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**On the Application of Diffusion Theory to Neutral Atom
Transport in Fusion Plasmas**

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ABSTRACT: It is found that energy dependent diffusion theory provides excellent accuracy in the modelling of transport of neutral atoms in fusion plasmas. Two reasons in particular explain the good accuracy. First, while the plasma is optically thick for low energy neutrals, it is optically thin for high energy neutrals and diffusion theory with Marshak boundary conditions gives accurate results for an optically thin medium even for small values of 'c', the ratio of the scattering to the total cross section. Second, the effective value of 'c' at low energy becomes very close to one due to the down-scattering via collisions of high energy neutrals. The first reason is proven both computationally and theoretically by solving the transport equation in a power series in 'c' and the diffusion equation with 'general' Marshak boundary conditions. The second reason is established numerically by comparing the results from a one-dimensional, general geometry, multigroup diffusion theory code, written for this purpose, with the results obtained using the transport code ANISN. Earlier work that compared one-speed diffusion and transport theory indicated diffusion theory would be inaccurate. A detailed analysis shows that this conclusion is limited to a very specific case. For a very wide range of conditions and when energy dependence is included, diffusion theory is surprisingly, and highly, accurate.

I. INTRODUCTION

Interest in calculating the neutral atom distribution in plasmas arises because of the very important role that the neutral atoms play in present experiments and in fusion reactors. Neutrals have an effect on both the plasma and the vacuum chamber, the former by affecting the plasma particle and energy balance, the latter by causing sputtering and erosion of the wall materials. Wall sputtering by the neutral atoms is of major importance. First, although a limiter can save the first wall from plasma ion bombardment, it cannot prevent the first wall from being bombarded by energetic atoms generated as a result of recycling and transport. Second, the energy of charge-exchange neutrals leaving the plasma can be high, often as high as the central ion energy. Sputtering of the first wall, caused mainly by the neutral atoms, can introduce high-Z impurities into the plasma thus enhancing the radiation loss. Charge-exchange neutrals can also be used as a diagnostic for the plasma ion temperature.

Analytical, semianalytical and numerical solutions to the problem of neutral atom transport in plasmas have been obtained. Since an analytical solution to the general Boltzmann transport equation is not possible, analytical and semianalytical solutions have been obtained only with many simplifying assumptions. The usual assumptions are slab or half-space geometry, constant plasma temperature and constant plasma density (i.e. a homogeneous medium) and simplified boundary conditions. Among others, solutions under such assumptions have been

obtained by Rehker and Wobig[1], Volkov and Igitkhanov[2] and Burrell[3]. Tendler and Ågren[4] have provided an analytical solution for the neutral atom distribution in the edge plasma with a nonhomogeneous temperature profile. They have assumed $(\sigma_{cx} v)$ to be constant. Among the numerical solutions are those of Hackman, et al.[5] and Audenaerde, et al.[6] in slab geometry. Garcia, et al.[7] have used the F_N -method to calculate the neutral atom distribution in half-space and slab plasmas. Marable and Obloz[8] appear to be the first to report the use of the one-dimensional neutron transport code ANISN for neutral atom transport in fusion plasmas. Duchs, et al.[9] have applied the generation method, allowing up to ten successive generations of charge-exchange neutrals, to neutral atom transport in one-dimensional cylindrical plasmas. Hughes and Post[10] have written a Monte Carlo code in one-dimensional cylindrical geometry. Multidimensional Monte Carlo codes for neutral atom transport have been reported by Heifetz, et al.[11], by Reiter and Nicolai[12], and others.

Although there are certain features, such as nearly isotropic charge-exchange cross sections and isotropic wall-originated neutral atom sources, which would imply that a diffusion theory solution would be accurate, no serious attempt has been made to investigate the possibility of applying diffusion theory to the transport of neutral atoms in plasmas. In some previous works [2,3], a one-group or energy independent diffusion approximation solution was obtained from the kinetic solution for the neutral atom density.

The primary objective of this paper is to establish that diffusion theory provides an accurate description of neutral atom transport in fusion plasmas. The significance of this finding will come in the numerical solution of two and three-dimensional problems where computation time will be crucial. Diffusion theory numerical solutions are generally obtained with orders of magnitude savings in computational time relative to numerical transport theory. A multi-energy group diffusion theory code for neutral atom calculations in two-dimensional plasmas of general cylindrical and toroidal geometries has been developed and is reported elsewhere [13].

In section II, we compare diffusion and transport theory in one-dimensional plasmas to show the accuracy of diffusion theory. The limitations of one-group diffusion theory and the range of its applicability are discussed in section III. This provides a partial understanding of why energy dependent diffusion theory provides good accuracy. In section IV, we investigate the reasons for this good accuracy. Section V contains a summary and conclusions.

