NEUTRAL TRANSPORT IN A PLASMA

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December, 1977

ABSTRACT

A solution procedure for the neutral transport equation in plasma slab geometry is developed. Half-angle scalar fluxes, currents and averaged cross sections are introduced to provide a convenient and simple method of calculating the neutral energy distribution as an adjunct to the neutral density calculation. A forward-backward sweep numerical solution procedure, which avoids matrix inversion, is outlined.
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A number of different computational techniques have been proposed to treat the transport of neutral hydrogen (H, D, T) atoms in the edge region of a hydrogen plasma. The computationally simpler methods, in which an analytical solution is obtained under certain simplifying assumptions or the distribution of neutrals which have undergone only a few interactions with the plasma is obtained analytically, generally suffer from a lack of accuracy. The more rigorous methods, in which neutral histories are followed in a Monte Carlo simulation or the energy-dependent neutral transport equation is solved in the multigroup discrete-ordinates approximation, generally suffer from an excess of computational effort. The purpose of this report is to propose a method for neutral transport which should be both adequately accurate and computationally attractive.

The principal interactions which affect the transport of neutrals in a plasma of the same species are charge-exchange (CX), ion-impact ionization (II), and electron-impact ionization (IE). The total interaction cross section for neutrals is thus,

\[
\sigma = \frac{N_p \langle \sigma_{CX} \rangle + \langle \sigma_{II} \rangle + N_e \langle \sigma_{IE} \rangle}{N_p \frac{\langle v \rangle_m}{\overline{v_n}}},
\]

where the brackets \(\langle \rangle\) indicate an average over the velocity distribution of the interacting particles, \(N_p\) and \(N_e\) are the plasma ion and electron densities, respectively, and \(\overline{v_n}\) is the average speed of the neutrals.

The effect of ionization is the loss of a neutral. The effect of charge exchange is to replace a neutral at one velocity by a neutral at another velocity. In this model, the neutrals resulting from charge-exchange...
events are assumed to be isotropically distributed in direction relative to the direction of the incident neutral and to be distributed in energy as are the plasma ions at that spatial location; these assumptions result in simplifications, but are not essential. The number of secondary neutrals per incident neutral is

\[
C = \frac{N_0 \langle v_{CX} \rangle}{\sigma}
\]  

(2)

Because neutral effects are important only in the outermost regions of large plasmas, slab geometry is appropriate. For generality, a two-side slab problem, as illustrated in Fig. 1, will be considered. Incident fluxes \( \Psi_{in} (x, \mu > 0) \) and \( \Psi_{in} (x, \mu < 0) \) are prescribed as boundary conditions. The flux is

\[
\Psi = N_n \left\langle v_n \right\rangle
\]  

(3)

where \( N_n \) is the neutral density.

At any interior surface \( x_o < x < x_n \), the neutral flux consists of uncollided incident neutrals and neutrals which are the progeny of incident neutrals after one or more charge-exchange events. The velocity distribution of the uncollided incident neutrals is known. The energy distribution of the progeny—"collided"—neutrals depends upon the plasma ion energy distributions at the locations at which the charge-exchange event occurred. The plasma temperature gradient may be steep in the edge region. Thus, there may be a significant difference in the energy distributions of collided neutrals crossing the plane at \( x \) from left-to-right.
and those crossing from right-to-left. Because the values of the interaction cross sections depend upon the energy distribution of the neutrals, it is useful to define separate cross sections for neutrals moving from left-to-right (+) and those moving from right-to-left (--). In addition, it is useful to distinguish between uncollided (u) and collided (c) neutrals.

The uncollided neutral flux satisfies

\[
\frac{d\psi}{dx} (x, \mu) + \sigma_u^+ (x) \psi_u (x, \mu) = 0
\]

and boundary conditions

\[
\psi_u (x, \mu) = \begin{cases} 
\psi_{in} (x_0, \mu), & \mu > 0 \\
0, & \mu < 0 
\end{cases}
\]

(4.b)

\[
\psi_u (x, \mu) = \begin{cases} 
0, & \mu > 0 \\
\psi_{in} (x_n, \mu), & \mu < 0 
\end{cases}
\]

(4.c)

Equations (4) have the solutions

\[
\psi_u (x, \mu) = \begin{cases} 
\frac{\psi_{in} (x_0, \mu) \mu}{\varepsilon}, & \mu > 0 \\
\frac{\psi_{in} (x_n, \mu) \mu}{\varepsilon}, & \mu < 0 
\end{cases}
\]

(5)

where

\[
y_u^+ (x_1, x_2) \equiv \int_{x_1}^{x_2} \sigma_u^+ (x') dx'
\]

