An interface current balance formulation of neutral atom transport theory in plasmas

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An interface current balance (ICB) method for neutral particle transport is presented and specialized to the calculation of neutral atom transport in background plasmas. A multigroup extension of the ICB methodology is presented which enables the direct calculation of neutral atom energy distributions and energy and momentum transport, as well as particle transport. Extension of the ICB methodology to multidimensions recovers the transmission/escape probability method. © *1997 American Institute of Physics.* [S1070-664X(97)02601-3]

I. INTRODUCTION

Integral transport methods are widely used for neutron transport calculations within heterogeneous reactor cores (e.g., Refs. 1–3) and more recently have been adopted for the calculation of neutral atom transport in the edge regions of fusion plasmas (e.g., Ref. 4), where they have found widespread usage. One of the attractions of integral transport methods is the physically intuitive nature of the various terms in the computational algorithm. The major drawback to integral transport methods is that all regions in the discretized problem are coupled, resulting in a $N\times N$ matrix to invert on each iteration, where N is the number of discretized regions. Although various approximations have been developed to circumvent this difficulty, the inherent coupling of all regions in an iterative solution procedure remains the major drawback of integral transport methods.

The purpose of this paper is to set forth an interface current balance (ICB) formulation of integral transport theory which results in coupling only among contiguous regions in the discretized problem. This ICB formulation provides a more efficient computational algorithm for neutral atom transport calculations in the plasma edge region than the integral transport models presently in plasma edge codes and is readily generalized to multidimension, where this advantage is retained. This ICB formulation is related to the response matrix method[1–2] of neutron transport theory and leads to and provides a theoretical basis for the transmission/escape probability method[5] for neutral atom transport in the edge regions of fusion plasmas.

The ICB formulation is developed in Secs. II–V in slab geometry by using integral transport theory to express the emergent currents from a discrete region and the reaction rates within that region in terms of the incident currents into that region and the source of particles within that region. The relation to the response matrix method is established in Sec. VI, and the ICB method is extended to treat energy dependence in Sec. VII. The ICB method is extended to two dimensions in Sec. VIII, and equivalence with the transmission/escape probability method is established. Specialization of the ICB formalism to neutral particle transport in the edge of fusion plasmas is discussed in Sec. IX, where a multigroup formulation is developed. Extensions of the methodology to handle higher levels of anisotropy in the neutral particle distribution and anisotropic scattering are discussed in Sec. X. The results of a model problem computation are described in Sec. XI. Finally, the work is summarized in Sec. XII.

II. EMERGENT CURRENTS AND REACTION RATES DUE TO INCIDENT CURRENTS

Consider the slab geometry configuration depicted in Fig. 1, in which a slab region i is bounded by surfaces i and $i+1$ with incident currents J_i^+ and J_{i+1}^- and emergent currents J_i^- and J_{i+1}^+. The angular flux of particles at x arising from a plane source of unit strength at $x'<x$ is[6]

$$\psi(x,x',\mu)=\frac{e^{-\Sigma_t(x-x')/\mu}}{\mu}, \tag{1}$$

where it is assumed that the total cross section, Σ_t, is uniform over Δ_i, and μ is the cosine of the angle that the particle direction makes with the x axis. Further assuming that the incident currents are isotropically distributed in angle over the incident hemisphere (i.e., a double P_0 approximation[7]), the uncollided currents emergent from the opposite surface are given by

$$\begin{aligned}\hat{J}_{un}^+(x_{i+1})&=J_i^+\int_0^1\mu\left(\frac{e^{-\Sigma_{ti}\Delta_i/\mu}}{\mu}\right)d\mu=E_2(\Delta_i\Sigma_{ti})J_i^+,\\ \hat{J}_{un}^-(x_i)&=J_{i+1}^-\int_{-1}^0\mu\left(\frac{e^{+\Sigma_t\Delta_i/\mu}}{\mu}\right)d\mu=E_2(\Delta_i\Sigma_{ti})J_{i+1}^-,\end{aligned} \tag{2}$$

where E_n is the exponential integral function

$$E_n(z)\equiv\int_0^1\mu^{n-2}e^{-z/\mu}\,d\mu. \tag{3}$$

The first collision rate for incident particles within Δ_i is given by

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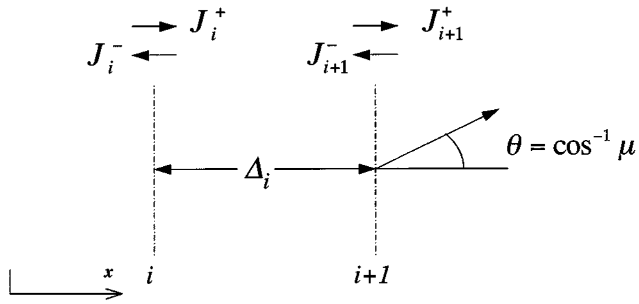

FIG. 1. Slab geometry configuration.

$$\hat{A}_{i1}=\Sigma_{ti}\left[J_i^+\int_0^1 d\mu\int_{x_i}^{x_{i+1}}dx\left(\frac{e^{-\Sigma_{ti}(x-x_i)/\mu}}{\mu}\right)\right.$$
$$\left.+J_{i+1}^-\int_{-1}^0 d\mu\int_{x_i}^{x_{i+1}}dx\left(\frac{e^{-\Sigma_{ti}(x-x_{i+1})/\mu}}{\mu}\right)\right]$$
$$=(J_i^+ + J_{i+1}^-)[1-E_2(\Delta_i\Sigma_{ti})]. \tag{4}$$

The fraction c_i of the collision rate which is due to scattering (i.e., to events which do not remove the particle) constitutes a source of once-collided particles, which we assume to be isotropic (1/2 emerge going to the right and 1/2 to the left) and uniformly distributed over Δ_i. The emergent currents of once-collided particles are then

$$\hat{J}_1^+(x_{i+1})=\int_{x_i}^{x_{i+1}}dx\int_0^1\mu\left(\frac{1}{2}\,c_i\,\frac{\hat{A}_{i1}}{\Delta_i}\right)\left(\frac{e^{-\Sigma_{ti}(x_{i+1}-x)/\mu}}{\mu}\right)d\mu$$
$$=\frac{1}{2}\,\frac{c_i\hat{A}_{i1}}{\Delta_i\Sigma_{ti}}\,[\tfrac{1}{2}-E_3(\Delta_i\Sigma_{ti})]=\tfrac{1}{2}c_iP_{oi}\hat{A}_{i1}, \tag{5}$$
$$\hat{J}_1^-(x_i)=\tfrac{1}{2}c_iP_{oi}\hat{A}_{i1}=\tfrac{1}{2}c_iP_{oi}(J_i^+ + J_{i+1}^-)[1-E_2(\Delta_i\Sigma_{ti})],$$

where the average first-flight escape probability for source particles distributed uniformly over Δ_i has been defined

$$P_{oi}\equiv\frac{\frac{1}{2}}{\Delta_i}\int_{x_i}^{x_{i+1}}dx\int_0^1 d\mu\;\mu\left(\frac{e^{-\Sigma_{ti}(x_{i+1}-x)/\mu}}{\mu}\right)$$
$$+\frac{\frac{1}{2}}{\Delta_i}\int_{x_i}^{x_{i+1}}dx\int_{-1}^0 d\mu\;\mu\left(\frac{e^{\Sigma_{ti}(x-x_i)/\mu}}{\mu}\right)$$
$$=\frac{1}{\Delta_i\Sigma_{ti}}\,[\tfrac{1}{2}-E_3(\Delta_i\Sigma_{ti})]. \tag{6}$$

Note that we are distinguishing between the total partial currents at x_i, denoted by $J_i^{+/-}$, and the various components of that current, denoted by $\hat{J}_z^{+/-}(x_i)$, where z is a descriptive subscript pertaining to the particular component.