II. COMPARISON OF MULTIGROUP DIFFUSION THEORY AND TRANSPORT THEORY RESULTS

In plasma-neutral interactions, ionization of the neutral atoms by plasma ions and electrons is equivalent to absorption, while charge-exchange is equivalent to scattering. This scattering has complete up-scattering and down-scattering in the sense that, in a multigroup energy treatment, a neutral atom in the lowest energy group can appear

in the highest energy group, and vice versa, upon a charge exchange event. An attempt to find a multigroup diffusion theory code which would allow complete up and down-scattering was not successful. Therefore, a one-dimensional, general geometry (slab, cylindrical and spherical), multigroup diffusion theory code has been written employing a finite difference method. In the multigroup method, the energy variable, E , is divided into a number of energy groups defined by the boundary energies: E_1 (highest energy), $E_2, \dots, E_g, E_{g+1}, \dots, E_G$ (lowest energy). The energy group 'g' refers to the group bounded by E_{g+1} and E_g . A review of multigroup energy dependent diffusion theory can be found in many texts [14-17]. The one-dimensional, general geometry, multigroup diffusion equation can be written as

$$-\frac{1}{r^2} \frac{d}{dr} (r^2 D_g \frac{d}{dr} \phi_g(r)) + \sigma_t^g(r) \phi_g(r) = \sum_{g'=1}^G \sigma_{g' \rightarrow g}(r) \phi_{g'}(r) + S_g(r) \quad (1)$$

$g=1, 2, \dots, G$

where g labels the particular energy group, ϕ_g is the neutral atom flux for group g , σ_t^g is the macroscopic total cross section (ionization plus charge-exchange) for group g , $\sigma_{g' \rightarrow g}$ is the group-to-group macroscopic scattering cross section, D_g is the diffusion coefficient in group g , and S_g is the volumetric source in group g .

The flux, $\phi_g(r)$, is equal to $\phi(r,E)$ integrated over the energy group g , i.e., from E_{g+1} to E_g , and ϕ is the product of density and speed. When the scattering cross section is isotropic, the diffusion coefficient, D_g , for isotropic diffusion theory is given by $1/(3\sigma_t^g)$. The source in group g , S_g , can contain a recombination neutral atom source which may become important for high density plasmas[18]. In this paper we provide results assuming only a wall-originated source of neutrals in order to address the issue of accuracy using diffusion theory. The parameter ρ is 0 in slab geometry, 1 in cylindrical geometry and 2 in spherical geometry.

The boundary conditions considered are:

1. free surface; $J_{in}=0$
2. reflection; $J_{net}=0$
3. albedo or white; $J_{in} = \alpha J_{out}$

where J represent the total current of neutral atoms (inward or outward) at the surface. Each of these, together with the surface source, can be represented as

$$J_{in} = S_o + \alpha J_{out} \quad (2)$$

There is one equation like equation (2) for each energy group. The P_1 Marshak expressions[16] for J_{in} and J_{out} are used in equation (2) and are:

$$J_{in} = \frac{\phi_s}{4} + \frac{D}{2} \hat{n} \cdot \nabla \phi_s \quad J_{out} = \frac{\phi_s}{4} - \frac{D}{2} \hat{n} \cdot \nabla \phi_s \quad (3)$$

where $\hat{n}$ is the unit outward normal vector at the surface and ϕ_s and $\nabla \phi_s$ are the neutral flux and its gradient at the surface, respectively.

In neutron transport theory, P_N equations corresponding to the Boltzmann's transport equation are obtained by expanding the angular flux in Legendre polynomials for one-dimensional problems and in spherical harmonics for problems that are multidimensional. The expansions are truncated after $(N+1)$ terms. The P_1 -approximation gives the diffusion equation. In one-dimensional slab geometry, the Marshak expressions [16,17] for free surface boundary conditions are given by the following equations:

$$\int_0^1 du \phi(0,u) P_k(u) = 0 ; \quad \int_{-1}^0 du \phi(a,u) P_k(u) = 0 \quad (4)$$

$$k=1,3,\dots,N \text{ odd.}$$

where μ is the cosine of the polar angle and $P_k(\mu)$ is the Legendre polynomial of order k . In the P_1 approximation, we only need $P_1(\mu)=\mu$. Then equation (4) simply states that at the boundary, $J_{in}=0$. The expression for J_{in} is the same as in equation (3).

At least three types of diffusion theories are available, namely, Isotropic Diffusion Theory (IDT) or the familiar P_1 -diffusion theory[14-17], asymptotic diffusion theory[19], and flux-limited diffusion theory[20]. Numerical comparisons reported in reference [21] show that IDT gives better accuracy for neutral transport compared to the other two. Likely reasons are that asymptotic diffusion theory solves for the asymptotic part of the total transport solution while suitable boundary conditions for flux-limited diffusion theory are not available at present. The diffusion theory results reported here are based on IDT.

