-eng-26

FUSION ENERGY DIVISION

ORNL/TM--8341

DE82 018207

IMPLEMENTATION OF THE REDUCED CHARGE STATE METHOD OF CALCULATING IMPURITY TRANSPORT

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Date Published - July 1982

Prepared by
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operated by
UNION CARBIDE CORPORATION
for the
DEPARTMENT OF ENERGY

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ABSTRACT

A recent review article by Hirshman and Sigmar includes expressions needed to calculate the parallel friction coefficients f_{ij}^{ab}, the essential ingredients of the plateau-Pfirsch-Schlüter transport coefficients, using the method of reduced charge states. These expressions have been collected and an expanded notation introduced in some cases to facilitate differentiation between reduced charge state and full charge state quantities. A form of the Coulomb logarithm relevant to the method of reduced charge states is introduced. This method of calculating the f_{ij}^{ab} has been implemented in the impurity transport simulation code IMPTAR and has resulted in an overall reduction in computation time of approximately 25% for a typical simulation of impurity transport in the Impurity Study Experiment (ISX-B). Results obtained using this treatment are almost identical to those obtained using an earlier approximate theory of Hirshman.

1. INTRODUCTION

At various stages in the development of our IMPurity Transport And Recycling computer simulation code, IMPTAR, we have used different formulations for the impurity transport coefficients. They have been, in approximate historical order, approximations based on a Lorentz plasma hierarchy, i.e., $m_1 << m_2 << \ldots << m_i$, where the m_i stand for the masses of the various hydrogenic and impurity chemical elements;[1] an exact treatment[2] that does not take into account the effects of the plateau-Pfirsch-Schlüter transition;[3] a reduced charge state formulation[4] of the theory of Ref. 2; and a treatment similar to that of Ref. 2 that incorporates an approximation to the effects of the plateau-Pfirsch-Schlüter transition.[5-7] Recently, Hirshman and Sigmar have published a review paper[8] in which the effects of the plateau-Pfirsch-Schlüter transition are taken into account in a reduced charge state formulation. We have now implemented the theory of Ref. 8 in IMPTAR and present here some preliminary results.

The Lorentz hierarchy approximation was unsatisfactory because the experiments we simulate contain impurities that do not satisfy the required mass relationship very well, e.g., oxygen (m = 16 amu) and argon (m = 40 amu). Before the introduction of the CRAY computer with its vector capabilities at the National Magnetic Fusion Energy Computing Center, limitations of computer time kept us from using the method of Ref. 2 except for cross checks. Even after we began using the CRAY, approximately 40% of the calculation time was used in computing coefficients for multispecies plasmas, primarily because the treatments of Refs. 2 and 5 require the solution of linear systems on the order of the number of different charge states of the chemical elements present. Thus, for example, a plasma containing hydrogen, oxygen, and argon requires solutions of 27 sets of coupled equations. The reduced charge state formalism introduced in Ref. 4 reduces the number of sets from n = number of charge states present to n′ = number of chemical elements present, which for the above example would be a reduction from 27 to 3. We implemented this method as a test and found considerable time savings, but by that time the theory had progressed to the point of considering the plateau-Pfirsch-Schlüter transition,[9]

which showed an important temperature screening effect not treated in Refs. 2 and 4, so we could not make use of the less time-consuming method. The implementation of the theory of Ref. 5 allowed us to take the temperature screening effect into account, but it was still necessary to solve large linear systems. Now, with the implementation of the theory of Ref. 8, we again have to invert only small matrices.

In Sect. 2 we review the reduced charge state method of calculation of the parallel friction coefficients f_{ij}^{ab}, which are central to the calculation of the impurity transport coefficients. In Sect. 3 we present preliminary numerical results, which show that the approximate method of including the plateau-Pfirsch-Schlüter transition[5] yields surprisingly good results for the cases considered, and discuss the savings in computing time. In Sect. 4 we present our conclusions and plans for future work. Finally, in the Appendix, we give an example of typical units used in a practical evaluation of one of the quantities needed for the calculation of the f_{ij}^{ab}.

2. NUMERICAL CALCULATION OF f_{ij}^{ab} FOR APPLICATION IN IMPURITY TRANSPORT SIMULATION

The parallel friction coefficients f_{ij}^{ab} of Ref. 8 play the same role in the calculation of the perpendicular Pfirsch-Schlüter fluxes that was played by the ℓ_{ij}^{ab} of Ref. 2, an earlier version of this calculation without plateau-Pfirsch-Schlüter transition effects. The relationship between the f_{ij}^{ab} and the ℓ_{ij}^{ab} is given by Eq. (6.39) of Ref. 8.

Numerical calculation of the f_{ij}^{ab} using the reduced charge state model rather than the full charge state model permits a considerable reduction in the time required for matrix manipulation because the full charge state model requires one matrix element for each charge state of each chemical element considered, while the reduced charge state model requires only one matrix element for each chemical element. The reduced charge state model is covered in Ref. 8 and the references therein; it is discussed here only as needed in presenting the equations to be used.