The collision rate for incident particles undergoing a second collision in Δ_i is

$$\hat{A}_{i2}=\Sigma_{ti}\tfrac{1}{2}c_i\,\frac{\hat{A}_{i1}}{\Delta_i}\left[\int_0^1 d\mu\int_{x_i}^{x_{i+1}}dx'\int_{x'}^{x_{i+1}}dx\left(\frac{e^{-\Sigma_{ti}(x-x')/\mu}}{\mu}\right)\right.$$
$$\left.+\int_{-1}^0 d\mu\int_{x_i}^{x_{i+1}}dx'\int_{x_i}^{x'}dx\left(\frac{e^{-\Sigma_{ti}(x-x')/\mu}}{\mu}\right)\right]$$
$$=c_i\hat{A}_{i1}(1-P_{oi})=c_i(J_i^+ + J_{i+1}^-)$$
$$\times[1-E_2(\Delta_i\Sigma_{ti})](1-P_{oi}). \tag{7}$$

As before, the fraction c_i of this collision rate constitutes a source of twice-collided particles which are assumed to be isotropic. The emergent currents of twice-collided particles are given by Eqs. (5) but with $\hat{A}_{i1}$ replaced by $\hat{A}_{i2}$

$$\hat{J}_2^+(x_{i+1})=\hat{J}_2^-(x_i)=\tfrac{1}{2}c_i\hat{A}_{12}P_{oi}$$
$$=\tfrac{1}{2}c_i^2(J_i^+ + J_{i+1}^-)[1-E_2(\Delta_i\Sigma_{ti})]$$
$$\times(1-P_{oi})P_{oi}. \tag{8}$$

Continuing this line of argument, we derive general expressions for the rate at which incident particles undergo their nth collision in Δ_i

$$\hat{A}_{in}=c_i^{n-1}(J_i^+ + J_{i+1}^-)[1-E_2(\Delta_i\Sigma_{ti})](1-P_{oi})^{n-1} \tag{9}$$

and for the emergent currents of n-collided incident particles

$$\hat{J}_n^+(x_{i+1})=\hat{J}_n^-(x_i)=\tfrac{1}{2}c_i^n(J_i^+ + J_{i+1}^-)[1-E_2(\Delta_i\Sigma_{ti})]$$
$$\times(1-P_{oi})^{n-1}P_{oi}. \tag{10}$$

The total collision rate in Δ_i due to incident currents is obtained by summing Eq. (9)

$$\hat{A}_i=\sum_{n=1}^{\infty}A_{in}=(J_i^+ + J_{i+1}^-)[1-E_2(\Delta_i\Sigma_{ti})]\sum_{n=0}^{\infty}[c_i(1-P_{oi})]^n$$
$$=\frac{(J_i^+ + J_{i+1}^-)[1-E_2(\Delta_i\Sigma_{ti})]}{1-c_i(1-P_{0i})} \tag{11}$$

and the total emergent currents due to incident currents are obtained by summing Eq. (10) and adding the uncollided contributions of Eqs. (2)

$$\hat{J}^+(x_{i+1})=\left[\frac{\frac{1}{2}c_iP_{oi}[1-E_2(\Delta_i\Sigma_{ti})]}{1-c_i(1-P_{oi})}+E_2(\Delta_i\Sigma_{ti})\right]J_i^+$$
$$+\left[\frac{\frac{1}{2}c_iP_{oi}[1-E_2(\Delta_i\Sigma_{ti})]}{1-c_i(1-P_{oi})}\right]J_{i+1}^-,$$
$$\hat{J}^-(x_i)=\left[\frac{\frac{1}{2}c_iP_{oi}[1-E_2(\Delta_i\Sigma_{ti})]}{1-c_i(1-P_{oi})}+E_2(\Delta_i\Sigma_{ti})\right]J_{i+1}^-$$
$$+\left[\frac{\frac{1}{2}c_iP_{oi}[1-E_2(\Delta_i\Sigma_{ti})]}{1-c_i(1-P_{oi})}\right]J_i^+. \tag{12}$$

III. EMERGENT CURRENTS AND REACTION RATES DUE TO INTERNAL SOURCES

We consider a uniform distribution of particle sources within Δ_i of strength s_i/Δ_i per unit length. This source is allowed to be anisotropic, with a number s_i^+ emitted to the right and s_i^- emitted to the left. The emergent currents of uncollided source particles are

$$
\begin{aligned}
J_{un,s}^+(x_{i+1}) &= \frac{s_i^+}{\Delta_i}\int_{x_i}^{x_{i+1}} dx \int_0^1 d\mu\ \mu\left(\frac{e^{-\Sigma_{ti}(x_{i+1}-x)/\mu}}{\mu}\right) \\
&= s_i^+ P_{oi}, \\
J_{un,s}^-(x_i) &= \frac{s_i^-}{\Delta_i}\int_{x_i}^{x_{i+1}} dx \int_{-1}^0 d\mu\ \mu\left(\frac{e^{-\Sigma_{ti}(x-x_i)/\mu}}{\mu}\right) \\
&= s_i^- P_{oi}.
\end{aligned}
\tag{13}
$$

The first collision rate of source particles within Δ_i is given by

$$
\begin{aligned}
A_{i1,s} &= \frac{s_i^+}{\Delta}\ \Sigma_{ti}\int_{x_i}^{x_{i+1}} dx' \int_{x'}^{x_{i+1}} dx \int_0^1 d\mu\left(\frac{e^{-\Sigma_{ti}(x-x')/\mu}}{\mu}\right) \\
&\quad + \frac{s_i^-}{\Delta_i}\ \Sigma_{ti}\int_{x_i}^{x_{i+1}} dx' \int_{x_i}^{x'} dx \int_{-1}^0 d\mu\left(\frac{e^{-\Sigma_{ti}(x-x')/\mu}}{\mu}\right) \\
&= (s_i^+ + s_i^-)\left\{1 - \frac{1}{\Delta_i\Sigma_{ti}}\left[\tfrac{1}{2} - E_3(\Sigma_{ti}\Delta_i)\right]\right\} \equiv s_i(1-P_{oi}).
\end{aligned}
\tag{14}
$$

As before, treating the fraction c_i of these particles that undergo scattering collisions as an isotropic source of once-collided particles, the emergent currents of once-collided source particles are given by

$$
\begin{aligned}
J_{1s}^+(x_{i+1}) &= \int_0^1 d\mu\ \mu\int_{x_i}^{x_{i+1}} dx\,\tfrac{1}{2}c_i\ \frac{A_{i1,s}}{\Delta_i}\left(\frac{e^{-\Sigma_{ti}(x_{i+1}-x)/\mu}}{\mu}\right) \\
&= \tfrac{1}{2}c_i A_{i1,s}P_{oi} = \tfrac{1}{2}c_s s_i(1-P_{oi})P_{oi}, \\
J_{1s}^-(x_i) &= \int_{-1}^0 d\mu\ \mu\int_{x_i}^{x_{i+1}} dx\,\tfrac{1}{2}c_i\ \frac{A_{i1,s}}{\Delta_i}\left(\frac{e^{\Sigma_{ti}(x-x_i)/\mu}}{\mu}\right) \\
&= \tfrac{1}{2}c_i A_{i1,s}P_{oi} = \tfrac{1}{2}c_i s_i(1-P_{oi})P_{oi}.
\end{aligned}
\tag{15}
$$

Continuing in this fashion, the general expression for the nth collision rate of source particles in Δ_i is

$$
A_{in,s} = c_i^{n-1}s_i(1-P_{oi})^n \tag{16}
$$

and the general expressions for the emergent currents of n-collided source particles are

$$
J_{ns}^+(x_{i+1}) = J_{ns}^-(x_i) = \tfrac{1}{2}s_i P_{oi}c_i^n(1-P_{oi})^n. \tag{17}
$$

The total collision rate of source particles within Δ_i is

$$
A_{i,s} = \sum_{n=1}^{\infty} A_{in,s} = \frac{s_i(1-P_{oi})}{1-c_i(1-P_{oi})} \tag{18}
$$

and the total emergent currents due to an anisotropic particle source within Δ_i are obtained by summing Eq. (17) and adding Eqs. (13)

$$
\begin{aligned}
J_s^+(x_{i+1}) &= (s_i^+ - \tfrac{1}{2}s_i)P_{oi} + \frac{\tfrac{1}{2}s_i P_{oi}}{1-c_i(1-P_{oi})}, \\
J_s^-(x_i) &= (s_i^- - \tfrac{1}{2}s_i)P_{oi} + \frac{\tfrac{1}{2}s_i P_{oi}}{1-c_i(1-P_{oi})}.
\end{aligned}
\tag{19}
$$