Transport results have been obtained using the one-dimensional transport theory code ANISN[22]. The changing properties of the plasma as a function of radius is treated by dividing the plasma into a number of zones along the radius. In each zone, the plasma-neutral interaction cross sections are assumed to be constant. These cross sections are calculated by integrating over each zone using the basic plasma-neutral interaction cross sections and the temperature and density profiles of the plasma. The basic cross sections are functions of plasma-neutral relative velocity. Each zone is referred to as a separate material in a multigroup treatment. The code PLASMX[23] has been used to find the multigroup plasma-neutral interaction cross sections. As explained later, only isotropic multigroup cross sections have been used.

Figures 1 to 3 show the comparison of multigroup IDT results with those from ANISN. Figures 1 and 2 are for a 40cm wide slab. Figure 1 also shows the solution using the 1-D slab geometry code SPUDNUT[6]. The accuracy of diffusion theory is quite good. SPUDNUT gives poor results at the plasma edge and center. Probable reasons are the approximations introduced by using the exponential integral of order one, E_1 , in the solution, and the use of successive generations of charge-exchange neutral atoms. The plasma temperature and density are assumed to have parabolic profiles.

In figure 3, the plasma slab width has been increased to 85cm, modelled after TFTR[11]. The multigroup structure used has 21 energy groups with a maximum energy of 40keV. The right surface($x=85\text{cm}$) of the plasma slab is reflected and the left surface($x=0\text{cm}$) is subject to either vacuum or reflection boundary conditions. The 85.0cm plasma is equivalent to about 200 mean free paths for a neutral atom in the lowest energy group, group 21. The ratio of scattering to total cross section, c , for this group is less than 0.8. Comparison of the neutral flux by the multigroup diffusion theory(IDT) and ANISN for group 21 is shown in Table I. For the case ' c ' less than 0.8 and a 200mfp slab, one-group diffusion theory would predict a very poor solution (see figure 6(c)). Yet the multigroup diffusion theory solution for group 21, given in table I, is clearly accurate. Figure 4 shows a comparison of the average neutral atom energy by the transport and diffusion theories for this problem. It shows that diffusion theory accurately predicts the average neutral atom energy.

These results clearly show that the multigroup diffusion theory provides good accuracy for the transport of neutral atoms in fusion plasmas. The maximum difference is within 20% of results from transport theory.

III. LIMITATIONS OF MONOENERGETIC DIFFUSION THEORY

In this section, we discuss the limitations of a one-group diffusion theory solutions and point out the conditions under which such a solution can provide good accuracy for the transport of neutral atoms in plasmas. The need for an energy dependent treatment becomes apparent from this discussion. A comparison of energy independent diffusion approximation solutions and energy dependent kinetic theory solutions reported in reference [3] support the observations made in this section. Figure 5 is a reproduction from reference [3] where the one-group diffusion solution has been obtained from the energy dependent transport solution by taking the limit as 'c' approaches one. A one-group treatment is equivalent to assuming that the neutral atoms have the same temperature as the plasma particles. This is true only when 'c' is very close to one. The reasons are as follow.

When 'c' is very close to unity, absorption is negligible, and, after a sufficient number of collisions, neutral particles assume the plasma particle distribution, i.e., a Maxwellian around v_{th} (see also figure 5(b)). As such, they can be treated as in the same energy group as the plasma particles even though the neutral source has a

different energy. Again, this is not true near the source, whatever the value of 'c', if the source neutrals have a different temperature from the plasma temperature. This can be seen from the energy distribution of the neutral atoms in figure 5(b). In this case (different source temperature), even with 'c' close to one, one-group diffusion theory will be very inaccurate near the source. That this is the case can be clearly seen from figure 5(a) where for $c=0.8$, for example, the diffusion theory result is about 10 times smaller than the kinetic theory result at the surface. Therefore, a one-group diffusion solution away from the source will closely represent the transport solution only when 'c' is very close to one.

When 'c' is not close to 1, absorption is appreciable, and the neutral particles will no longer assume the plasma velocity distribution. As such, v_{th} is no longer the representative velocity for the neutral particles in the plasma, and a one-group diffusion solution will not be applicable. In fact, the distribution of the neutral particles in the plasma will greatly deviate from a Maxwellian, and only an energy dependent treatment will be accurate in this case.