2.1 THE PARALLEL FRICTION COEFFICIENTS f_{ij}^{ab}

The symmetric parallel friction coefficients f_{ij}^{ab} for the interaction of charge state species a with charge state species b are given in Ref. 8 as

$$f_{ij}^{ab} = \xi_a(\bar{M}_a^{i-1,j-1}\delta_{ab} - \bar{M}^{i-1,2}\alpha_{ab}^{j} + \xi_b \bar{N}_{ab}^{i-1,j-1} - \sum_{m_k} \bar{N}_{ak}^{i-1,2}A_{ab}^{j}) , \quad (6.41)\ (1)$$

where the indices i and j range from 1 to 2. (Here and in what follows, the corresponding equation number from Ref. 8 is shown immediately to the left of our equation number for reference.) In Eq. (1),

$$\xi_a = \frac{n_a e_a^2}{\sum_{i_a} n_a e_a^2} \quad , \tag{2}$$

where the summation is over the various charge states of the chemical element of mass m_a and a specific charge state is indicated in the numerator. In clearer but more cumbersome notation, Eqs. (1) and (2) may be written as

$$f_{ij}^{a_\mu b_\nu} = \xi_{a_\mu}(\bar{M}_a^{i-1,j-1}\delta_{a_\mu b_\nu} - \bar{M}_a^{i-1,2}\alpha_{a_\mu b_\nu}^{j} + \xi_{b_\nu}\bar{N}_{ab}^{i-1,j-1} - \sum_{m_k}\bar{N}_{ak}^{i-1,2}A_{ab_\nu}^{j}) \tag{3}$$

and

$$\xi_{a_\mu} = \frac{n_{a_\mu} e_{a_\mu}^2}{\sum_\nu n_{a_\nu} e_{a_\nu}^2} \quad , \tag{4}$$

where μ and ν index the densities n_{a_μ} and electric charge e_{a_μ}, respectively, of distinct charge states of chemical element a.

Other terms in Eq. (1) are defined as follows:

$$\bar{M}_a^{ij} = \sum_{m_b} m_a \left\langle\!\left\langle \frac{n_a}{\tau_{ab}} \right\rangle\!\right\rangle M_{ab}^{ij} \tag{5.28) (5}$$

and

$$\bar{N}_{ab}^{ij} = m_a \left\langle\!\left\langle \frac{n_a}{\tau_{ab}} \right\rangle\!\right\rangle N_{ab}^{ij} \quad , \tag{5.29) (6}$$

where

$$\left\langle\!\left\langle \frac{n_a}{\tau_{ab}} \right\rangle\!\right\rangle = \sum_{i_a} \sum_{i_b} \frac{n_a}{\tau_{ab}} = \frac{4}{3\sqrt{\pi}} \frac{4\pi\left(\sum_{i_a} n_a e_a^2\right)\left(\sum_{i_b} n_b e_b^2\right) \ell n\ \Lambda}{m_a^2 v_{T_a}^3} \quad . \qquad (5.25)\ (7)$$

We discuss the α_{ab}^j and the A_{ab}^j in Sects. 2.2 and 2.3, respectively. Here we point out only that the determination of the α_{ab}^j and A_{ab}^j is at the heart of the numerical problem of determining the f_{ij}^{ab}. In Eqs. (1), (3), (5), and (6), the overbars denote reduced charge state quantities, i.e., quantities that do not explicitly depend on the density and charge state of a given species. However, the notation of Ref. 8 is not complete in that regard, no doubt in an attempt to reduce cumbersomeness [cf. Eqs. (3) and (4)], because the M_{ab}^{ij} and N_{ab}^{ij} are also free of those dependences. Explicitly,

$$M_{ab}^{00} = -(1 + \frac{m_a}{m_b})(1 + x_{ab}^2)^{-3/2} = -N_{ab}^{00} \quad , \qquad (4.11)\ (8)$$

$$M_{ab}^{01} = M_{ab}^{10} = -\frac{3}{2}(1 + \frac{m_a}{m_b})(1 + x_{ab}^2)^{-5/2} = -N_{ab}^{10} \quad , \qquad (4.12)\ (9)$$

$$M_{ab}^{11} = -(\frac{13}{4} + 4x_{ab}^2 + \frac{15}{2} x_{ab}^4)(1 + x_{ab}^2)^{-5/2} \quad , \qquad (4.13)\ (10)$$

$$M_{ab}^{02} = M_{ab}^{20} = -\frac{15}{8}(1 + \frac{m_a}{m_b})(1 + x_{ab}^2)^{-7/2} = x_{ba} N_{ba}^{02} \quad , \qquad (4.15)\ (11)$$

$$M_{ab}^{12} = M_{ab}^{21} = (\frac{69}{16} + 6x_{ab}^2 + \frac{63}{4} x_{ab}^4)(1 + x_{ab}^2)^{-7/2} \quad , \qquad (4.16)\ (12)$$

$$N_{ab}^{11} = \frac{27}{4} \frac{T_a}{T_b} x_{ab}^2 (1 + x_{ab}^2)^{-5/2} = \frac{27}{4} \frac{m_a}{m_b} (1 + x_{ab}^2)^{-5/2} \quad , \qquad (4.14).\ (13)$$

