Discrete and Continuous Interactions in Charged Particle Transport Theory

In a recent paper,[1] Hoffman et al. proposed applying the neutral particle transport code, ANISN, to the calculation of sputtering yields (inner wall erosion of a controlled thermonuclear reactor). In other words, they solved a fast ion transport problem by using a DSN method. Bartine et al. made a similar attempt for electron penetration in several materials.[2]

As is well known, the scattering cross sections are very anisotropic for charged particle interactions, so the energy transfer operator is usually split into two parts. The first one, as in neutron transport theory, represents rather large energy transfers (LET) or "discrete interactions," while the second, the so-called continuous slowing down (CSD) differential operator, allows only small energy transfers (SET). As pointed out by Hoffman et al., this division is quite arbitrary, and, in principle, a pure integral operator could include all kinds of interactions. Unfortunately, such an approach would require too many Legendre scattering kernels.

Generally, the CSD term is obtained by using a Taylor expansion for the flux in the SET operator. As shown by Greenspan and Shvarts,[3] this procedure is correct for uniform space distributions of particles. For space-dependent problems, another approximation is needed, and usually it is assumed that no deflection occurs during a "continuous interaction." This last approximation is inconsistent because a CSD should result from a continuous deflection.

It is known, in plasma physics, for example, that a full continuous interaction approximation leads to the so-called Fokker-Planck operator of the following form:

$$\frac{\partial}{\partial E} S(E)\phi(x,E,\mu) + T(E)\frac{\partial}{\partial \mu}(1-\mu^2)\frac{\partial \phi}{\partial \mu}(x,E,\mu) \ , \qquad (1)$$

when the thermal motion of target particles can be neglected.[4] Then, in the general case, the SET operator should have the same form as Eq. (1) and should not reduce to the first term only. This can be derived directly from the Boltzmann equation.

For plane geometry, one can write[5]

$$\mu \frac{\partial \phi}{\partial x} + \Sigma\phi(x,E,\mu) = \sum_{l=0}^{\infty} \frac{2l+1}{2} P_l(\mu) \int_0^{\infty} dE' \, \Sigma_{s,l}(E' \to E) \Phi_l(x,E') + Q(x,E,\mu) \ , \qquad (2)$$

with

$$\Sigma_{s,l}(E' \to E) = 2\pi \int_{-1}^{1} \Sigma_s(E' \to E, \mu_L) P_l(\mu_L) d\mu_L \qquad (3)$$

and

$$\Phi_l(x,E) = \int_{-1}^{1} \phi(x,E,\mu) P_l(\mu) d\mu \ , \qquad (4a)$$

$$\phi(x,E,\mu) = \sum_{l=0}^{\infty} \frac{2l+1}{2} P_l(\mu) \Phi_l(x,E) \ . \qquad (4b)$$

In the above equations, μ and μ_L are the cosine of the pitch angle and the cosine of the scattering angle in the laboratory system, respectively. The standard versions of DSN codes are based on Eq. (2). The Legendre expansion has to be truncated somehow; in other words, $\Sigma_{s,l}(E' \to E)$ is set to zero when $l > l_M$. In practice, for neutron transport problems, $l_M = 5$ is a very good approximation. For charged particles, on the other hand, a large value of l_M is needed, as shown by Hoffman et al.,[1] although they introduced CSD terms in the formalism. Another strategy is therefore required.

Let us call m_1 and m_2 the masses of test particles described by Eq. (2) and field particles (targets), respectively, assumed to be at rest with a density n_2. Then, the Legendre scattering kernels are given by[5]

$$\Sigma_{s,l}(E' \to E) = \Sigma_{s,l}(E', T) = n_2 \frac{4\pi}{E'} \cdot \frac{1}{\gamma_2} P_l(\mu_L) \sigma_s(E', \mu_c) \qquad (5)$$

for $\alpha E' < E < E'$ and cancel elsewhere. In this equation, $T = E' - E$ represents the recoil target energy, and

$$\gamma_2 = \frac{4m_2 m_1}{(m_2 + m_1)^2} = 1 - \alpha$$

is the parameter given by Hoffman et al.[1] In the above equation, the differential microscopic cross section $\sigma_s(E', \mu_c)$ depends very much on the value of μ_c, the scattering angle cosine in the center of mass. Because of the energy angle correlation, one has[5]

$$\begin{cases} \mu_c\left(\dfrac{T}{E'}\right) = 1 - \dfrac{2}{\gamma_2}\dfrac{T}{E'} \ , & (6) \\ \mu_L\left(\dfrac{T}{E'}\right) = \dfrac{1}{2m_1}\left[(m_1+m_2)\left(1-\dfrac{T}{E'}\right)^{1/2} + (m_1-m_2)\dfrac{1}{\left(1-\dfrac{T}{E'}\right)^{1/2}}\right] . & (7) \end{cases}$$

Let us define a small scattering angle θ_{cm} below which interactions can be considered as continuous. The corresponding energy transfer [Eq. (6)] is

$$T_m = \gamma_1 E' \text{ with } \gamma_1 = (1 - \cos\theta_{cm})\frac{\gamma_2}{2} \ll 1 \ . \qquad (8)$$

The γ_1 parameter is expressed here as a function of the scattering angle in the center of mass. The choice of θ_{cm} can be roughly determined from the shape of

$$\sigma_s(E', \mu_c) \ ,$$

which is a very sharp function near $\mu_c \cong 1$.