High energy neutrals have longer mean free paths. Absorption always shifts the neutral spectrum towards higher energy. A one-group (especially for low energy) diffusion solution will show faster decay of the neutral density away from the wall(source) than is proper. Again, in reference[3], the diffusion coefficient, D , is $c/2$. As a

result, the neutral density decays faster away from the wall for smaller values of 'c' in the diffusion theory solution in reference[3]. This is evident from figure 5(a). When $c=1$, the diffusion coefficient of $1/2$ is proper for particles with a Maxwellian distribution, which the neutral atoms assume when 'c' is very close to one.

In summary, the limited applicability of monoenergetic diffusion theory for neutral atom transport in plasmas may be stated as follows: The neutral particle density in a constant temperature plasma can be closely approximated by a one-energy group diffusion theory with mean energy given as $3/2$ the plasma temperature only when 'c' is very close to unity and only away from the source, unless the source neutrals have the same temperature as the plasma temperature.

IV. ACCURACY OF ENERGY DEPENDENT DIFFUSION THEORY

The numerical comparisons presented in figures 1 to 4 establish that multigroup diffusion theory provides good accuracy for the transport of neutral atoms in fusion plasmas. Here we present some of the reasons which make multigroup diffusion theory accurate. First we examine the effects of 'c' and the slab thickness 'a' (in mean free path) on the diffusion theory solution. Figures 6(a) to 6(c) show these effects for $c=0.1, 0.5, 0.9$, and $a=0.1, 1.0$, and 10.0 mean free paths. These are one-group solutions. The following conclusions can be drawn from these results:

1. For 'c' close to one, diffusion theory gives accurate results for all values of 'a', the slab thickness.
2. For 'a' small (optically thin slab), diffusion theory gives good results even for small values of 'c'.

There are certain features in fusion plasmas which are helpful in improving the accuracy of diffusion theory calculations. Among these are:

1. The value of $c (= \sigma_{cx} / \sigma_t)$ for plasma-neutral interactions is around 0.6 in the temperature range important to fusion application.
2. The plasma is optically thick for low energy neutrals but thin for high energy neutrals. As a consequence, the high energy neutral flux is more or less flat in the plasma.
3. The temperature and density of the plasma vary in such a way that they are low near the edge. This tends to give a higher value of 'c' and longer mean free path near the edge.
4. The neutral source at the wall is isotropic or nearly isotropic, and the charge-exchange cross section is also very nearly isotropic. Gilligan, et al. [24] have shown in their application of ANISN that in going from a P_0 to a P_3 cross section representation (using ANISN), the neutral density at the center changed from 5.29×10^3 to 5.26×10^3 (less than 1%). The P_0 cross section is the isotropic part of the total charge-exchange cross section, σ_{cx} , while P_1 , P_2 , P_3 , etc. correspond

to the higher orders of anisotropy in σ_{cx} . Similar results have also been obtained by El Derini and Gelbard[25]. The charge-exchange cross section is a function of the ion-neutral relative velocity, v_r . Angular effects are prominent only when a neutral atom and a plasma ion have comparable velocities. And the number of such pairs is not significant compared to the total number of particles. Hence anisotropy in the charge-exchange cross section is very small.

5. A consequence of point number 2 is that away from the surface with the source, fluxes in the high energy groups are larger than fluxes in the low energy groups. Down-scattering from the high energy groups prevents the rapid decay of the flux in the low energy groups. If 'c' is defined for an energy group as the total number of particles emerging in that group per collision in it, that is, as

$$c_g^{eff} = \left(\sum_{g'=1}^G \sigma_{g' \rightarrow g} \phi_{g'} \right) / (\sigma_{t,g} \phi_g), \quad (5)$$

then it is found that the value of 'c' is very close to one for the lower groups away from the source.

Figure 3 shows the comparison between diffusion theory and transport theory results for a 85.0cm slab with cross sections (21 groups) for TFTR plasma parameters. The value of 'c' as defined by equation (5) for the lowest energy group is very close to one. This group contains the surface source. Although

- the 85.0cm plasma corresponds to about 200 m.f.p. for a neutral in this lowest energy group, and the flux for this group decays by about 9 orders of magnitude, the difference between the flux at $x=0$ as computed by diffusion theory and by transport theory is less than 10%, a remarkable result. The source is at $x=85.0\text{cm}$.
6. As shown by the figures 6(a) and 6(b), for an optically thin medium, as is the case for high energy neutral atoms, diffusion theory with Marshak boundary conditions provides good accuracy even for small values of 'c'. In addition to the numerical evidence in figures 6(a) and 6(b), an analytical proof is provided in the appendix.

V. SUMMARY AND CONCLUSIONS

The multigroup diffusion equation with Marshak boundary conditions provides good accuracy for the transport of neutral atoms in fusion plasmas. Contributing factors are that the wall-originated source neutrals and the charge-exchange cross sections are very nearly isotropic. In addition, although the plasma is optically thick for low energy neutrals, it is optically thin for high energy neutrals. Finally, diffusion theory with Marshak boundary conditions provides good accuracy for an optically thin medium even for small values of 'c', the ratio of scattering to total cross sections.