(6)
The collided flux satisfies

\[
\frac{d\psi_c}{dx}(x,\mu) + \sigma^+_c(x) \psi_c(x,\mu) = S(x),
\]

(7)

and \( \psi_c(x_o,\mu>0) = \psi_c(x_n,\mu<0) = 0 \) boundary conditions, where \( S(x) \) is the charge-exchange source

\[
S(x) \equiv \frac{1}{2} C^+_c(x) \sigma^+_c(x) \phi^+_c(x) + \frac{1}{2} C^-_c(x) \sigma^-_c(x) \phi^-_c(x) +
\]

\[
\frac{1}{2} C^+_u(x) \sigma^+_u(x) \phi^+_u(x) + \frac{1}{2} C^-_u(x) \sigma^-_u(x) \phi^-_u(x),
\]

(8)

where the half-angle scalar fluxes are defined

\[
\phi^+_c(x) = \int_0^1 \psi(x,\mu) d\mu, \quad \phi^-_c(x) = \int_{-1}^0 \psi(x,\mu) d\mu,
\]

(9)

and the isotropy of the charge-exchange event has been used. The solution of Eq. (7) is

\[
\psi_c(x,\mu) = \begin{cases} 
\int_{x_o}^{x} e^{-\frac{y^+_c(x',x)/\mu}{S(x')}} \frac{S(x')}{\mu} dx', & \mu > 0 \\
\int_{x_n}^{x} e^{-\frac{y^-_c(x,x'/\mu}{S(x')}} \frac{S(x')}{\mu} dx', & \mu < 0
\end{cases}
\]

(10)
where $y_+^+$ is defined as in Eq. (6), but with $\sigma^+_{\nu}$ rather than $\sigma^+_{\mu}$.

Substituting Eqs. (10) into Eqs. (9) results in a coupled pair of integral equations which must be solved for the half-angle scalar fluxes

$$\phi^+_c(x) = \int_{x_0}^{x} E_1([y^+_c(x'), x')] S(x') dx' , \quad (11.a)$$

$$\phi^-_c(x) = \int_{x}^{x_n} E_1([y^-_c(x'), x]) S(x') dx'^- , \quad (11.b)$$

where $E_1$ is the exponential integral function

$$E_n(z) \equiv \int_0^1 \mu^{n-2} e^{-z/\mu} d\mu , \quad (12)$$

for which tables exist.\(^5\)

Thus, the neutral transport problem has been reduced to the solution of coupled integral equations for the scalar half-angle fluxes, which are proportional to the neutral densities. Others (e.g. Ref. 6) have reduced the neutral transport problem to an integral equation for the neutral density under the assumption that the $<\sigma \nu>$ terms were constant, or at least independent of the neutral velocity distribution. However, $<\sigma_{CX} \nu>$ varies by an order of magnitude and $<\sigma_{II \nu}>$ varies by even more for the regime of interest. By introducing the half-angle cross sections, the present method is able to avoid the assumption of constant rate coefficients, and to provide a convenient means for constructing energy-dependent rate coefficients, as will be discussed.

The structure of Eqs. (11) suggests a forward and backward sweep solution. First, a discrete mesh (with $x_0$ and $x_n$ the end points) would be superimposed on the slab. Second, the uncollided half-angle scalar flux

...
fluxes would be computed at each mesh point from Eqs. (5) and (9). The discrete version of Eq. (11.a), which is of the form

\[ \phi_c^+(x_i) = \sum_{j=0}^{i-1} \phi_{cj}^+(x_i) \]  

(13.a)

can then be evaluated by sweeping from \( x_1 \) to \( x_n \). Only the \( \phi_c^- \) contributions to \( S(x) \) are unknown and must be estimated from an initial guess or previous iteration in solving Eq. (13.a). The discrete version of Eq. (11.b), which is of the form

\[ \phi_c^-(x_i) = \sum_{j=i+1}^{n} \phi_{cj}^-(x_i) \]  

(13.b)

can then be evaluated by sweeping backwards from \( x_{n-1} \) to \( x_0 \), using values of \( \phi_c^+ \) from the forward sweep. Because the charge-exchange neutrals created at \( x_j \) are assumed to have the energy distribution of the plasma ions at \( x_j \), the \( E_1 \) function is independent of the iteration and the energy distribution of the collided half-angle scalar fluxes can be computed from

\[ f_c^+(x_i, E) = \sum_{j=0}^{i-1} f_p(x_j, E) \phi_{cj}^+(x_i) / \phi_c^+(x_i) \]  

(14.a)

\[ f_c^-(x_i, E) = \sum_{j=i+1}^{n} f_p(x_j, E) \phi_{cj}^-(x_i) / \phi_c^-(x_i) \]  

(14.b)

where \( f_p(x_j, E) \) is the energy distribution of the plasma ions at \( x = x_j \).

Equations (14) indicate a straightforward procedure for constructing \( \phi_c^\pm \).
The forward (+) and backward (−) neutral currents are defined

\[ J^+(x) = \int_0^1 \mu \Psi(x, \mu) \ d\mu, \quad J^-(x) = \int_0^1 \mu \Psi(x, \mu) \ d\mu. \tag{15} \]

The uncollided current is obtained by using Eqs. (5) in Eqs. (15).

\[ J^+_u(x) = \int_0^1 \mu \left. e^{-y^+_u(x_o, x)/\mu} \Psi_{in}(x_o, \mu) \right| \right. \tag{16.a} \]

\[ J^-_u(x) = \int_0^1 \mu \left. e^{-y^-_u(x, x_n)/\mu} \Psi_{in}(x_n, \mu) \right| \right. \tag{16.b} \]

Differentiating Eq. (16.a) with respect to \( x \) and integrating the result from \( x_o \) to \( x \), and likewise for Eq. (16.b) except integrating from \( x_n \) to \( x \), yields.

\[ J^+_u(x) = J^+_u(x_o) - \int_{x_o}^x \sigma^+_u(x') \phi^+_u(x') \ dx' \tag{17.a} \]

\[ J^-_u(x) = J^-_u(x_n) + \int_{x_n}^x \sigma^-_u(x') \phi^-_u(x') \ dx' \tag{17.b} \]

(Note that the sign of \( J^-_u \) is −, so Eq. (17.b) does describe an attenuation in magnitude.)

The collided neutral currents are obtained by using Eqs. (10) in Eqs. (15).

\[ J^+_c(x) = \int_{x_o}^x E_2(|y^+_c(x', x)|) S(x') \ dx' \tag{18.a} \]

\[ J^-_c(x) = -\int_{x_n}^x E_2(|y^-_c(x, x')|) S(x') \ dx' \tag{18.b} \]
Differentiating and integrating as for $J_\text{u}$, noting

$$\frac{dE_2}{dx} \left( |y^+(x,x^-)| \right) = \pm \sigma_\pm E_1 \left( |y^+(x,x^-)| \right),$$

and recalling that the incident collided currents at $x_\text{o}$ and $x_\text{n}$ are zero by definition, leads to

$$J_\text{c}^+(x) = \int_{x_\text{o}}^x [S(x', x') - \sigma_\text{c}^+(x') \phi_\text{c}^+(x')] \, dx', \quad \text{(19.a)}$$

$$J_\text{c}^-(x) = \int_{x_\text{n}}^x [S(x', x') - \sigma_\text{c}^-(x') \phi_\text{c}^-(x')] \, dx'. \quad \text{(19.b)}$$

Once the half-angle flux equations have been solved, the current can be simply evaluated from the discrete approximations to either Eqs. (16) and (18), or (17) and (19). The former requires the additional evaluation of the $E_2$ functions, from table lookup or recursion relations, but has the advantage of providing a means of computing the energy distribution of the currents. The discrete forms of Eqs. (18) can be written in a form similar to Eqs. (13), and weighting schemes similar to Eqs. (14) can be used to construct the collided current energy distribution. The energy distribution of the uncollided current is known.

This formalism can be specialized to calculate various quantities of interest. For example, if neutrals are incident upon a plasma from the left at $x_\text{o}$, and if $x_\text{n}$ is chosen sufficiently deep into the plasma that the neutral density is negligible, then the plasma albedo (reflection coefficient) is given by
all quantities being evaluated for $\psi_{in}(x_n, \mu < 0) = 0$. A second example is energetic neutrals emerging from the plasma core at $x_0$ and transversing a cooler plasma or neutral gas edge region before striking a wall at $x_n$. The transmission coefficient for neutrals through the edge region is

$$R \equiv \frac{J_c^-(x_0)}{J_c^+(x_0)}$$

all quantities again being evaluated for $\psi_{in}(x_n, \mu < 0) = 0$. (This transmission formalism may also be appropriate, under certain conditions, for neutral beam transmission through a plasma.) The energy distribution for the reflected or transmitted neutral currents could be constructed from the weighting scheme discussed previously.
Figure 1. Two-Sided Slab Problem
References


Acknowledgement

This work was supported by the U. S. Department of Energy.