By using these definitions, the transport equation [Eq. (2)] can be written as follows:

$$\begin{cases} \mu \dfrac{\partial \phi}{\partial x} + \Sigma\phi(x,E,\mu) \\ \quad = \displaystyle\sum_{l=0}^{\infty} \frac{2l+1}{2} P_l(\mu) \int_{E+T_m}^{E/\alpha} dE' \, \Sigma_{s,l}(E', T) \Phi_l(x,E') \\ \quad + \displaystyle\sum_{l=0}^{\infty} \frac{2l+1}{2} P_l(\mu) I_l(x,E) + Q(x,E,\mu) \ , \end{cases} \qquad (2 \text{ bis})$$

with the SET operator,

$$I_l(x,E) = \int_E^{E+T_m} dE' \, \Sigma_{s,l}(E', T) \Phi_l(x,E') \ . \qquad (9)$$

---

[1] T. J. HOFFMAN, H. L. DODDS, Jr., M. T. ROBINSON, and D. K. HOLMES, *Nucl. Sci. Eng.*, **68**, 204 (1978).

[2] D. E. BARTINE, R. G. ALSMILLER, Jr., F. R. MYNATT, W. W. ENGLE, Jr., and J. BARISH, *Nucl. Sci. Eng.*, **48**, 159 (1972).

[3] E. GREENSPAN and D. SHVARTS, *Nucl. Fusion*, **16**, 2 (1976).

[4] P.-A. HALDY and J. LIGOU, *Nucl. Fusion*, **17**, 6 (1977).

[5] G. I. BELL and S. GLASSTONE, *Nuclear Reactor Theory*, pp. 175-177, Van Nostrand Reinhold Company, New York (1970).

In this last expression, the integrand is a smooth function of E' over the small interval $(E, E + T_m)$, and therefore a first-order Taylor expansion around E can be performed while the T value is fixed:

$$\Sigma_{s,l}(E',T)\Phi_l(x,E') = \Sigma_{s,l}(E,T)\Phi_l(x,E) + (E' - E) \times \frac{\partial[\Sigma_{s,l}(E,T)\Phi_l(x,E)]}{\partial E} .$$

With the new variable T, Eq. (9) becomes

$$I_l(x,E) = \left[\int_0^{T_m} \Sigma_{s,l}(E,T)dT\right]\Phi_l(x,E) + \frac{\partial}{\partial E}\left[\int_0^{T_m} T\Sigma_{s,l}(E,T)dT\,\Phi_l(x,E)\right] . \quad (10)$$

From Eq. (5), one sees that

$$\Sigma_{s,l}(E,T) = \Sigma_{s,0}(E,T)P_l[\mu_L]$$

where μ_L is given by Eq. (7) ($E' = E$). Since $T \leqslant T_m$ is small, $P_l(\mu_L)$ can be approximated by a linear function of T. (This is not true, of course, for $\Sigma_{s,0}$, which is almost singular for $T \cong 0$.) A first-order expansion of $P_l(\mu_L)$ gives

$$P_l\left[\mu_L\left(\frac{T}{E}\right)\right] = \left|P_l[\mu_L]\right|_{T=0} + T\left|\dot{P}_l(\mu_L)\frac{\partial\mu_L}{\partial T}\right|_{T=0} .$$

From the definition of Legendre polynomials,

$$(1 - \mu^2)\ddot{P}_l(\mu) - 2\mu\,\dot{P}_l(\mu) = -l(l+1)P_l(\mu) \quad (11)$$

and $P_l(1) = 1$, one finds

$$\dot{P}_l(1) = \frac{l(l+1)}{2} .$$

Moreover, the derivation of $\mu_L(T/E)$ given by Eq. (7) provides

$$\left(\frac{\partial\mu_L}{\partial T}\right)_{T=0} = -\frac{m_2}{2m_1E} .$$

Finally, the scattering kernel can be approximated as

$$\Sigma_{s,l}(E,T) \cong \Sigma_{s,0}(E,T)\left[1 - l(l+1)\frac{m_2}{4m_1}\frac{T}{E}\right] \text{ for } T \text{ small} ,$$

and Eq. (10) becomes

$$I_l(x,E) \cong \left[\Sigma_{\text{SET}}(E) - l(l+1)\frac{m_2}{4m_1E}S(E)\right]\Phi_l(x,E) + \frac{\partial}{\partial E}S(E)\Phi_l(x,E) , \quad (12)$$

where

$$\Sigma_{\text{SET}}(E) = \int_0^{T_m} \Sigma_{s,0}(E,T)dT , \quad (13)$$

$$S(E) = \int_0^{T_m} T\Sigma_{s,0}(E,T)dT . \quad (14)$$

Here, $S(E)$ is the usual stopping power restricted to SET interactions, and $\Sigma_{\text{SET}}(E)$ is the corresponding macroscopic scattering cross section. In the above derivation, the T^2 terms have been neglected.