Although we have not compared our one-dimensional, multigroup diffusion theory code with all other available 1-D neutral atom transport codes, we feel that it will compete favorably with them both in terms of accuracy and computation time. In addition, the present code accommodates several types of boundary conditions and provides solutions in slab, cylindrical and spherical geometries. Volumetric sources such as due to recombination can also be used with this code. We have not done calculations using a volumetric source. However, in view of the importance of the recombination source on neutral atom distributions especially in high density plasmas[18], we intend to carry out such calculations in the future.

The good accuracy of multigroup diffusion theory has a very important implication. Calculations of neutral atom distributions in multidimensional fusion plasmas (such as in a torus) using a multigroup diffusion theory code will be much faster than either transport or Monte Carlo codes. A multigroup, multidimensional diffusion theory Finite Element Neutral Atom Transport (FENAT) code has been developed for use on CRAY computers. FENAT solves the multigroup diffusion equation in X-Y and R-Z cylindrical/toroidal geometries[13,21]. The code is fast and compact and has been applied to the calculation of the neutral atom distribution and the wall material erosion rates in tokamak devices such as TEXTOR and TFTR. The results are reported elsewhere[13,26]. The method permits an accurate and time-efficient analysis of neutral atom transport in fusion

devices of complex geometries, such as noncircular cross section tokamaks with toroidal belt limiters or magnetic divertors.

Appendix

DIFFUSION SOLUTION IN AN OPTICALLY THIN SLAB

In this appendix we provide an analytical proof of the observation made earlier that diffusion theory with Marshak boundary conditions provides accurate results in an optically thin medium even for small values of 'c'. We prove this by showing that, in order to obtain the same particle loss as by the transport theory from an optically thin slab with small values of 'c', the diffusion theory must use the P_1 -Marshak boundary conditions. Figure 7 shows the geometries, the boundary conditions, and defines some terms used in the following transport and diffusion solutions.

Transport solution: The one-dimensional energy and time independent transport equation in a homogeneous slab can be written as [15]

$$\mu \frac{\partial \phi(z, \mu)}{\partial z} + \phi(z, \mu) = \frac{c}{2} \int_{-1}^1 d\mu' \phi(z, \mu') \quad (A-1)$$

where z is measured in terms of a mean free path, μ is the cosine of the angle between the flight motion and the positive z -axis, $\phi(z, \mu)$ is the angular flux, and 'c' is the ratio of the scattering to the total cross section, constant for this homogeneous slab. The boundary conditions are

$$\begin{aligned}\phi(0, \mu) &= 2S_0 \quad ; \quad \mu > 0 \\ \phi(a, \mu) &= 0 \quad ; \quad \mu < 0\end{aligned}\tag{A-2}$$

The boundary condition at $z=0$ is the incidence of an isotropic flux of magnitude of $2S_0$. This gives a surface source of S_0 per unit area per second at the surface at $z=0$. The expressions for reflection, R and transmission, T are

$$R = -\int_{-1}^0 d\mu \, \mu \, \phi(0, \mu)\tag{A-3}$$

$$T = \int_0^1 d\mu \, \mu \, \phi(a, \mu)$$

For small values of ' c ' or for thin slabs, the neutrals experience only a few collisions, and $\phi(z, \mu)$ can be expanded in a power series in ' c ', as

$$\phi(z, \mu) = \sum_{n=0}^{\infty} c^n \phi_n(z, \mu) = \phi_0(z, \mu) + c \phi_1(z, \mu) + c^2 \phi_2(z, \mu) + \dots$$

Putting this series in equation (A-1) and equating the powers of ' c ', equations for ϕ_0 , ϕ_1 , etc. can be obtained as

$$\mu \frac{\partial \phi_0(z, \mu)}{\partial z} + \phi_0(z, \mu) = 0$$

$$\mu \frac{\partial \phi_1(z, \mu)}{\partial z} + \phi_1(z, \mu) = \frac{1}{2} \phi_r(z)$$

where $\phi_t(z)$ is the total uncollided flux, i.e., $\phi_0(z, \mu)$ integrated over μ .