IV. TOTAL REACTION RATES AND EMERGENT CURRENTS

The total reaction rate in Δ_i due to incident currents and to internal sources is obtained by adding Eqs. (11) and (18)

$$
A_i = \frac{(J_i^+ + J_{i+1}^-)(1-T_{oi}) + s_i(1-P_{oi})}{1-c_i(1-P_{oi})}, \tag{20}
$$

where the first-flight, or uncollided, transmission probability has been identified

$$
T_{oi} \equiv E_2(\Delta_i\Sigma_{ti}). \tag{21}
$$

Further identifying the total escape probability

$$
P_i \equiv P_{oi}\sum_{n=0}^{\infty}[c_i(1-P_{oi})]^n = \frac{P_{oi}}{1-c_i(1-P_{oi})} \tag{22}
$$

the total reflection probability

$$
R_i \equiv \frac{\tfrac{1}{2}c_i P_{oi}[1-E_2(\Delta_i\Sigma_{ti})]}{1-c_i(1-P_{oi})} = \tfrac{1}{2}c_i P_i(1-T_{oi}) \tag{23}
$$

and the total transmission probability

$$
T_i = T_{oi} + R_i = T_{oi} + \tfrac{1}{2}c_i P_i(1-T_{oi}). \tag{24}
$$

Equations (12) and (19) can be summed to obtain expressions for the total emergent currents due to incident currents and internal particle sources

$$
\begin{aligned}
J_{i+1}^+ &= T_i J_i^+ + R_i J_{i+1}^- + \tfrac{1}{2}s_i P_i + (s_i^+ - \tfrac{1}{2}s_i)P_{oi}, \\
J_i^- &= T_i J_{i+1}^- + R_i J_i^+ + \tfrac{1}{2}s_i P_i + (s_i^- - \tfrac{1}{2}s_i)P_{oi}.
\end{aligned}
\tag{25}
$$

The inherent advantage of an ICB formulation of integral transport theory is evident from Eqs. (25). In order to solve for the currents across interface i, one needs only the currents at interface $i+1$ and the source in the intervening region. By contrast, in the standard integral transport formulation, the fluxes in all other regions in the problem and the transition probabilities from these regions to the region in question are needed in order to solve for the flux in a given region. In both formulations, an iterative solution is needed, but each iteration should be much quicker with the ICB formulation.

It is informative to sum Eqs. (25) to obtain an intuitively obvious balance between incident and emergent currents and internal sources

$$
(J_{i+1}^+ + J_i^-) = (T_i + R_i)(J_i^+ + J_{i+1}^-) + s_i P_i
$$

or

$$
J_{\text{out}} = (T_{oi} + (1-T_{oi})c_i P_i)J_{\text{in}} + s_i P_i. \tag{26}
$$

V. BOUNDARY CONDITIONS

Boundary conditions take on a particularly simple form for an interface current formulation of integral transport. Let $x=0$, $i=0$ represent the leftmost surface of the transport medium. If a vacuum or nonscattering medium with no particle source exists for $x<0$, then $J_0^+=0$ is the appropriate boundary condition. If, on the other hand, a source-free scattering medium exists for $x<0$, an albedo or reflection condition of the form $J_0^+=\alpha J_0^-$, where α is the reflection coefficient or albedo, is appropriate. Finally, if a known current of particles Γ_{in} is incident upon the medium from the left at $x=0$, the appropriate boundary condition is $J_0^+=\Gamma_{\text{in}}$.

VI. RESPONSE MATRIX FORMULATION

Solving the first of Eqs. (25) for J_i^+ and using the result in the second equation leads to a matrix relation between the currents at adjacent surfaces

$$\begin{bmatrix} J_i^+ \\ J_i^- \end{bmatrix} = \begin{bmatrix} (T_i^{-1}) & (-T_i^{-1}R_i) \\ (R_iT_i^{-1}) & (T_i-R_iT_i^{-1}R_i) \end{bmatrix} \begin{bmatrix} J_{i+1}^+ \\ J_{i+1}^- \end{bmatrix} + \tfrac{1}{2}s_i\left\{ P_i \begin{bmatrix} -T_i^{-1} \\ 1-R_iT_i^{-1} \end{bmatrix} + P_{oi}\begin{bmatrix} -T_i^{-1}(s_i^+-\frac{1}{2}s_i) \\ (s_i^- -\frac{1}{2}s_i)-R_iT_i^{-1}(s_i^+-\frac{1}{2}s_i) \end{bmatrix}\right\}. \tag{27}$$

Equation (27) has the form of the response matrix formalism[1,2] of neutron transport theory, which is well suited for numerical evaluation by simply marching from one boundary of the problem to the other.

VII. ENERGY DEPENDENCE

A. Component summation method

Integral transport in general, and the ICB formulation in particular, provides a natural methodology for calculating the energy dependence of the flux or current in a given region or at a given interface by summing over the contributions to that flux or current from the different regions of the problem. Again, the ICB formulation has some inherent computational advantages because only the region in question and those next to it must be considered in the sum.

We rewrite the first of Eqs. (25) in a form that now reflects the different energy dependence of currents incident from the left and right and the corresponding differences in cross sections and hence in the parameters of the model

$$\overline{J_{i+1}^+}\psi_{i+1}^+(E) = T_{oi}^i\overline{J_i^+}\psi_i^+(E)+\overline{s_i^+}\chi_i^s(E)P_{oi}^s+[\tfrac{1}{2}(1-T_{oi}^i)\times\overline{J_i^+}c_i^iP_{oi}^i+\tfrac{1}{2}(1-T_{oi}^{i+1})\overline{J_{i+1}^-}c_i^{i+1}P_{oi}^{i+1}+\tfrac{1}{2}\overline{s_i}\overline{c_i^c}(1-P_{oi}^c)]\,\frac{\chi_i^c(E)}{1-c_i^c(1-P_{oi}^c)}. \tag{28}$$

In this equation, $\psi_i^+(E)$ is the energy distribution of $J_i^+(E)$, $\chi_i^s(E)$ is the energy distribution of the source $s_i(E)$ within Δ_i, and $\chi_i^c(E)$ is the energy distribution taken on by either incident or source particles as a result of scattering collisions within Δ_i, all normalized to integrate over energy to unity. The overbar indicates the average over energy, i.e., the total value, of the quantity. The superscripts i and $i+1$ on T_{0i}, P_{0i}, and c_i indicate that these quantities are to be evaluated with cross sections averaged over the incident current spectra $\psi_i^+(E)$ and $\psi_{i+1}^+(E)$, respectively; the superscript s indicates that the corresponding quantity is to be evaluated with cross sections averaged over $\chi_i^s(E)$; and the superscript c indicates that the corresponding quantity is to be evaluated with cross sections averaged over $\chi_i^c(E)$.

Integrating Eq. (28) over energy yields the equation for the total emergent current

$$\overline{J_{i+1}^+}=T_{oi}^i\overline{J_i^+}+\overline{s_i^+}P_{oi}^s+\left[\frac{\frac{1}{2}(1-T_{oi}^i)\overline{J_i^+}c_i^iP_{oi}^i+\frac{1}{2}(1-T_{oi}^{i+1})\overline{J_{i+1}^-}c_i^{i+1}P_{oi}^{i+1}+\frac{1}{2}\overline{s_i}\overline{c_i^c}(1-P_{oi}^c)}{1-c_i^c(1-P_{oi}^c)}\right] \tag{29}$$

and dividing Eq. (28) through by $\overline{J_{i+1}^+}$ yields the equation for the spectrum of the emergent current at $i+1$

$$\psi_{i+1}^+(E)=T_{oi}^i\,\frac{\overline{J_i^+}}{\overline{J_{i+1}^+}}\,\psi_i^+(E)+\overline{s_i^+}\,\frac{P_{oi}^s}{\overline{J_{i+1}^+}}\,\chi_i^s(E)+\chi_i^c(E)\left[\frac{\frac{1}{2}(1-T_{oi}^i)\overline{J_i^+}c_i^iP_{oi}^i+\frac{1}{2}(1-T_{oi}^{i+1})\overline{J_{i+1}^-}c_i^{i+1}P_{oi}^{i+1}+\frac{1}{2}\overline{s_i}\overline{c_i^c}(1-P_{oi}^c)}{\overline{J_{i+1}^+}[1-c_i^c(1-P_{oi}^c)]}\right]. \tag{30}$$

The second of Eqs. (25) can be similarly recast.