The quantity $I_l(x,E)$ can now be introduced in Eq. (2 bis). By using Eqs. (11) and (4b), the transport equation takes the final form:

$$\mu\frac{\partial\phi}{\partial x} + \Sigma_{\text{LET}}\phi(x,E,\mu) = \sum_{l=0}^{\infty}\frac{2l+1}{2}P_l(\mu) \times \int_{\text{LET}} dE'\Sigma_{s,l}(E',T)\Phi_l(x,E') + \frac{\partial}{\partial E}[S(E)\phi(x,E,\mu)] + \frac{m_2}{4m_1}\frac{S(E)}{E}\frac{\partial}{\partial\mu}(1-\mu^2)\frac{\partial\phi}{\partial\mu}(x,E,\mu) + Q(x,E,\mu) . \quad (15)$$

As expected, the Fokker-Planck operator appears naturally when the continuous interactions are correctly handled.

The scattering cross section, Σ_{SET}, has been eliminated from the formalism. This is very important because it takes a large value for Coulomb interactions (it goes to infinity for unscreened potentials). In the left side of Eq. (15), the total cross section involves only the LET part of all scattering processes (discrete interactions) and of course all absorptions.

Let us consider a few cases:

1. The test particles are fast ions. For electronic interactions ($m_2 = m_e$), the ratio $m_2/4m_1$ is very small, and the deflection operator is negligible. Moreover, all energy transfers can be considered as small, $\theta_{cm} = \pi$, $\gamma_1 = \gamma_2$ [Eq. (8)], and no LET term occurs in Eq. (15). For nuclear interactions, on the other hand, $m_2/4m_1$ can be large, when, for example, light ions are impinging on a heavy material ($m_2/m_1 \gg 1$). In this case, the deflection term has to be kept in Eq. (15). This is probably the reason why Hoffman et al. have met numerical difficulties for protons incident on a nickel target.

2. The test particles are electrons. Here, also, in most cases there is a need for a "deflection operator." Some of the discrepancies between experimental data and ANISN calculations could be explained in this way.[2]

NUMERICAL ASPECTS

The usual DSN codes are not able to solve Eq. (15), although the method itself should allow such a Fokker-Planck operator. For example, a finite difference scheme for μ derivatives will lead to connections among three directions, and inner iteration schemes can incorporate such a scattered particle source.

Another problem arises when the multigroup form of Eq. (15) is derived. After integration over the range (E_g, E_{g-1}), the CSD part of this equation becomes

$$S(E_{g-1})\phi(x,E_{g-1},\mu) - S(E_g)\phi(x,E_g,\mu) .$$

The first term represents particles slowing down from group $(g - 1)$ to group (g), and the second term the removal from group (g) to group $(g + 1)$. One must then write this expression as proposed by Greenspan and Shvarts[3]:

$$\Sigma_{R,g-1}\phi_{g-1}(x,\mu) - \Sigma_{R,g}\phi_g(x,\mu) , \quad (16)$$

with

$$\Sigma_{R,g} = S(E_g)W(E_g)\Big/\int_{E_g}^{E_{g-1}} W(E)dE ,$$

in which $\phi(x,E,\mu)$ is approximated by a known weighting function $W(E)$ over the interval (E_g, E_{g-1}).

The simplest way is to assume that both $\phi(x,E_{g-1},\mu)$ and $\phi(x,E_g,\mu)$ are proportional to the group flux $\phi_g(x,\mu)$, as done by Hoffman et al.[1] Unfortunately, by doing that, the CSD process is smeared out, since connections between group fluxes are absent in the formalism.

On the other hand, the deflection term in Eq. (15), which does not involve any slowing down, can be expressed only as a function of $\phi_g(x, \mu)$:

$$T_g \frac{\partial}{\partial \mu} (1 - \mu^2) \frac{\partial}{\partial \mu} \phi_g(x, \mu) \ , \tag{17}$$

with

$$T_g = \frac{m_2}{4m_1} \int_{E_g}^{E_{g-1}} \frac{S(E)}{E} W(E) dE \Big/ \int_{E_g}^{E_{g-1}} W(E) dE \ .$$

In the framework of a general study on ion beam-plasma interactions, we intend to develop a DSN code based on the multigroup form of Eq. (15) by keeping only the Fokker-Planck operator. This will show how to handle the deflection operator

$$\frac{\partial}{\partial \mu} (1 - \mu^2) \frac{\partial}{\partial \mu}$$

from the numerical point of view. The conclusions to be drawn should keep their meaning when discrete interactions are introduced.

J. Ligou

Laboratoire de Génie Atomique
de l'Ecole Polytechnique Fédérale de Lausanne
Lausanne, Switzerland

December 12, 1978