The boundary conditions for ϕ_0 and ϕ_1 are obtained by putting the series in equation (A-2). These are

$$\phi_0(0, \mu) + c\phi_1(0, \mu) + \dots = 2S_0 \quad ; \quad \mu > 0$$

$$\phi_0(a, \mu) + c\phi_1(a, \mu) + \dots = 0 \quad ; \quad \mu < 0$$

With only the first two terms kept in the series, the solution to the equations (A-1) and (A-2), skipping the algebra, is

$$\begin{aligned} \phi(z, \mu) &= 2S_0 e^{-z/\mu} + 2S_0 c \left[\frac{1+E_2(z)}{4} (1-e^{-z/\mu}) \right] \quad ; \quad \mu > 0 \\ &= 2S_0 c \left[\frac{1+E_2(a)}{4} (1-e^{a/\mu}) e^{-z/\mu} + \frac{1+E_2(z)}{4} (1-e^{-z/\mu}) \right] \quad ; \quad \mu < 0 \end{aligned}$$

where $E_2(z)$ is the exponential integral of order 2. The expressions for R and T, from equation (A-3), are

$$R = 2S_0 \frac{c}{4} [1+E_3(a)] \left[\frac{1}{2} - E_3(a) \right]$$

$$T = 2S_0 E_3(a) + 2S_0 \frac{c}{4} [1+E_2(a)] \left[\frac{1}{2} - E_3(a) \right]$$

Differentiating T and R with respect to 'a' and taking the limit as 'a' approaches zero, we get

$$\left. \frac{\partial T}{\partial a} \right|_{a=0} + \left. \frac{\partial R}{\partial a} \right|_{a=0} = -2S_0(1-c) \quad (A-4)$$

Diffusion solution: Now the same problem is solved by diffusion theory without any restriction on 'c'. The homogeneous one-group steady state diffusion equation in a homogeneous slab is

$$\frac{d^2 \phi(z)}{dz^2} - L^2 \phi(z) = 0 \quad (A-5)$$

$$\text{where, } L^2 = 3(1-c). \quad (A-6)$$

The boundary conditions are taken as

$$J_{in}(0) = S_0 = \alpha \phi(0) - \beta D \sigma_t \left. \frac{d\phi}{dz} \right|_{z=0} \quad (A-7)$$

$$J_{in}(a) = 0 = \alpha \phi(a) + \beta D \sigma_t \left. \frac{d\phi}{dz} \right|_{z=a}$$

For P_1 Marshak boundary conditions, $\alpha=1/4$ and $\beta=1/2$. The reflection, R and transmission, T are then given by

$$R = \alpha \phi(0) + (1-\beta) D \sigma_t \left. \frac{d\phi}{dz} \right|_{z=0} \quad (A-8)$$

$$T = \alpha \phi(a) - (1-\beta) D \sigma_t \left. \frac{d\phi}{dz} \right|_{z=a}$$

The solution to equations (A-5) and (A-7) is

$$\phi(z) = A e^{Lz} + B e^{-Lz} \quad (A-9)$$

where,

$$A = \frac{-S_o (\alpha - \beta D\sigma_t L) e^{-aL}}{M}$$

$$B = \frac{S_o (\alpha + \beta D\sigma_t L) e^{aL}}{M}$$

$$M = (\alpha + \beta D\sigma_t L)^2 e^{aL} - (\alpha - \beta D\sigma_t L)^2 e^{-aL}$$

Now inserting equation (A-9) in equation (A-8), α and β can be solved for in terms of R and T , after a straightforward but rather lengthy algebra. These are given by

$$\alpha = D\sigma_t L \frac{S_o \sinh(aL)}{(S_o - T - R)(S_o + T - R)} \quad (A-10)$$

$$\beta = \frac{S_o (S_o - R - T \cosh(aL))}{(S_o - R - T)(S_o - R + T)}$$

Now as 'a' approaches zero (optically thin slab), $\sinh(aL) \rightarrow aL$, $R \rightarrow 0$, $\cosh(aL) \rightarrow 1$ and $T \rightarrow S_o$. From equation (A-4)

$$\left. \frac{\partial T}{\partial a} \right|_{a=0} + \left. \frac{\partial R}{\partial a} \right|_{a=0} = -2S_o(1-c)$$

Using this result and taking the limit of equation (A-10) as 'a' $\rightarrow 0$, we get, for small 'c',

$$\lim_{a \rightarrow 0} \alpha = \frac{1}{4}, \quad \text{and} \quad \lim_{a \rightarrow 0} \beta = \frac{1}{2}$$

These are the same as those for the Marshak boundary conditions which we have used with the multigroup diffusion equation for calculating neutral atom transport in fusion plasmas. This shows that even for small values of 'c', total particle loss (=R+T) given by transport theory and diffusion theory are the same for an optically thin medium. To conserve particles, the absorption rates will also be the same by transport theory and diffusion theory. Since the flux attenuation is small in an optically thin medium, the flux given by the diffusion theory using Marshak boundary conditions will be accurate for such a medium even for small values of 'c'.