$$N_{ab}^{12} = \frac{225}{16}\frac{T_a}{T_b}\, x_{ab}^4 (1 + x_{ab}^2)^{-7/2} = \frac{225}{16}\frac{m_a}{m_b}\, x_{ab}^2 (1 + x_{ab}^2)^{-7/2} \quad , \qquad (4.17)\ (14)$$

where

$$x_{ab}^2 = \frac{v_{T_b}^2}{v_{T_a}^2} = \frac{2T_b/m_b}{2T_a/m_a} = \frac{m_a}{m_b}\frac{T_b}{T_a} \qquad (15)$$

and x_{ab} is defined in Ref. 8 in text just preceding Eq. (4.11). We have used Eq. (15) to obtain the second equivalences in Eqs. (13) and (14); the symmetry properties of the matrix elements, some of which are indicated in Eqs. (8)-(14), are given by

$$M_{ab}^{ij} = M_{ab}^{ji} \qquad (4.8)\ (16a)$$

and

$$(T_a v_{T_a})^{-1} N_{ab}^{ij} = (T_b v_{T_b})^{-1} N_{ba}^{ji} \quad . \qquad (4.9)\ (16b)$$

We can use Eq. 15 to rewrite Eq. (16b) as

$$N_{ba}^{ji} = \frac{m_b}{m_a}\, x_{ab}^3\, N_{ab}^{ij} = \frac{T_b}{T_a}\, x_{ab} N_{ab}^{ij} \quad . \qquad (16c)$$

We note, however, that (as in Ref. 2) the fact that $T_a \neq T_b$ for $m_a \neq m_b$ has been accounted for only in the evaluation of the $j = 0$ matrix elements.

Using the definition of the thermal speed v_{T_a} implicit in Eq. (15), we can rewrite the right-hand side of Eq. (7) in the familiar form

$$\left\langle\left\langle \frac{n_a}{\tau_{ab}} \right\rangle\right\rangle = \frac{4\sqrt{2\pi}}{3} \frac{\sum_{i_a} n_a e_a^2 \sum_{i_b} n_b e_b^2 \ln \Lambda}{m_a^{1/2} T_a^{3/2}} \quad . \tag{17}$$

In Ref. 8, Hirshman and Sigmar state that the Coulomb logarithm, $\ln \Lambda$, is "taken to be the same large constant ($\ln \Lambda \approx 20$) independent of species." It can readily be shown that the Coulomb logarithm may vary by as much as 50%, depending on the interacting species; because it is a multiplicative factor in the f_{ij}^{ab}, a more accurate estimate is desirable. An analysis of the Coulomb collision terms in the reduced charge state problem[4] leads to the following expression for the Coulomb logarithm in terms of the interacting reduced charge states:

$$\ln \Lambda = \overline{\ln \Lambda_{ab}} = 23.46 + 0.5 \ln \frac{T_i^3 \text{ (eV)}}{n_e \text{ (cm}^{-3}) \cdot \bar{z}_a^2 \bar{z}_b^2 \left(\frac{T_i}{T_e} + Z_{eff} \right)} \quad , \tag{18}$$

where

$$\bar{z}_a^2 = \frac{\bar{e}_a^2}{e^2} = \frac{1}{\tilde{n}_a e^2} \sum_{i_a} = \frac{1}{e^2} \frac{\sum_{i_a} n_a e_a^2}{\sum_{i_a} n_a} \tag{19}$$

and e is the unit electric charge. In the notation of Eq. (4),

$$\overline{z}_a^2 = \frac{1}{e^2} \frac{\sum_\mu n_{a_\mu} e_{a_\mu}^2}{\sum_\mu n_{a_\mu}} \quad . \tag{20}$$

In Eq. (18) we have assumed that all of the interacting ions have a common (local) temperature T_i. This approximation requires further scrutiny involving the analysis of heat transfer among the ions, which is addressed in Sect. 6.4.3 of Ref. 8. At present, however, we note that even a factor of 2 error in the value of T_i would lead to less than a 10% correction in $\overline{\ell n\, \Lambda_{ab}}$. We use the overbar in our definition of the Coulomb logarithm to indicate its reduced charge state nature. Finally, we point out that Z_{eff} takes its usual form because

$$\overline{Z_{eff}} = \frac{\sum_a \tilde{n}_a e_a^2}{n_e} = \frac{\sum_a \sum_\mu \frac{\sum_\mu n_{a_\mu} e_{a_\mu}}{\sum_\mu n_{a_\mu}}}{n_e} = \frac{\sum_a \sum_\mu n_{a_\mu} e_{a_\mu}^2}{n_e} \quad . \tag{21}$$