This component summation method should be able to provide an accurate energy dependence of the neutral particle currents, in principle. In practice, it is necessary to calculate the energy distribution, $\chi_i^c(E)$, taken on by incident and source particles as a result of scattering collisions within Δ_i. If these scattering collisions are sufficient to bring the neutral particle distribution into equilibrium, then $\chi_i^c(E)$ can be readily determined. We next consider a method that can be used when local equilibration is not a good approximation.

B. Multigroup method

If the energy interval $0\leqslant E\leqslant\infty$ is subdivided into G subintervals, or groups, and the neutral particle reaction rates are integrated over each group g within $E_g \leqslant E \leqslant E_{g-1}$, effective total cross sections $\Sigma_{\rm tot}^g$ may be defined for each group and effective group-to-group ''scattering'' transfer cross sections $\Sigma_{\rm sc}^{gg'}$ can be defined. The choice of group structure is usually dictated by the physics, but may be made as detailed as required to obtain an adequate approximation to the energy dependence.

A pair of Eqs. (25) can be written for each group. The approximate value of c_i^g is now defined in terms of the fraction of collisions which do not remove a neutral from group g

$$c_i^g = \Sigma_c^{gg} / \Sigma_{\rm tot}^g . \tag{31}$$

The current balance equations for the different groups are coupled through the scattering transfer of particles between groups, which can be represented as a scattering source $S_{i,\rm sc}^{g'g}$, so that the total source to group g may be written

$$S_i^g = S_{i,\rm true}^g + \sum_{g' \neq g} S_{i,\rm sc}^{g'g} , \tag{32}$$

where $S_{i,\rm true}^g$ is the ''true'' source of new particles introduced into group g by some ''external'' means.

Detailed definitions of the parameters in the multigroup method will be presented in Sec. IX.

VIII. EXTENSION TO MULTIDIMENSION

The ICB formulation of integral transport theory can be extended to two and three dimensions. First, for conceptual purposes, we make the identification $J_i^+ = J_i^{\rm in}$, $J_i^- = J_i^{\rm out}$, $J_{i+1}^+ = J_{i+1}^{\rm out}$, $J_{i+1}^- = J_{i+1}^{\rm in}$ and

$$\begin{aligned} \Lambda_{i+1}^s s_i P_i &\equiv \tfrac{1}{2} s_i P_i + (s_i^+ - \tfrac{1}{2} s_i) P_{oi} , \\ \Lambda_i^s s_i P_i &\equiv \tfrac{1}{2} s_i P_i + (s_i^- - \tfrac{1}{2} s_i) P_{oi} , \end{aligned} \tag{33}$$

where Λ_i^s is the fraction of escaping source particles which escapes to the left across surface i and Λ_{i+1}^s is the fraction escaping to the right across surface $i+1$. Then, using Eqs. (20)–(24), Eqs. (25) may be rewritten

$$\begin{aligned} J_{i+1}^{\rm out} &= T_{oi} J_i^{\rm in} + (1 - T_{oi})(J_i^{\rm in} + J_{i+1}^{\rm in}) c_i P_i \Lambda_{i+1} \\ &\quad + \Lambda_{i+1}^s s_i P_i , \\ J_i^{\rm out} &= T_{oi} J_{i+1}^{\rm in} + (1 - T_{oi})(J_i^{\rm in} + J_{i+1}^{\rm in}) c_i P_i \Lambda_i + \Lambda_i^s s_i P_i , \end{aligned} \tag{34}$$

where $\Lambda_i = \Lambda_{i+1} = 1/2$ is the fraction of the escaping scattered incident particles which escape across surfaces i and $i+1$, respectively.

In this form, the terms in Eqs. (34) for the emergent currents have a direct physical interpretation which leads immediately to a generalization to multidimension. The outward current across surface $i+1$ consists of three terms: (1) the inward current across surface i times the probability T_{oi} that it is transmitted across region i without collision to surface $i+1$; (2) the inward currents across all surfaces times the probability $(1 - T_{oi})$ that these currents are not transmitted across region i without collision, times the probability c_i that the first collision is a scattering event, times the probability P_i that the scattered particles subsequently escape from region i, times the probability Λ_{i+1} that escaping particles escape across surface $i+1$; and (3) the total particle source s_i in region i times the probability P_i that these particles will escape from region i, times the probability Λ_{i+1}^s that escaping source particles escape across surface $i+1$. Note that Λ_{i+1} and Λ_{i+1}^s can differ because an anisotropic source is allowed, i.e., $\Lambda_{i+1} = 1/2$ and Λ_{i+1}^s is given by Eq. (33) for slab geometry.

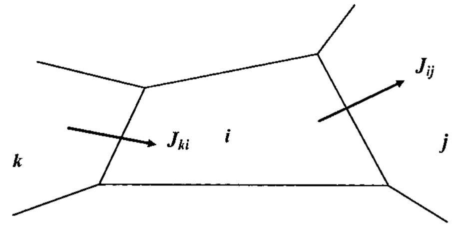

FIG. 2. Two-dimensional geometry configuration.

Generalization to multidimension is straightforward in principle. Consider the two-dimensional (2D) configuration in Fig. 2. The current from region k into region i is denoted J_{ki}, the probability that the current entering region i from region k is transmitted across region i without collision to contribute to the current from region i into region j is denoted T_{0i}^{kj}, and the probability that a particle escaping from region i escapes into region j is denoted Λ_{ij}. The generalization of Eqs. (34) to 2D is then

$$J_{ij} = \sum_k^i T_{oi}^{kj} J_{ki} + \sum_k^i \left(1 - \sum_l^i T_{oi}^{kl} \right) J_{ki} c_i P_i \Lambda_{ij} + \Lambda_{ij}^s s_i P_i , \tag{35}$$

where the summation Σ_k^i is over all regions k that are contiguous to region i. The three terms in Eq. (35) correspond physically to: (1) the sum of the currents incident into region i from all contiguous regions times the probability that each is transmitted across region i without collision to exit into region j (note that the possibility of concave surfaces is allowed by including uncollided transmission from region j across region i back into region j); (2) the sum of the currents incident into region i from all contiguous regions times the probability that each is not transmitted without collision across region i to any of the contiguous regions, times the probability that the first collision is a scattering event, times the probability that the scattered particle eventually escapes from region i into region j; and (3) the source of particles in region i times the probability that a source particle in region i eventually escapes into region j. Equation (35) is identical to the equation previously derived[5] purely from these same physical considerations for a 2D model; the present derivation now provides a more rigorous theoretical basis.

Thus, extension of the ICB formulation of integral transport theory to 2D [and three dimensions (3D)] is formally straightforward. Practically, one must calculate the first flight transmission probabilities T_{0i}^{kj} and the first flight escape probabilities P_{0i}. Calculation of the former is straightforward analytically for regular geometries[5] and may readily be done by numerical integration for any geometry. Analytical expressions for P_{0i} exist only for slabs, spheres, cylinders, and other regular geometries,[6] but a useful approximate form is given by[5]

$$P_{oi} \simeq \frac{1}{1+4V_i\Sigma_{ti}/S_i}, \tag{36}$$

where V_i and S_i are the area (volume) and bounding surface perimeter (area) of region i in a 2D (3D) configuration. Since P_{0i} is the average first flight escape probability for a uniform distribution of particle sources over region i, it may readily be calculated by Monte Carlo methods for irregular geometries. Once the geometry is fixed, these first flight transmission and escape probabilities depend only on the total cross section in region i and hence may be precomputed as a function of total cross section for later table lookup.

IX. SPECIALIZATION TO NEUTRAL ATOM TRANSPORT IN THE PLASMA EDGE

A. Component summation method

The total cross section for neutral atoms in the plasma edge can be written

$$\Sigma_t = N_i\left[\frac{Ne}{N_i}\langle\sigma_{\rm ion}\rangle + \langle\sigma_{\rm cx}\rangle + \langle\sigma_{\rm el}\rangle\right] + N_n\langle\sigma_{\rm eln}\rangle, \tag{37}$$

where N_i, N_e, and N_n are the ion, electron, and atom densities and

$$\langle\sigma_{\rm ion}\rangle \equiv \frac{\int_0^\infty dE_n\, f_n(E_n)\int_0^\infty dE_e\, f_e(E_e)|v_e-v_n|\sigma_{\rm ion}(v_e-v_n)}{[\int_0^\infty dE_n\, f_n(E_n)v_n(E_n)][\int_0^\infty dE_e\, f_e(E_e)]}, \tag{38a}$$

$$\langle\sigma_{\rm cx}\rangle \equiv \frac{\int_0^\infty dE_n\, f_n(E_n)\int_0^\infty dE_i\, f_i(E_i)|v_i-v_n|\sigma_{\rm cx}(v_i-v_n)}{[\int_0^\infty dE_n\, f_n(E_n)v_n(E_n)][\int_0^\infty dE_i\, f_i(E_i)]}, \tag{38b}$$

$$\langle\sigma_{\rm el}\rangle \equiv \frac{\int_0^\infty dE_n\, f_n(E_n)\int_0^\infty dE_i\, f_i(E_i)|v_i-v_n|\sigma_{\rm el}(v_i-v_n)}{[\int_0^\infty dE_n\, f_n(E_n)v_n(E_n)][\int_0^\infty dE_i\, f_i(E_i)]}, \tag{38c}$$

$$\langle\sigma_{\rm eln}\rangle \equiv \frac{\int_0^\infty dE_n\, f_n(E_n)\int_0^\infty dE_n'\, f_n(E_n')|v_n'-v_n|\sigma_{\rm eln}(v_n'-v_n)}{[\int_0^\infty dE_n\, f_n(E_n)v_n(E_n)][\int_0^\infty dE_n'\, f_n(E_n')]}, \tag{38d}$$

where f is a distribution function, v is the velocity, E is the energy and the n, i, e subscripts refer to neutral atoms, ions, and electrons, respectively. The quantity $\sigma_{\rm ion}$ is the electron-impact ionization cross section; the definition can be extended in an obvious way to include also ion-impact ionization. The quantities $\sigma_{\rm cx}$ and $\sigma_{\rm el}$ are the neutral-ion charge exchange and elastic scattering cross sections, and $\sigma_{\rm eln}$ is the neutral–neutral scattering cross section.

The scattering probability is

$$c_i \equiv \{N_i[\langle\sigma_{\rm cx}\rangle + \langle\sigma_{\rm el}\rangle] + N_n\langle\sigma_{\rm eln}\rangle\}_i/\Sigma_{ti}. \tag{39}$$

The source term is

$$s_i = \int_{x_i}^{x_{i+1}} dx\left[s_{\rm ext} + \int_0^\infty dE_i\, f_i(E_i)\int_0^\infty dE_e\, f_e(E_e) \times |v_e-v_i|\sigma_{\rm rec}(v_i-v_e)\right], \tag{40}$$

where $\sigma_{\rm rec}$ is the recombination cross section and $s_{\rm ex}$ is any external source (e.g., pellet fueling, molecular dissociation). Equation (40) is written for two-body recombination processes. It can be extended to handle three-body processes by appropriate modification of the energy integral term.

If the charge exchange is highly anisotropic (e.g., plasma ions flowing towards the divertor plate with near sonic average speed will produce neutrals directed predominantly towards the divertor plate[8]), this anisotropy can be incorporated by treating charge exchange as a removal plus an anisotropic source. The energy spectra χ^s associated with the components of the source are the calculated energy spectrum of atoms ablating from a pellet, the Franck–Condon energy for atoms formed by molecular dissociation, and the local ion energy distribution for atoms formed from ions by recombination and charge exchange.

The energy spectra $\psi_w(E)$ associated with the current of neutral atoms reflected from a wall at one boundary of the transport problem would be taken from wall reflection data (e.g., as discussed in Ref. 8). The energy spectrum $\psi_b(E)$ associated with the current ''reflected'' (albedo condition) from the plasma at the other boundary of the neutral atom transport problem would be taken as the energy spectrum of the plasma ions at that location.

B. Multigroup method

For the multigroup energy treatment, the above results are generalized by writing

$$\Sigma_t^g \equiv N_e\langle\sigma_{\rm ion}\rangle^g + N_i\sum_{g'=1}^{G}\{\langle\sigma_{\rm cx}\rangle^{gg'} + \langle\sigma_{\rm el}\rangle^{gg'}\} + \sum_{g''=1}^{G} N_n^{g''}\sum_{g'=1}^{G}\langle\sigma_{\rm eln}\rangle_{g''}^{gg'}, \tag{41}$$

where

$$N_n^g \equiv \int_{Eg}^{Eg-1} dE_n\, f_n(E_n) \tag{42}$$

is the particle density of the neutral species with energy in the group $E_g \leqslant E_n \leqslant E_{g-1}$, and

$$\langle \sigma_{\rm ion}\rangle^{g} \equiv \frac{\int_{E_g}^{E_{g-1}} dE_n\ f_n(E_n) \int_0^\infty dE_e\ f_e(E_e) |v_e - v_n| \sigma_{\rm ion}(v_e - v_n)}{[\int_{E_g}^{E_{g-1}} dE_n\ f_n(E_n) v_n(E_n)][\int_0^\infty dE_e\ f_e(E_e)]}, \tag{43a}$$

$$\langle \sigma_{\rm cx}\rangle^{gg'} \equiv \frac{\int_{E_g}^{E_{g-1}} dE_n\ f_n(E_n) \int_{Eg'}^{Eg'-1} dE_i\ f_i(E_i) |v_i - v_n| \sigma_{\rm cx}(v_i - v_n)}{[\int_{E_g}^{E_{g-1}} dE_n\ f_n(E_n) v_n(E_n)][\int_0^\infty dE_i\ f_i(E_i)]}, \tag{43b}$$

$$\langle \sigma_{\rm el}\rangle^{gg'} \equiv \frac{\int_{E_g}^{E_{g-1}} dE_n\ f_n(E_n) \int_0^\infty dE_i\ f_i(E_i) |v_i - v_n| \sigma_{\rm el}(v_i - v_n) \int_{Eg'}^{Eg'-1} dE_n'\ P_{\rm el}(E_i, E_n \to E_n')}{[\int_{E_g}^{E_{g-1}} dE_n\ f_n(E_n) v_n(E_n)][\int_0^\infty dE_i\ f_i(E_i)]}, \tag{43c}$$

$$\langle \sigma_{\rm eln}\rangle^{gg'}_{g''} \equiv \frac{\int_{E_g}^{E_{g-1}} dE_n\ f_n(E_n) \int_{Eg''}^{Eg''-1} dE_n''\ f_n(E_n'') |v_n'' - v_n| \sigma_{\rm eln}(v_n'' - v_n) \int_{Eg'}^{Eg'-1} dE_n'\ P_{\rm eln}(E_n'', E_n \to E_n')}{[\int_{E_g}^{E_{g-1}} dE_n\ f_n(E_n) v_n(E_n)][\int_{Eg''}^{Eg''-1} dE_n''\ f_n(E_n'')]}, \tag{43d}$$

where $P_{\rm el}(E_i, E_n \to E_n')$ is the probability that a neutral atom of energy E_n upon scattering from an ion of energy E_i will have a final energy E_n', and $P_{\rm eln}(E_n'', E_n \to E_n')$ is similarly defined for scattering from a neutral atom of energy E_n''.

We define the average group speed

$$\langle v_n\rangle^{g} \equiv \frac{\int_{E_g}^{E_{g-1}} dE_n\ v_n(E_n) f_n(E_n)}{\int_{E_g}^{E_{g-1}} dE_n\ f_n(E_n)}. \tag{44}$$

The definitions of Eqs. (42)–(44) are such that $N_n^g \langle v_n\rangle^g N_{i,e,n} \langle \sigma_x\rangle^{gg'}$ preserves the corresponding x-reaction rate—the numerator on the right side of Eqs. (43)—when the actual neutral and ion/electron/neutral distribution functions are used to evaluate Eqs. (43). The exact distribution functions are, of course, not known; however it should be possible to make reasonable approximations to the distribution functions for the purpose of evaluating Eqs. (43) and (44).

The scattering probability, c^g, for each group equation is given by

$$c^g = \frac{N_i\{\langle \sigma_{\rm cx}\rangle^{gg} + \langle \sigma_{\rm el}\rangle^{gg}\} + \Sigma_{g''=1}^{G} N_n^{g''} \langle \sigma_{\rm eln}\rangle^{gg}_{g''}}{\Sigma_t^g}, \tag{45}$$

i.e., the probability that the collision event results in a neutral particle in group g.

The appropriate source term for each group in each region is

$$s_i^g = s_{i,\rm ext}^g + s_{i,\rm rec}^g + s_{i,\rm sc}^g, \tag{46}$$

where

$$s_{i,\rm ext}^g \equiv \int_{x_i}^{x_{i+1}} dx \int_{E_g}^{E_{g-1}} dE_n\ s_{\rm ext}(x, E_n) \tag{47}$$

is the external fueling (pellet, neutral beam) source

$$s_{i,\rm rec}^g \equiv \int_{x_i}^{x_{i+1}} dx \int_{E_g}^{E_{g-1}} dE_i\ f_i(E_i) \times \int_0^\infty dE_e\ f_e(E_e) |v_e - v_i| \sigma_{\rm rec}(v_e - v_i) \tag{48}$$

is the recombination source, and

$$s_{i,\rm sc}^g \equiv \int_{x_i}^{x_{i+1}} dx \sum_{g' \neq g} \langle v_n\rangle^{g'} N_n^{g'} \Bigg[N_i\{\langle \sigma_{\rm cx}\rangle^{g'g} + \langle \sigma_{\rm el}\rangle^{g'g}\} + \sum_{g''=1}^{G} N_n^{g''} \langle \sigma_{\rm eln}\rangle^{g'g}_{g''} \Bigg] \tag{49}$$

is the scattering source.

The multigroup version of Eqs. (25) then becomes

$$\begin{aligned} J_{i+1}^{+g} &= T_i^g J_i^{+g} + R_i^g J_{i+1}^{-g} + \tfrac{1}{2} s_i^g P_i^g + (s_i^{+g} - \tfrac{1}{2} s_i^g) P_{oi}^g \\ J_i^{-g} &= T_i^g J_{i+1}^{-g} + R_i^g J_i^{+g} + \tfrac{1}{2} s_i^g P_i^g + (s_i^{-g} - \tfrac{1}{2} s_i^g) P_{oi}^g, \\ g &= 1, \ldots, G, \end{aligned} \tag{50}$$

where the source, s_i^g, is given by Eqs. (46)–(49) and

$$R_i^g = \tfrac{1}{2} c_i^g P_i^g (1 - T_{oi}^g), \tag{51}$$

$$T_{oi}^g = E_2(\Delta_i \Sigma_{ti}^g), \tag{52}$$

$$P_{oi}^g = \frac{1}{\Delta_i \Sigma_{ti}^g} [\tfrac{1}{2} - E_3(\Delta_i \Sigma_{ti}^g)], \tag{53}$$

$$P_i^g = \frac{P_{oi}^g}{1 - c_i^g (1 - P_{oi}^g)}, \tag{54}$$

$$T_i^g = T_{oi}^g + R_i^g \tag{55}$$

with Σ_{ti}^g given by Eq. (41).

The response matrix formulation of Eqs. (27) generalizes immediately to multigroup by replacing the currents and sources with multigroup column vectors, i.e.,

$$J_i^+ \to \mathbf{J}_i^+ \equiv \begin{bmatrix} J_i^{+1} \\ \vdots \\ J_i^{+g} \\ \vdots \\ J_i^{+G} \end{bmatrix}, \tag{56}$$

$$s_i P_i \to \mathbf{SP}_i \equiv \begin{bmatrix} s_i^1 P_i^1 \\ \vdots \\ s_i^g P_i^g \\ \vdots \\ s_i^G P_i^G \end{bmatrix} \tag{57}$$

and replacing the transmission and reflection coefficients with diagonal multigroup matrices, i.e.,

$$T_i \to \mathbf{T}_i \equiv \begin{bmatrix} T_i^1 & 0 & \cdots & & & 0 \\ 0 & T_i^2 & 0 & & \cdots & \vdots \\ \vdots & & \ddots & & & \\ \vdots & & 0 & T_i^g & 0 & \\ & & & & \ddots & \vdots \\ 0 & \cdots & & & \cdots & T_i^G \end{bmatrix}. \tag{58}$$

The proper choice of group structure and within-group weighting function, $f_n(E)$, for evaluating the ''group constants'' of Eq. (43) must be guided by the physics. Energy ranges over which important cross sections change rapidly (e.g., low eV range for ionization and recombination) should be represented by several groups, while a large energy range over which the important cross sections vary slowly can probably be represented by a single group. For sufficiently fine energy groups, a uniform weighting may suffice, while choosing $f_n(E)$ as a Maxwellian at the local background plasma temperature may be a better choice for broader energy groups. Numerical experimentation is required to investigate the choice of group structure and weighting function.

X. ANISOTROPY

A certain degree of isotropy has been assumed in the preceding development. The neutral particle flux has been assumed to be isotropic in the forward $(+)$ directional hemisphere and to be isotropic in the background $(-)$ directional hemisphere; i.e., any direction in the forward hemisphere is equally probable and any direction in the backward hemisphere is equally probable, but the probability for a direction in the forward hemisphere is different than the probability for a direction in the backward hemisphere. These forward and backward probabilities are related to J^+ and J^-

$$\psi(x,\mu) = \begin{cases} 2J^+(x), & 0<\mu<1, \\ 2J^-(x), & -1<\mu<0, \end{cases} \tag{59}$$

where μ is the cosine of the angle with respect to the positive axis.

Since the Legendre polynomials, $P_l(\mu)$, constitute a complete set on the interval $-1 \leqslant \mu \leqslant 1$, the half-range Legendre polynomials[8]

$$\begin{aligned} p_l^+(\mu) &\equiv P_l(2\mu-1), \\ p_l^-(\mu) &\equiv P_l(2\mu+1), \end{aligned} \tag{60}$$

constitute complete sets on the intervals $0 \leqslant \mu \leqslant 1$ and $-1 \leqslant \mu \leqslant 0$, respectively. Thus, we can expand

$$\begin{aligned} \psi(x,\mu) &= \sum_{l=0}^{L} (2l+1)\psi_l(x) p_{(l)}^+(\mu), \quad 0<\mu<1, \\ &= \sum_{l=0}^{L} (2l+1)\psi_l(x) p_{(l)}^-(\mu), \quad -1<\mu<0, \end{aligned} \tag{61}$$

with the assurance that the expansion could exactly represent any angular flux distribution in the limit $L \to \infty$. The approximation used in the preceding derivation corresponds to terminating the summation after the first term $(L=0)$. The calculation can obviously be extended to handle higher degrees of anisotropy by retaining $l>0$ terms, at the price of increased complexity. In an essentially one-dimensional (1D) configuration, the only phenomenon which could produce $l>0$ components of the angular distribution is the injection (reflection from the wall) of neutral atoms with a distribution which contained $l>0$ components. However, scattering would be expected to quickly isotropize the injected distribution. Thus, the $L=0$ approximation should be valid for essentially 1D configurations, and certainly is valid for a 1D model which can only represent 1D configurations. The issue becomes more complicated for multidimensional configurations.

Isotropic elastic scattering and charge exchange in the laboratory system have also been assumed in the preceding derivation by the assumption that 1/2 of the neutral particles resulting from such an event are directed forward $(+)$ and 1/2 directed backward $(-)$. If these events are highly anisotropic, as would be the case at least for charge exchange with ions flowing towards the plate with sonic average speeds,[8] there are ways to incorporate scattering anisotropy into the calculational model. The scattering or charge-exchange event may be treated as a particle loss event coupled with an anisotropic particle source event, or the assumption of 1/2 of the particles going in each the forward and backward directions may be removed. We will develop the latter option.

Let $f_{+/-}$ be the fraction of neutral particles emerging from a charge-exchange or scattering event going in the same direction $(+/-)$ as the incident particle. In the case of neutral particles interacting with a near sonic plasma flow, f_+ and f_- will be different.[8] The average scattering sources of once-collided incident neutral particles per unit length within $x_i \leqslant x \leqslant x_{i+1}$ emerging in the forward $(+)$ direction and the backward $(-)$ direction are

$$\begin{aligned} \hat{S}_{i1}^+ &\equiv \frac{c_i}{\Delta_i}\{f_+[J_i^+ - \hat{J}_{un}^+(x_{i+1})] + (1-f_-) \\ &\quad \times [J_{i+1}^-(x_i) - \hat{J}_{un}^-(x_i)]\} \\ &= \frac{c_i}{\Delta_i}[f_+ J_i^+ + (1-f_-)J_{i+1}^-][1 - E_2(\Delta_i \Sigma_{ti})], \end{aligned} \tag{62}$$

$$\hat{S}_{i1}^- = \frac{c_i}{\Delta_i}[(1-f_+)J_i^+ + f_- J_{i+1}^-][1 - E_2(\Delta_i \Sigma_{ti})].$$

The emergent currents of once-collided neutral particles resulting from incident currents are

$$\hat{J}_1^+(x_{i+1}) \equiv \int_{x_i}^{x_{i+1}} dx \int_0^1 d\mu (\hat{S}_{i1}^+) \left(\frac{e^{-\Sigma_{ti}(x_{i+1}-x)/\mu}}{\mu} \right) \mu$$

$$= c_i[f_+ J_i^+ + (1-f_-)\hat{J}_{i+1}] P_{oi}[1 - E_2(\Sigma_{ti}\Delta_i)], \quad (63)$$

$$\hat{J}_1^-(x_i) = c_i[(1-f_+)J_i^+ + f_- J_{i+1}^-] P_{oi}[1 - E_2(\Sigma_{ti}\Delta_i)].$$

Equations (63) generalize Eqs. (5), to which they reduce when $f_{+/-} = 1/2$.

The average scattering sources of twice-collided incident neutral particles per unit length within $x_i \leq x \leq x_{i+1}$ in the forward (+) and the backward (−) directions are

$$\hat{S}_{i2}^+ = f_+ \frac{c_i}{\Delta_i} \Sigma_{ti} \int_0^1 d\mu \int_{x_i}^{x_{i+1}} dx' \int_{x'}^{x_{i+1}} dx\ \hat{S}_{i1}^+(x') \times \left(\frac{e^{-\Sigma_{ti}(x-x')/\mu}}{\mu} \right) + (1-f_-) \frac{c_i}{\Delta_i} \Sigma_{ti} \int_{-1}^0 d\mu \int_{x_i}^{x_{i+1}} dx' \times \int_{x_i}^{x'} dx\ \hat{S}_{i1}^-(x') \left(\frac{e^{-\Sigma_{ti}(x-x')/\mu}}{\mu} \right)$$

$$= [\hat{S}_{i1}^+ f_+ + \hat{S}_{i1}^-(1-f_-)] c_i (1 - P_{oi}), \quad (64)$$

$$\hat{S}_{i2}^- = (1-f_+) \frac{c_i}{\Delta_i} \Sigma_{ti} \int_0^1 d\mu \int_{x_i}^{x_{i+1}} dx' \int_{x'}^{x_{i+1}} dx\ \hat{S}_{i1}^+(x') \times \left(\frac{e^{-\Sigma_{ti}(x-x')/\mu}}{\mu} \right) + f_- \frac{c_i}{\Delta_i} \Sigma_{ti} \int_{-1}^0 d\mu \int_{x_i}^{x_{i+1}} dx' \times \int_{x_i}^{x'} dx\ \hat{S}_{i1}^-(x') \left(\frac{e^{-\Sigma_{ti}(x-x')/\mu}}{\mu} \right),$$

$$= [\hat{S}_{i1}^+(1-f_+) + \hat{S}_{i1}^- f_-] c_i (1 - P_{oi}).$$

In general, the scattering source of nth-collided incident neutral particles per unit length within $x_i \leq x \leq x_{i+1}$ in the forward (+) and backward (−) directions are

$$\hat{S}_{\mathrm{in}}^+ = [\hat{S}_{\mathrm{in}-1}^+ f_+ + \hat{S}_{\mathrm{in}-1}^-(1-f_-)] c_i (1 - P_{oi}),$$
$$\hat{S}_{\mathrm{in}}^- = [\hat{S}_{\mathrm{in}-1}^+(1-f_+) + \hat{S}_{\mathrm{in}-1}^- f_-] c_i (1 - P_{oi}), \quad \mathbf{n} \geq 2. \quad (65)$$

The emergent currents of n-collided incident neutral particles are

$$\hat{J}_n^+(x_{i+1}) = \int_{x_i}^{x_{i+1}} dx \int_0^1 d\mu \hat{S}_{\mathrm{in}}^+(x) \left(\frac{e^{-\Sigma_{ti}(x_{i+1}-x)/\mu}}{\mu} \right) \mu$$

$$= \hat{S}_{\mathrm{in}}^+ \Delta_i P_{oi}, \quad (66)$$

$$\hat{J}_n^-(x_i) = \hat{S}_{\mathrm{in}}^- \Delta_i P_{oi}, \quad n \geq 2.$$

Equations (66) generalize Eq. (10) and reduce to it when $f_{+/-} = 1/2$.

The total emergent currents due to incident currents are

$$\hat{J}^+(x_{i+1}) = \sum_{n=1}^{\infty} \hat{J}_n^+ + E_2(\Delta_i \Sigma_{ti}) J_i^+,$$
$$\hat{J}^-(x_i) = \sum_{n=1}^{\infty} \hat{J}_n^- + E_2(\Delta_i \Sigma_{ti}) J_{i+1}^-. \quad (67)$$

Equations (67) generalize Eqs. (12) and reduce to them when $f_{+/-} = 1/2$, which allows the summation to be performed analytically.

When the deviation from isotropic scattering is small ($|f_{+/-} - \frac{1}{2}| \ll 1$), only linear terms in ($|f_{+/-} - \frac{1}{2}|$) need be retained in the above analysis and the summations can be performed analytically to obtain

$$\hat{J}^+(x_{i+1}) = [\tfrac{1}{2} c_i [1 - E_2(\Delta_i \Sigma_{ti})] P_i \{1 + 2g_+ - c_i[1 - P_{oi}(g_+ + g_-)]\} + E_2(\Delta_i \Sigma_{ti})] J_i^+ + \{\tfrac{1}{2} c_i [1 - E_2(\Delta_i \Sigma_{ti})] P_i \{1 - 2g_- + c_i[1 - P_{oi}(g_+ + g_-)]\}\} J_{i+1}^-,$$

$$\hat{J}^-(x_i) = [\tfrac{1}{2} c_i [1 - E_2(\Delta \Sigma_{ti})] P_i \{1 + 2g_- - c_i[1 - P_{oi}(g_+ + g_-)]\} + E_2(\Delta_i \Sigma_{ti})] J_{i+1}^- + \{\tfrac{1}{2} c_i [1 - E_2(\Delta_i \Sigma_{ti})] P_i \{1 - 2g_+ + c_i[1 - P_{oi}(g_+ + g_-)]\}\} J_i^+, \quad (68)$$

where

$$g_{+/-} \equiv f_{+/-} - 1/2. \quad (69)$$

Equations (68) reduce to Eqs. (12) when $g_{+/-} = 0$.

Generalization of the results related to internal particle sources follows the same general procedure. The emergent currents of n-collided source particles are given by

$$\hat{J}_{n,s}^+ = \hat{S}_{\mathrm{in},s}^+ P_{oi},$$
$$\hat{J}_{n,s}^- = \hat{S}_{\mathrm{in},s}^- P_{oi}, \quad n \geq 1, \quad (70)$$

where the scattering sources per unit length of n-collided internal source particles in the forward (+) and backward (−) direction are calculated recursively

$$\hat{S}_{\mathrm{in},s}^+ = [\hat{S}_{\mathrm{in}-1,s}^+ f_+ + \hat{S}_{\mathrm{in}-1,s}^-(1-f_-)] c_i (1 - P_{oi}),$$
$$\hat{S}_{\mathrm{in},s}^- = [\hat{S}_{\mathrm{in}-1,s}^+(1-f_+) + \hat{S}_{\mathrm{in}-1,s}^- f_-] c_i (1 - P_{oi}), \quad n \geq 1 \quad (71)$$

from the scattering sources per unit length for once-collided source particles

$$\hat{S}_{i1,s}^+ = \left[\left(\frac{s_i^+}{\Delta_i} \right) f_+ + \left(\frac{s_i^-}{\Delta_i} \right) (1-f_-) \right] c_i (1 - P_{oi}),$$
$$\hat{S}_{i1,s}^- = \left[\left(\frac{s_i^+}{\Delta_i} \right) (1-f_+) + \left(\frac{s_i^-}{\Delta_i} \right) f_- \right] c_i (1 - P_{oi}). \quad (72)$$

Equations (68)–(70) generalize Eqs. (15) and (17) and reduce to them when $f_{+/-} = 1/2$. The total emergent currents due to internal sources are

$$\hat{J}_s^+(x_{i+1}) = s_i^+ P_{oi} + \sum_{n=1}^{\infty} \hat{J}_{\mathrm{ns}}^+,$$
$$\hat{J}_s^-(x_i) = s_i^- P_{oi} + \sum_{n=1}^{\infty} \hat{J}_{\mathrm{ns}}^-. \quad (73)$$

Equations (73) generalize Eqs. (19) and reduce to them when $f_{+/-}=1/2$, which allows the summation to be performed analytically.

When the deviation from isotropic scattering is small ($|g_{\pm}|\ll 1$), only linear terms in $g_{\pm}$ need be retained, and the summations can be performed analytically to obtain

$$\begin{aligned}
\hat{J}_s^+(x_{i+1}) &= \{s_i^+ - \tfrac{1}{2}s_i[1+(g_+-g_-)]\}P_{oi} \\
&\quad + \tfrac{1}{2}P_{oi}\left\{ \frac{[1+(g_+-g_-)]s_i}{1-c_i(1-P_{oi})} + c_i(1-P_{oi}) \right. \\
&\quad \left. \times\left[g_+(s_i^+ - \tfrac{1}{2}s_i) - g_-\left(s_i^- - \frac{1}{2}s_i\right)\right]\right\}, \\
\hat{J}_s^-(x_i) &= \{s_i^- - \tfrac{1}{2}s_i[1+(g_--g_+)]\}P_{oi} \\
&\quad + \tfrac{1}{2}P_{oi}\left\{ \frac{[1+(g_--g_+)]s_i}{1-c_i(1-P_{oi})} + c_i(1-P_{oi}) \right. \\
&\quad \left. \times\left[g_-\left(s_i^- - \frac{1}{2}s_i\right) - g_+(s_i^+ - \tfrac{1}{2}s_i)\right]\right\}.
\end{aligned} \tag{74}$$

Equations (74) reduce to Eqs. (19) when $g_{+/-}=0$.

The formalism of Secs. IV and V can be reconstituted with anisotropic scattering by defining directional-dependent reflection coefficients and modifying the source terms.

The anisotropic scattering functions are defined, with reference to Fig. 1, as

$$\begin{aligned}
f_+ &\equiv \frac{\int_0^1 d\mu \int_0^1 d\mu' P(\mu'\to\mu)}{\int_{-1}^1 d\mu \int_0^1 d\mu' P(\mu'\to\mu)}, \\
f_- &\equiv \frac{\int_{-1}^0 d\mu \int_{-1}^0 d\mu' P(\mu'\to\mu)}{\int_{-1}^1 d\mu \int_{-1}^0 d\mu' P(\mu'\to\mu)},
\end{aligned} \tag{75}$$

where $P(\mu'\to\mu)$ is the probability that a neutral particle entering a scattering event with direction cosine μ' results in a neutral particle emerging from the scattering event with directional cosine μ. For scattering from ions or other neutral particles with an isotropic velocity distribution, $f_+=f_-$. However, for scattering from ions streaming towards the divertor plate at near sonic speeds, $f_+\neq f_-$, as discussed in Ref. 8.

XI. MODEL PROBLEM CALCULATION

We solved Eqs. (25) for the physical situation of deuterium plasma ions incident upon a plate and reflected as neutral atoms. The reflected neutral flux at the plate was $1.55\times 10^{23}/\mathrm{m}^2$ s. The fixed plasma density and temperature varied linearly from ($n=5\times 10^{18}/\mathrm{m}^3$, $T=10$ eV) just in front of the plate to ($n=1\times 10^{19}/\mathrm{m}^3$, $T=100$ eV) at a distance of 50 cm away. The dominant atomic processes in this plasma regime are electron-impact ionization, charge exchange and elastic scattering. We assume that the neutral atoms acquire the same local average energy as the plasma ions via scattering and charge exchange and use the Maxwellian-averaged data from Ref. 8. The resulting neutral atom distribution shown in Fig. 3 appears to be nearly exponential but, since

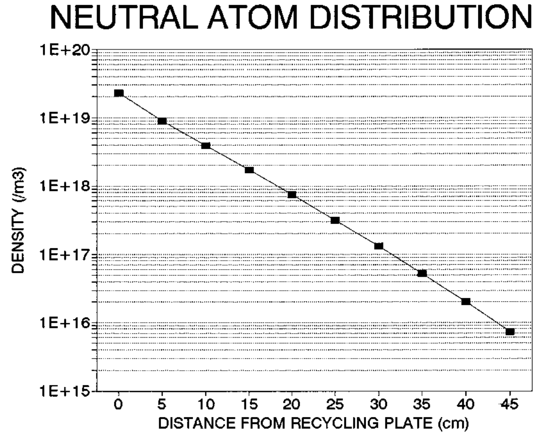

FIG. 3. One-dimensional model problem.

the mean free paths for the various atomic processes vary by a factor of 5 or more over the model problem dimensions, this is coincidental.

The numerics of the code used to solve Eqs. (25) to give the results shown in Fig. 3 have been checked by repeating the calculation with the transmission/escape probability code GTNEUT[5]; the results are indistinguishable from those shown in Fig. 3. Since GTNEUT solves essentially the same equations, this provides a check on the coding. However, since GTNEUT has been successfully benchmarked[5] against DEGAS Monte Carlo calculations, this comparison also provides an indirect benchmark of the methodology presented in this paper.

We plan to undertake an extensive comparison of the interface current balance method with other methods of neutral particle transport, which will be published at a future date.

XII. SUMMARY

A new interface current balance (ICB) formulation of neutral particle transport theory has been developed. The partial current exiting a region across a surface is formulated in terms of (1) the currents entering the region across other surfaces times a transmission probability; plus (2) the current entering the region across the surface in question times a reflection probability; plus (3) the internal source of particles within the region times an escape probability. Integral transport theory is employed to calculate the transmission, reflection, and escape probabilities exactly in slab geometry. The method is shown to be similar to the response matrice method in neutron transport theory, but extends the latter by providing analytical results for the transmission, reflection, and escape probabilities. When extended to multidimension, the interface current balance formulation is shown to be identical to the transmission/escape probability method[5] of neutral atom transport theory, thus providing a more rigorous theoretical formulation for the latter.

The ICB formulation of general neutral particle transport theory is specialized to the transport of neutral atoms in a background plasma. The reflection, transmission, and escape probabilities are specified in terms of suitably averaged ionization, charge exchange, and atom-ion and atom–atom elastic scattering cross sections; and the internal sources are specified in terms of pellet fueling and recombination sources.

The methodology is extended to obtain a multigroup ICB formulation of neutral atom transport theory. This formulation allows the direct calculation of the neutral atom energy distribution, in the multigroup approximation, and the direct calculation of neutral atom momentum and energy currents, as well as particle currents.

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