It is instructive to see how α and β vary with 'c' and 'a' to give the same R and T as given by transport theory. R and T can be calculated as functions of 'c' and 'a' by using ANISN. Maynard[27] has tabulated such values. Using these values of R and T, equation (A-10) has been used to calculate α and β . These are shown in figure 8 plotted as functions of 'a' for values of 'c' of 0.1, 0.5 and 0.9. We can very easily see that for small 'a' α and β are very close to 1/4 and 1/2 respectively for all values of 'c' and, for 'c' close to one, for all values of 'a' as is expected for a diffusion theory. This proves the observation made in point 6 earlier in section IV.

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REFERENCE

1. S. Rehker & H. Wobig, Plasma Phys. vol 15, 1083(1973).
2. T.F. Volkov & Y.L. Igithkanov, Sov. J. Plasma Phys. 3, 668(1977).
3. K.H. Burrell, Phys. Fluids, 21(12), 2282(1978).
4. M.B. Tendler and O. Ågren, Phys. Fluids, 25, 1037(1982).
5. J. Hackmann, Y.C. Kim, E.K. Souw and J. Uhlenbusch, Plasma Phys. vol 20, 309(1978).
6. K. Audenaerde, G.A. Emmert, & M. Gordinier, J. of Comp. Phys. 34, 268(1980).
7. R.D. Garcia, G.C. Pomraning & C.E. Siewert, Plasma Phys. vol 24, no.8, 903(1982).
8. J.H. Marable & E.M. Oblow, Nucl. Sci. & Eng. 61, 90(1976).
9. D.F. Ducks, D.E. Post and P.H. Rutherford, Nuc. Fusion, 17, 565(1977).
10. M.W. Hughes & D.E. Post, J. Comp. Phys. 28, 43(1978).
11. D. Heifetz, D. Post, M. Petravic, J. Weisheit and G. Bateman, J. Comp. Phys. 46, 309(1982).
12. D. Reiter and A. Nicolai, J. Nuclear Materials, 128&129, 453(1984).
13. M. Z. Hasan and R. W. Conn, "A Two-Dimensional Finite Element Multigroup Diffusion Theory for Neutral Atom Transport in Plasmas", (submitted to J.Computational Physics).
14. M. Clark, Jr. and K.F. Hansen, Numerical Methods for Reactor Analysis, Academic Press, N.Y. 1964.
15. G. I. Bell and S. Glasstone, Nuclear Reactor Theory, Robert E. Krieger Publishing Co., N.Y., 1979.
16. J. J. Duderstadt and L. J. Hamilton, Nuclear Reactor Analysis, John Wiley & Sons, Inc., N.Y., 1976.

17. J.J. Duderstadt and W.R. Martin, Transport Theory, John Wiley & Sons, Inc., 1979.
18. Y.N. Dnestrovskij, S.E. Lysenko and A.I. Kislyakov, Nuc. Fusion, 19, 293(1979).
19. B. Davison, Neutron Transport Theory. Oxford Univ. Press, Oxford, U.K., 1957.
20. C.D. Levermore & G.C. Pomraning, A Flux-limited Diffusion Theory, Astrophysical J. 248, 321(1981).
21. M. Z. Hasan, Application of Diffusion Theory to the Transport of Neutral Particles in Fusion Plasmas, Ph.D. Dissertation, University of California, Los Angeles, 1985.
22. W. W. Engle, Jr., "A Users Manual for ANISN: A One-Dimensional Discrete Ordinate Transport Code with Anisotropic Scattering", K-1693, Oak Ridge National Laboratory (1967).
23. PLASMX: "A Multigroup Ionization and Charge Exchange Cross Section Code for Neutral Hydrogen Transport in Plasmas", PSR-106, RSIC, Oak Ridge National Laboratory, (1977).
24. J. G. Gilligan, S.L. Gralnick, W.G. Price, Jr., and T. Kammash, Nuclear Fusion, 18, 63(1978).
25. Z. ElDerini and E. M. Gelbard, Trans. Am. Nucl. Soc. 23, 45(1976).
26. M. Z. Hasan and R. W. Conn, "Two-Dimensional Toroidal Geometry Neutral Atom Transport and Material Erosion Rates in the TEXTOR and TFTR Tokamaks", (submitted to Fusion Technology).
27. C. W. Maynard, Nucl. Sci. Eng., 6, 174(1959).

Table 1: Comparison of neutral atom flux for the lowest energy group by diffusion and transport theory for a slab with TFTR plasma properties. The surface at $x = 85$ cm has unit surface source and is subject to reflection boundary condition.