2.2 THE EXPANSION COEFFICIENTS A_{ab}^j OF THE REDUCED CHARGE STATE HIGHER ORDER FLOW $\overline{u}_{a2}$

In Ref. 8, Hirshman and Sigmar have inverted the system of linear algebraic equations for the reduced charge state higher order flow $\overline{u}_{a2}$ to obtain

$$\overline{u}_{a2} = -\sum_b A_{ab}^1 u_{\|b} = \frac{2}{5} \sum_b A_{ab}^2 \frac{q_{\|b}}{p_b} \quad , \tag{6.32) (22}$$

or, in expanded notation,

$$\bar{u}_{a2} = -\sum_b \sum_\nu A^1_{ab_\nu} u_{\|b_\nu} + \frac{2}{5} \sum_b \sum_\nu A^2_{ab_\nu} \frac{q_{\|b_\nu}}{p_{b_\nu}} \quad , \tag{23}$$

where $u_{\|b_\nu}$ is the parallel flow velocity of species b_ν, $q_{\|b_\nu}$ is its random heat flux, and p_{b_ν} is the pressure. The A^j_{ab} are given by

$$A^j_{ab} = \bar{A}_{ab}\bar{M}^{2,j-1}_b \xi_b \frac{I_b}{\bar{I}_b} + \left(\sum_{m_k} \bar{A}_{ak}\bar{N}^{2,j-1}_{kb}\right)\xi_b$$

$$+ \left[\sum_{m_k} \bar{A}_{ak}\bar{D}_k\bar{D}_b\left(\frac{\bar{g}_k}{\bar{n}_k}\right)\left(\frac{\bar{M}^{22}_k\bar{P}_k}{\bar{M}^{22}_b}\right)\left(\frac{T_b}{T_k}\right)\Delta P_{kb}\bar{M}^{2,j-1}_b\right]\delta n_b \quad . \quad (6.33) \tag{24}$$

In Eq. (24), the $\bar{A}_{ab}$ are symmetric matrix coefficients,

$$\bar{A}_{ab} = (\overleftrightarrow{M}^{-1})_{ab} = \bar{A}_{ba} \quad , \tag{25}$$

the matrix elements of the inverse of the symmetric reduced charge state matrix $\overleftrightarrow{M}$, where

$$(\overleftrightarrow{M})_{ab} = \bar{M}^{22}_a\bar{D}_a\delta_{ab} + \bar{N}^{22}_{ab} + \bar{g}_a\left(\frac{\bar{n}_b}{\bar{n}_a}\right)\left(\frac{T_b}{T_a}\right)\bar{P}_a\bar{M}^{22}_a\bar{D}_a(\overleftrightarrow{P}^{-1})_{ab} = (\overleftrightarrow{M})_{ba} \quad , \quad (6.34) \tag{26}$$

and the matrix $\overleftrightarrow{P}$ is also a symmetric reduced charge state matrix,

$$(\overleftrightarrow{P})_{ab} = \bar{P}_a\bar{D}_a\bar{\delta}_{ab} + \bar{Q}_{ab} = (\overleftrightarrow{P})_{ba} \quad . \quad (6.35) \tag{27}$$

We may rewrite Eq. (24) in expanded notation to indicate its lack of dependence on the actual charge state of the chemical element with mass m_a and its dependence on the charge state of the chemical element with mass m_b:

$$A^{j}_{ab_\nu} = \bar{A}_{ab}\bar{M}_b^{2,j-1}\xi_{b_\nu}\frac{I_{b_\nu}}{\bar{I}_b} + \left(\sum_{m_k}\bar{A}_{ak}\bar{N}_{kb}^{2,j-1}\right)\xi_{b_\nu}$$

$$+ \left[\sum_{m_k}\bar{A}_{ak}\bar{D}_k\bar{D}_b\left(\frac{\bar{g}_k}{\bar{n}_k}\right)\left(\frac{\bar{M}_k^{22}\bar{P}_k}{\bar{M}_b^{22}}\right)\left(\frac{T_b}{T_a}\right)\Delta P_{kb}\bar{M}_b^{2,j-1}\right]\delta n_{b_\nu} \quad . \quad (28)$$

We now continue defining the symbols in Eqs. (24), (26), and (27). We have

$$I_a = \left[1 + \bar{g}_a\left(\frac{n_a}{\bar{n}_a\xi_a}\right)^2\right]^{-1} \qquad (6.27)\ (29)$$

and

$$\bar{I}_a = \sum_{i_a}\xi_a I_a \quad , \qquad (6.29)\ (30)$$

where, in expanded notation,

$$I_{a_\mu} = \left[1 + \bar{g}_a\left(\frac{n_{a_\mu}}{\bar{n}_a\xi_{a_\mu}}\right)^2\right]^{-1} \qquad (31)$$

and

$$\bar{I}_a = \sum_{\mu} \xi_{a\mu} I_{a\mu} \quad . \tag{32}$$

In Eqs. (24), (25), (28), (29), and (31),

$$\bar{g}_a = \left(\frac{35}{6} \frac{n_a T_a}{L_c}\right)^2 (\bar{M}_a^{22} \bar{P}_a)^{-1} \tag{6.28} (33)$$

and

$$\bar{n}_a = \sum_{i_a} \frac{n_a I_a}{\bar{I}_a} = \bar{I}_a^{-1} \sum_{\mu} n_{a\mu} I_{a\mu} \quad . \tag{6.29} (34)$$

[Henceforth, where desirable, we write the original and the expanded notation forms in the same equation, as in Eq. (34).] The connection length L_c, which appears in Eq. (33), is defined by Hirshman and Sigmar in the relation

$$-\frac{1}{L_c} \equiv \frac{\vec{n} \cdot \nabla[\vec{B} \cdot \nabla(u_{a2}/B)]}{u_{a2}} \simeq \frac{(\vec{B} \cdot \nabla)^2 (I/B^2)}{I - \langle I \rangle (B^2/\langle B^2 \rangle)} \quad , \tag{6.25} (35)$$

where I is related to the toroidal magnetic flux [cf. the paragraph preceding Eq. (2.18) of Ref. 8]. In the large aspect ratio, low beta limit,

$$L_c = Rq \quad , \tag{36}$$

where R is the major radius of the plasma and q is the safety factor.

Recalling Eqs. (5) and (6), we have

$$M_{ab}^{22} = \left(\frac{433}{64} + 17x_{ab}^2 + \frac{459}{8}\, x_{ab}^4 + 28x_{ab}^6 + \frac{175}{8}\, x_{ab}^8\right)(1 + x_{ab}^2)^{-7/2} \qquad (5.21)\ (37)$$

and

$$N_{ab}^{22} = \frac{2625}{64}\frac{T_a}{T_b}\, x_{ab}^4(1 + x_{ab}^2)^{-9/2} = \frac{2625}{64}\frac{m_a}{m_b}\, x_{ab}^2(1 + x_{ab}^2)^{-9/2} \quad ; \qquad (5.22)\ (38)$$

we need Eq. (38) to solve Eq. (26). The remaining undefined quantity in Eq. (33) is

$$\bar{P}_a = \sum_{m_b} T_a \left\langle\!\!\left\langle \frac{n_a}{\tau_{ab}} \right\rangle\!\!\right\rangle P_{ab}^{22} \quad , \qquad (6.10)\ (39)$$

where

$$P_{ab}^{22} = -3x_{ab}^2\left(\frac{13}{4} + 2x_{ab}^2 + \frac{5}{2}\, x_{ab}^4\right)(1 + x_{ab}^2)^{-7/2} \quad . \qquad (6.11)\ (40)$$

We define the remaining undefined quantities in Eqs. (24) and (26)-(28) as

$$\bar{D}_a = [\bar{I}_a(1 + \bar{g}_a)]^{-1} \qquad (41)$$

[from the text following Eq. (6.31) of Ref. 8] and the ΔP_{ab}, which are also elements of a symmetric reduced charge state matrix, as

$$\Delta P_{ab} = (\overleftrightarrow{P}^{-1})_{ab} - \bar{\delta}_{ab}(\bar{P}_a \bar{D}_a)^{-1} = \Delta P_{ba} \quad , \qquad (6.36)\ (42)$$

where $\bar{\delta}_{ab}$ is the reduced charge state Kronecker delta

$$\bar{\delta}_{ab} = \sum_{i_a, i_b} \xi_a \delta_{ab} = \delta_{m_a, m_b} \qquad (5.30)\ (43a)$$

$$= \sum_{\mu} \sum_{\nu} \xi_{a_\mu} \delta_{a_\mu b_\nu} \begin{cases} = 1, & m_a = m_b \quad . \\ = 0, & m_a \neq m_b \quad . \end{cases} \qquad (43b)$$

Returning to Eqs. (24) and (28), we have

$$\delta n_a = (\bar{n}_a \xi_a - n_a) I_a \qquad (44a)$$

or

$$\delta n_{a_\mu} = (\bar{n}_a \xi_{a_\mu} - n_{a_\mu}) I_{a_\mu} \quad . \qquad (44b)$$

The symmetric matrix element $\bar{Q}_{ab}$, which appears in Eq. (27), is defined as

$$\bar{Q}_{ab} = T_a \left\langle\!\!\left\langle \frac{n_a}{\tau_{ab}} \right\rangle\!\!\right\rangle Q^{22}_{ab} = \bar{Q}_{ba} \quad , \qquad (6.20)\ (45)$$

where*

$$Q^{22}_{ab} = \frac{45}{4} x^4_{ab} (1 + x^2_{ab})^{-7/2} \quad . \qquad (6.12)\ (46)$$

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*As in the evaluation of the N^{ij}_{ab}, this equation does not satisfy Eq. (45) unless $T_a = T_b$.

Thus, in the determination of the A^j_{ab}, the only computational problem is the inversion of the two reduced charge state matrices, $\overleftrightarrow{P}$ and $\overleftrightarrow{M}$, and their rank will be low, ~2-5, for problems of interest. We note from Eq. (26) that $\overleftrightarrow{P}$ must be formed and inverted before $\overleftrightarrow{M}$ can be formed.

2.3 THE EXPANSION COEFFICIENTS α^j_{ab} OF THE HIGHER ORDER FLOW u_{a2}

In Ref. 8, the higher order flow u_{a2} (= $u_{a_\mu 2}$), which is expressible in terms of the parallel flow velocities and random heat fluxes as

$$u_{a2} = -\sum_b \alpha^1_{ab} u_{\|b} + \frac{2}{5} \sum_b \alpha^2_{ab} \frac{q_{\|b}}{p_b} \tag{47}$$

[from text following Eq. (6.39) of Ref. 8] or

$$u_{a_\mu 2} = -\sum_b \sum_\nu \alpha^1_{a_\mu b_\nu} u_{\|b_\nu} + \frac{2}{5} \sum_b \sum_\nu \alpha^2_{a_\mu b_\nu} \frac{q_{\|b_\nu}}{p_{b_\nu}} \ , \tag{48}$$

is eliminated by finding the relation between the α^j_{ab} and the A^j_{ab}.

$$\alpha^j_{ab} = \frac{I_a}{\bar{I}_a} A^j_{ab} + \frac{I_a \bar{M}^{2,j-1}_a}{I_a \bar{M}^{22}_a} \left(\delta_{ab} - \frac{\bar{\delta}_{ab} \xi_b I_b}{\bar{I}_b} \right)$$

$$+ \frac{\delta n_a \bar{D}_a}{\bar{n}^2_a \xi_a} \frac{\bar{g}_a \bar{P}_a}{T_a} \left[\sum_{m_k} \bar{n}_k T_k \bar{D}_k (\Delta P_{ak}) A^j_{kb} - \delta n_b T_b \bar{D}_b (\Delta P_{ab}) \frac{M^{2,j-1}_b}{\bar{M}^{22}_b} \right]$$

(6.40) (49)

or

$$\alpha^{j}_{a_\mu b_\nu} = \frac{I_{a_\mu}}{\bar{I}_a} A^{j}_{ab_\nu} + \frac{I_{a_\mu} \bar{M}^{2,j-1}_a}{\bar{M}^{22}_a} \left(\delta_{a_\mu b_\nu} - \frac{\bar{\delta}_{ab} \xi_{b_\nu} I_{b_\nu}}{\bar{I}_b} \right)$$

$$+ \frac{\delta n_{a_\mu} \bar{D}_a}{\pi^2_a \xi_{a_\mu}} \frac{\bar{g}_a \bar{P}_a}{T_a} \left[\sum_{m_k} \bar{n}_k T_k \bar{D}_k (\Delta P_{ak}) A^{j}_{kb_\nu} - \delta n_{b_\nu} T_b \bar{D}_b (\Delta P_{ab}) \frac{M^{2,j-1}_b}{\bar{M}^{22}_b} \right] . \quad (50)$$

There are no previously undefined quantities in Eqs. (49) and (50). At the risk of pointing out the obvious, we note that the A^{j}_{ab} must be completely determined before the α^{j}_{ab} can be calculated.

3. IMPLEMENTATION AND RESULTS

We have implemented the calculation of the f_{ij}^{ab} in the impurity transport simulation program IMPTAR and have compared the results obtained using this treatment to results obtained using previous formulations.

3.1 COMPARISON OF NUMERICAL RESULTS

We make three sets of numerical comparisons. First, we compare the effects of using the reduced charge state method[4] to the effects of using the full charge state method[2] without the additional encumbrance of the plateau-Pfirsch-Schlüter transition, for which the most advanced treatment[8] has been done only using the reduced charge state method. Second, we compare the effects of using the approximate treatment of the plateau-Pfirsch-Schlüter transition in the full charge state method[5] to the effects of using the treatment of Hirshman and Sigmar.[8] Third, we illustrate the importance of including the effect of the plateau-Pfirsch-Schlüter transition in the calculations. While this last comparison is not strictly speaking part of the topic of this report, the results obtained from it clarify our motivation for including this effect.

For the purpose of these comparisons, we consider a deuterium plasma with an oxygen impurity content of 1.6% of the local electron density. This impurity level leads to a central $Z_{eff} \approx 1.9$ and an edge $Z_{eff} \approx 1.3$. The plasma characteristics are typical of an ohmically heated ISX-B plasma at about 100 ms. We make comparisons both near the plasma center, Rq = 56 cm, and near the plasma edge, Rq = 454 cm, where R is the plasma major radius and q is the safety factor. This case is considered as a matter of convenience, since it is part of our current study of titanium injection experiments in ISX-B.

We modified the IMPTAR code to print out various friction coefficients f_{ij}^{ab}, to which the transport coefficients are directly proportional. We use the coefficient f_{12}^{ab} for comparison because its magnitude determines whether there can be a temperature screening effect on the impurities. If the plateau-Pfirsch-Schlüter transition

is not taken into account, there can be no temperature screening effect in the Pfirsch-Schlüter regime of the impurities except in special cases.[10,11]

The numerical results are presented in terms of ratios in Tables 1-3. In all three cases, results typical of the edge of the plasma (Rq = 454 cm) and results typical of the center of the plasma (Rq = 56.2 cm) are given. The tables are arranged in matrix form, with charge state species a listed in the rows and charge state species b listed in the columns. Thus, in Table 1, the entry in the fourth column of the second row has to do with the interaction of O^{3+} and O^{5+} at Rq = 454 cm. No entries are given for oxygen charge states that represent less than 0.1% of the total oxygen.

3.1.1 Effects of Using the Reduced Charge State Model

If the plateau-Pfirsch-Schlüter transition is not taken into account, the coefficients f_{ij}^{ab} of Ref. 8 reduce to the coefficients ℓ_{ij}^{ab} of Ref. 2. In Table 1, we give the ratios of the ℓ_{ij}^{ab} calculated using the full charge state method (i.e., solving systems of linear equations with one equation for each charge state of each element present, which means nine equations in this case) to the ℓ_{ij}^{ab} calculated using the reduced charge state method (i.e., inverting square matrices of order n, where n is the number of elements present; here n = 2).

It is seen that the entries in Table 1 are generally within 2% of unity; the deviations are most prominent for the O^{5+} interactions at the plasma edge and for the O^{6+} interactions near the plasma center. The O^{5+} density of the edge plasma is less than 5% of the total oxygen content and the O^{6+} density of the central plasma is less than 0.3% of the total energy content; in each case these are the lowest densities.

These small deviations are almost entirely due to differences in the Coulomb logarithms used in the calculations. In the full charge state calculation, there is a different Coulomb logarithm for each interaction of a given charge state of a given element; in the reduced charge state calculation, there is a different Coulomb logarithm only for each interaction of a given element. If a fixed Coulomb logarithm

Table 1. Ratios of ℓ_{12}^{ab} calculated using method of Ref. 2 to ℓ_{12}^{ab} calculated using method of Ref. 4

$Rq = L_c = 454$ cm

Charge state species a	Charge state species b: D^+	O^{3+}	O^{4+}	O^{5+}	O^{6+}
D^+	0.998	1.038	1.014	0.996	0.981
O^{3+}	1.036	1.037	1.054	1.033	1.016
O^{4+}	1.012	1.054	1.005	1.007	0.990
O^{5+}	0.994	1.033	1.007	0.995	0.970
O^{6+}	0.979	1.016	0.990	0.970	0.979

$Rq = L_c = 56.2$ cm

Charge state species a	Charge state species b: D^+	O^{6+}	O^{7+}	O^{8+}
D^+	1.000	1.019	1.009	1.000
O^{6+}	1.019	1.022	1.032	1.022
O^{7+}	1.009	1.032	1.010	1.010
O^{8+}	1.000	1.022	1.010	1.014

Table 2. Ratios of f_{12}^{ab} calculated using method of Ref. 5 to f_{12}^{ab} calculated using method of Ref. 8

$Rq = L_c = 454$ cm

Charge state species a	Charge state species b: D^+	O^{3+}	O^{4+}	O^{5+}	O^{6+}
D^+	0.998	1.042	1.015	0.995	0.980
O^{3+}	1.036	1.037	1.054	1.033	1.016
O^{4+}	1.012	1.053	1.006	1.007	0.990
O^{5+}	0.994	1.032	1.006	0.995	0.969
O^{6+}	0.978	1.015	0.989	0.969	0.979

$Rq = L_c = 56.2$ cm

Charge state species a	Charge state species b: D^+	O^{6+}	O^{7+}	O^{8+}
D^+	1.000	1.018	1.008	1.000
O^{6+}	1.019	1.022	1.027	1.026
O^{7+}	1.009	1.028	1.010	1.014
O^{8+}	1.000	1.022	1.010	1.002

Table 3. Ratios of ℓ_{12}^{ab} calculated using method of Ref. 2 to f_{12}^{ab} calculated using method of Ref. 8

$Rq = L_c = 454$ cm

Charge state species a	Charge state species b: D^+	O^{3+}	O^{4+}	O^{5+}	O^{6+}
D^+	0.699	0.584	0.569	0.558	0.549
O^{3+}	0.726	1.034	1.168	1.146	1.128
O^{4+}	0.709	1.017	0.966	1.117	1.099
O^{5+}	0.696	1.144	1.116	0.929	1.076
O^{6+}	0.685	1.125	1.097	1.076	0.961

$Rq = L_c = 56.2$ cm

Charge state species a	Charge state species b: D^+	O^{6+}	O^{7+}	O^{8+}
D^+	0.477	0.039	0.039	0.039
O^{6+}	0.486	0.888	0.885	1.000
O^{7+}	0.481	0.989	0.887	0.994
O^{8+}	0.477	0.986	0.986	0.097

is used in both calculations, the deviations are reduced to 0.1% or less.

3.1.2 Effects of Using an Approximate Treatment of the Plateau-Pfirsch-Schlüter Transition

In Table 2 we give the ratios of the f_{12}^{ab} calculated using the approximate method of Ref. 5 to the f_{12}^{ab} calculated using the exact method of Ref. 8. It is immediately apparent, when Tables 1 and 2 are compared, that the deviations from unity of the ratios in Table 2 are almost entirely due to the forms of the Coulomb logarithm used, as discussed in Sect. 3.1.1. This is very encouraging because it indicates that work done since the implementation of the method of Ref. 5, such as that appearing in Refs. 6 and 7, apparently needs no revision. Implementing the method of Ref. 8 does provide significant time savings, as discussed in Sect. 3.2, and there may be regimes of impurity concentration in which the method of Ref. 5 does not compare so favorably with that of Ref. 8; however, we have not yet done an extensive survey.

3.1.3 Effects of Including the Plateau-Pfirsch-Schlüter Transition

As a final numerical comparison, we give in Table 3 the ratios of the ℓ_{12}^{ab} of Ref. 2, which do not include the plateau-Pfirsch-Schlüter transition, to the f_{12}^{ab} of Ref. 8, which do. It is seen, especially for interactions with D^+, that use of the ℓ_{12}^{ab} would lead to severe underestimates of the coefficients of the temperature gradient term in the fluxes, both at the plasma edge and near the plasma center. As indicated above, this could completely obscure any temperature screening effect on the impurities.

3.2 COMPARISON OF COMPUTING TIME

For the purposes of comparing overall numerical results and CPU time requirements, we have used the new version of IMPTAR, which incorporates the reduced charge state theory of Ref. 8, to run two cases that were originally run with the previous version, which employed the full charge state theory of Ref. 5. As expected from the ratios in Tables 1 and 2, only very minor numerical differences appear in the simulation results, and we will not discuss that aspect further.

The first case run with the new version of IMPTAR was a simulation of the first 50 ms following the puffing of a small amount of titanium into an ISX-B-like deuterium plasma with an oxygen impurity level large enough to make the central $Z_{eff} \simeq 1.9$. The original calculation required 6.65 min of CPU time; the second run required only 4.75 min, a reduction of ~29%. The savings are of this magnitude, rather than larger or smaller, because calculation of the transport coefficients previously took about 40% of the CPU time for this type of run. Thus, the time saved in calculating the transport coefficients alone is about 71%. A more complete simulation of 200 ms of the same ISX-B discharge, in which oxygen was present throughout the simulation but titanium only during the last 100 ms, originally required 16.2 min of CPU time; the second run required only 12.2 min, representing a saving of ~24% in total CPU time. The percentage is smaller in this case because the savings increase with the number of chemical elements present, and only two elements were present for part of this run.

4. CONCLUSIONS AND PLANS FOR FUTURE WORK

We have shown that implementation of a new treatment[8] of impurity transport in the Pfirsch-Schlüter regime in the IMPTAR code leads to significant savings in computer time. For the cases we have considered, it appears to lead to simulation results that are not significantly different from those obtained with the approximate treatment[5] we were using. (However, this merely indicates that the approximation is very good for these cases.)

In the immediate future, we plan to tighten up the programming of the new method and may gain further slight savings in computer time. Also, we have discussed with S. P. Hirshman the possibility of deriving a method of obtaining the transport coefficients that is more direct than actual computation of the f_{ij}^{ab}, which may yield additional time savings.

A subroutine FFRIC to calculate the f_{ij}^{ab} on a vector computer such as the CRAY is available from the authors over the Magnetic Fusion Energy Computer Network.

ACKNOWLEDGMENT

The authors are grateful to S. P. Hirshman for elucidating certain aspects of the theory of Ref. 8 and thus easing our task of implementing it.

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APPENDIX

Typical Units for Calculating $\bar{g}_a$

We define $\bar{g}_a$ in Eq. (33) as

$$\bar{g}_a = \left(\frac{35}{8}\frac{\bar{n}_a T_a}{L_c}\right)^2 (\bar{M}_a^{22}\bar{P}_a)^{-1} \quad . \tag{A.1}$$

For practical calculations, the units of the quantities in which $\bar{g}_a$ is defined are as follows:

Quantity	Definition	Units
$\bar{n}_a$	Eq. (34)	cm^{-3}
T_a	temperature	eV
L_c	Eq. (35)	cm
$\bar{M}_a^{22}$	Eq. (5)	$amu \cdot cm^{-3} \cdot s^{-1}$
$\bar{P}_a$	Eq. (39)	$eV \cdot cm^{-3} \cdot s^{-1}$

Substituting to obtain the units of $\bar{g}_a$, we have

$$(\bar{g}_a)_{units} \sim eV \cdot amu^{-1} \cdot cm^{-2} \cdot s^{-1} \quad .$$

Now, $eV \cdot amu^{-1}$ has the units $cm^2 \cdot s^{-1}$, so $\bar{g}_a$ is, as one would expect, dimensionless. Using a standard conversion factor to obtain the thermal velocity in these units,

$$\frac{1}{2} v_T^2 = \frac{T}{m} = 9.648452 \times 10^{11} \frac{T\ (eV)}{m\ (amu)} \quad , \tag{A.2}$$

we can write Eq. (A.1) as

$$\overline{g}_a = 9.648452 \times 10^{11} \left[\frac{35}{8} \frac{\overline{n}_a\ (cm^{-3})\ T_a\ (eV)}{L_c\ (cm)}\right] [\overline{M}_a^{22}\ (amu \cdot cm^{-3} \cdot s^{-1}) \times \overline{P}_a\ (eV \cdot cm^{-3} \cdot s^{-1})] \quad . \tag{A.3}$$