Boundary Condition	Diffusion Theory Result (IDT)		Transport Theory Result (ANISN)		% Difference	
	<u>$x=0$</u>	<u>$x=85$</u>	<u>$x=0$</u>	<u>$x=85$</u>	<u>$x=0$</u>	<u>$x=85$</u>
Vacuum Boundary Condition at $x=0$	6.56×10^{-9}	1.734	7.5×10^{-9}	1.966	12.6	11.8
Reflection Boundary Condition at $x=0$	2.6×10^{-8}	1.734	2.44×10^{-8}	1.966	6.1	11.8

Figure captions:

Figure 1: Total neutral atom density by IDT, SPUDNUT[6] and ANISN[22] in a one-dimensional slab plasma with reflection boundary conditions at each surface. A unit surface source is located at $x=40\text{cm}$. The density and temperature profiles are parabolic with a central density of $5 \times 10^{13} \text{cm}^{-3}$, a central T_e of 2keV and a central T_i of 1keV.

Figure 2: Total neutral atom density by IDT and ANISN[22] in a one-dimensional cylindrical plasma with reflection boundary conditions. A unit surface source is located at $r=40\text{cm}$. Plasma properties are same as indicated for figure 1.

Figure 3: Total neutral atom density in a one-dimensional slab with TFTR plasma properties[11]. Twenty-one energy groups have been used with maximum energy of 40keV. The right surface is reflected and the left surface is subject to vacuum boundary condition. A unit surface source is located at $x=85\text{cm}$. Source energy is a few eV. Plasma density and temperature profiles are parabolic, with $n(0) = 5.44 \times 10^{13} \text{cm}^{-3}$ and $T_i(0)=T_e(0)=16.5\text{keV}$ at the center and $n(a)=1.33 \times 10^{13} \text{cm}^{-3}$ and $T_i(a)=T_e(a)=110\text{eV}$ at the plasma edge.

Figure 4: Average neutral atom energy (eV) for the problem in figure 3 by diffusion theory (IDT) and transport theory (ANISN). It can be seen that diffusion theory accurately predicts the average neutral atom energy in the plasma.

Figure 5: Result from reference [3]. Neutral density is normalized to the source strength, and the neutral energy is normalized to the plasma temperature. In (a), the solid lines represent kinetic solution and the dashed lines, the diffusion approximation solution. $B/A='c'$ and z is in mean free path. Notice the large difference in solution near the wall in (a) and the corresponding difference in the neutral energy from the plasma energy near the wall for all values of ' c ' in (b).

Figure 6(a): Effect of ' c ' and slab thickness ' a ' on diffusion theory solution with P_1 -Marshak boundary conditions. This is a one-group solution in an optically thin ($a=.1$ mean free path) homogeneous slab. There is a unit surface source at the right surface. Both faces of the slab are subject to vacuum boundary conditions. The particle flux ($\text{cm}^{-2}\text{sec}^{-1}$) is shown for three values of ' c ' (.1, .5 and .9). Diffusion theory gives good accuracy for all values of ' c ' for this thin slab.

Figure 6(b): Effect of 'c' and slab thickness 'a' on diffusion theory solution with P_1 -Marshak boundary conditions. This is a one-group solution in an optically thin($a=1$ mean free path) homogeneous slab. There is a unit surface source at the right surface. Both faces of the slab are subject to vacuum boundary conditions. The particle flux($\text{cm}^{-2}\text{sec}^{-1}$) is shown for three values of 'c' (.1, .5 and .9). Diffusion theory gives good accuracy for all values of 'c' for this thin slab.

Figure 6(c): Effect of 'c' and slab thickness 'a' on diffusion theory solution with P_1 -Marshak boundary conditions. This is a one-group solution in an optically thick($a=10$ mean free paths) homogeneous slab. There is a unit surface source at the right surface. Both faces of the slab are subject to vacuum boundary conditions. The particle flux($\text{cm}^{-2}\text{sec}^{-1}$) is shown for three values of 'c' (.1, .5 and .9). In contrast to the results in figures 6(a) and 6(b), this figure shows that, for an optically thick medium, diffusion theory is accurate for values of 'c' close to one and becomes increasingly less accurate for smaller values of 'c'.

Figure 7: Transport and diffusion theory solutions in a homogeneous slab. This figure shows the boundary conditions and defines R and T , the number of particles reflected at the left surface and transmitted across the right surface, respectively.

Figure 8: Variation of α and β with ' c ' and slab thickness, ' a '. α and β are calculated using equation (A-10). The values of R and T are taken from reference [27]. $\alpha=1/4$ and $\beta=1/2$ for P_1 -Marshak boundary conditions. This figure shows that for an optically thin slab (small ' a '), α and β approach $1/4$ and $1/2$ respectively for all values of ' c '.

Figure 1:

Figure # 2

Figure 3:

Figure # 4

(a)

(b)

Figure 5:

Figure 6(a):

Figure 6(b):

Figure 6(c):

(a) Transport Solution

(b) Diffusion Solution

Figure 7:

Figure 8: