UCRL-ID-122423

950809
**Charged Particle Transport
Updated Multi-group Diffusion**

E. Gary Corman, Sterrett T. Perkins, Ned T. Dairiki
Lawrence Livermore National Laboratory
L-059
P.O. Box 808
Livermore, CA 945510

September, 1995

This is an informal report intended primarily for internal or limited external distribution. The opinions and conclusions stated are those of the author and may or may not be those of the Laboratory.
Work performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under Contract W-7405-Eng-48

MASTER
DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED *DLC*

DISCLAIMER

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the University of California nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial products, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or the University of California, and shall not be used for advertising or product endorsement purposes.

**This report has been reproduced
directly from the best available copy.**

**Available to DOE and DOE contractors from the
Office of Scientific and Technical Information
P.O. Box 62, Oak Ridge, TN 37831
Prices available from (615) 576-8401, FTS 626-8401**

**Available to the public from the
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Rd.,
Springfield, VA 22161**

CHARGED PARTICLE TRANSPORT

Updated Multi-group Diffusion

E. Gary Corman, Sterrett T. Perkins[†], Ned T. Dairiki

University of California Lawrence Livermore National Laboratory

Livermore, California

I. INTRODUCTION

In 1974, a charged particle transport scheme was introduced which utilized a multi-group diffusion method for the spatial transport and slowing down of energetic ions in a hot plasma¹. In this treatment a diffusion coefficient was used which was "flux-limited" to provide, hopefully, some degree of accuracy when the slowing down of an energetic charged particle is dominated by Coulomb collisions with thermal ions and electrons in a plasma medium. An advantage of this method was a very fast, memory-contained program for calculating the behavior of energetic charged particles which resulted in smoothly varying particle number densities and energy depositions.

The main limitation of the original multi-group charged particle diffusion scheme is its constraint to a basic ten group structure; the same ten group structure for each of the five energetic ions tracked. This is regarded as a severe limitation, inasmuch as more groups would be desired to simulate more accurately the corresponding Monte Carlo results of energies deposited over spatial zones from a charged particle source. More generally, it seems preferable to have a different group structure for each particle type since they are created at inherently different energies.

In 1986, one of the authors (STP) developed a new model for charged particle transport in an ionized plasma². A standard multi-group discretization of the Boltzmann-Fokker-Plank equation is transport corrected to include implicitly the anisotropic effects of both Coulomb scattering and nuclear reactions. It should be noted that Coulomb scattering is composed of two components, a small angle component and a large angle component. The small angle component

[†] Sterrett T. (Ted) Perkins passed away April, 1995, due to complications of double pneumonia and lung cancer. Ted was a very productive physicist as well as an enjoyable friend, and he will be greatly missed by all of his many colleagues who worked with him. We extend our heartfelt condolences to his family on their loss, including his wife, children, his many grandchildren and great-grandchild.

is developed through the Fokker-Planck term i.e., continuous energy slowing down, and the large angle component is described as a two body scattering event under nuclear reactions.

In the next two sections, the basic theory and multi-group description will be given. This is followed by the specific techniques that were used to solve the resultant equations. Finally, the modifications that were made to the cross section data as well as the methods used for energy and momentum deposition are described.

II. BASIC THEORY

The basic Boltzmann-Fokker-Planck equation³ can be expressed as (ignoring the spatial and time variables for convenience):

$$\begin{aligned} \left(\frac{\partial}{\partial t} + v \bar{\Omega} \cdot \bar{\nabla} \right) n(E, \bar{\Omega}) &= \frac{1}{t_E} \frac{\partial}{\partial E} [F(E) n(E, \bar{\Omega})] + \frac{v}{2} \Sigma_c(E) \\ &\cdot \left[\frac{\partial}{\partial \mu} (1 - \mu^2) \frac{\partial}{\partial \mu} + \frac{1}{1 - \mu^2} \frac{\partial^2}{\partial \phi^2} \right] n(E, \bar{\Omega}) - v \Sigma_t(E) n(E, \bar{\Omega}) \\ &+ \int dE' \int d\bar{\Omega}' \Sigma(E' \rightarrow E, \bar{\Omega}' \rightarrow \bar{\Omega}) v' n(E', \bar{\Omega}') + S(E, \bar{\Omega}) \end{aligned} \quad (1)$$

where

v = the incident particle speed

μ = cosine of the polar angle

ϕ = azimuthal angle

$n(E, \bar{\Omega})$ = angular particle density [particles per energy per steradian per volume]

$\Sigma_t(E)$ = total nuclear reaction cross section

$\Sigma(E' \rightarrow E, \bar{\Omega}' \rightarrow \bar{\Omega})$ = nuclear reaction transference cross section

t_E , $F(E)$, $\Sigma_c(E)$ are small angle Coulomb scattering terms, viz,

t_E = charged particle relaxation time in collisions with electrons,

$\Sigma_c(E)$ = total Coulomb cross-section,

$$F(E) = (E + \gamma t_E) / E^{1/2} \text{ and } \gamma = \frac{\Gamma_I m_p^{3/2}}{\sqrt{2}}$$

$$\text{where } \Gamma_I = \frac{4\pi e^4 Z^2 \ell n \Lambda_I}{m_p} \sum_i \frac{n_i Z_i^2}{m_i},$$

m_p , the particle mass,

and Λ_I is the ion Coulomb logarithm.

$S(E, \bar{\Omega}) = \text{external source.}$

III. THE MULTI-GROUP SCHEME

For a specific incident particle, a given multi-group structure of energy group boundaries is introduced, in *descending* order, $E_1 > E_2 > \dots > E_{G+1}$:

The number of particles per volume in energy group g can be expressed as:

$$n_g = \int_{E_{g+1}}^{E_g} dE \int d\bar{\Omega} n(E, \bar{\Omega}) \quad (2)$$

Eq. (1) is now simplified by:

- (a) casting into a multi-group form by integrating over group g ,
- (b) transport correcting⁴ the multi-group equation, and
- (c) applying the Levermore flux-limited diffusion theory⁵,

to obtain

$$\frac{\partial n_g}{\partial t} + \bar{\nabla} \cdot \bar{J}_g + \frac{n_g}{\tau_{0g+1}} = \frac{n_{g-1}}{\tau_{0g}} + \hat{S}_{0g} \quad (3)$$

where $\hat{S}_{0g}$ is a generalized particle source, excluding small angle Coulomb scattering, and

$$\bar{J}_g = v_g \bar{\mu}_g n_g = v_g \int_{E_g}^{E_{g-1}} dE \int d\bar{\Omega} d\bar{\Omega}' n(E, \bar{\Omega}) \quad (4)$$

is the particle current in group g . Also,

$$\tau_{0g} = t_E \int_{E_{g+1/2}}^{E_{g-1/2}} \frac{dE}{F(E)} \quad (5)$$

is the transition time across group boundary g for a particle undergoing small angle Coulomb collisions. Referring to Eq. (4), the mean cosine for particle flow is $\bar{\mu}_g \equiv \bar{\mu}_g(\bar{\nabla} N_g, \bar{J}_{g-1})$. Note also that $\bar{\mu}_g \rightarrow 0$ in the isotropic limit and $\bar{\mu}_g \rightarrow 1$ in the free streaming limit. The general set of equations to be solved becomes:

$$\frac{\partial n_{p,g,j}}{\partial t} = -\bar{\nabla} \cdot \bar{J}_{p,g,j} - \frac{n_{p,g,j}}{\tau_{0g+1}} + \frac{n_{p,g-1,j}}{\tau_{0g}} + S_{0g} \quad (6a)$$

Time rate of change
Diffusion
Sink
(Small angle Coulomb)
Source
External source, thermonuclear reactions, plus neutron induced reactions

$$- n_{p,g,j} v_{p,g} \sum_{T,R} \sigma_{p,g,T,R} n_T \quad (6b)$$

Sum over all target isotopes, T , and collision type, R , of the macroscopic total cross section

$$+ \sum_{p'} \sum_{g'} n_{p',g',j} \Sigma_{p',g' \rightarrow p,g}^0 n_{p',g'} \quad (6c)$$

Sum over all particles, p' , and groups, g' , of the macroscopic generalized transfer matrices

for particles $p = 1, 2, \dots, 5$ $\{p, d, \dots, \alpha\}$,
energy groups $g = 1, \dots, G(p)$,
zones $j = 1, \dots, M$.

Σ^0 is a generalized macroscopic zone-dependent transfer matrix which gives the cross-section for the conversion of incoming particle of type p' and group g' to an outgoing particle of type p in group g by scattering or reactions.

For simplicity in the use of the variable, $J_{p,g,j}$, the spatial zone index j will be suppressed in our equations unless it is considered important to the discussion. However, bear in mind that when the solution of $n_{p,g}$ is indicated, it is for all zones, $j=1, \dots, M$. $n_{p,g}$ is the density [number/cm³] of energetic charged particles of species p in energy group g . S_{0g} is the external charged particle source rate which includes thermonuclear reactions plus neutron induced sources. $v_{p,g}$ is the speed of particle p in group g . n_T is the density of thermal target particles of species T . Index R is the 'type of collision', which is summed over; it includes large angle Coulomb, nuclear elastic, and all possible nuclear reactions of charged particle projectile p on target isotope T . As noted later in Section VII, group splitting is done for charged particles.

This requires the redefinition of τ_{0g} , as defined originally by Eq. (5). It is redefined to be the transition time from group g to group $g+1$ for particles undergoing small angle Coulomb scattering. The integral in Eq. (5) then goes from the group centered energy of group $g-1$ to the group centered energy of group g .

Eq. (6) is now rewritten with the positive scattering term summation (6c) broken into two parts; a term with particle and group index, p,g (beginning with $p,g=1$) and the remainder as a partial sum:

$$\frac{n'_{p,g} - n_{p,g}}{\Delta t} = -\nabla \cdot J'_{p,g} - \frac{n'_{p,g}}{\tau_{0g+1}} + \frac{n'_{p,g-1}}{\tau_{0g}} + S_{0g} - n'_{p,g} v_{p,g} \sum_{T,R} \sigma_{p,g,T,R} n_T \quad (7a)$$

$$+ \sum_{p',g' < p,g} n'_{p',g'} v_{p',g'} \sum^0_{p',g' \rightarrow p,g} \quad (7b)$$

$$+ \sum_{p',g' \geq p,g} n'_{p',g'} v_{p',g'} \sum^0_{p',g' \rightarrow p,g} \quad (7c)$$

This permits solution of the equations in two main steps, the first of which is implicit and includes only term Eq. (7b) of the total positive scattering contributions, since Eq. (7b) contains the only known n' terms, already solved at the end of the major cycle of length Δt , for a given particle p and group g . In a second step term Eq. (7c) is incorporated for an explicit calculation of $n'_{p,g}$ for each subsequent group index and charged particle index in turn. This is described in further detail in the following sections.

IV. THE SWEEP OVER SPACE AND TIME FOR THE IMPLICIT COMPONENT

The equation set to be solved implicitly becomes the following

$$\frac{\partial n'_{p,g}}{\partial t} = \nabla \cdot J'_{p,g} - \frac{n'_{p,g}}{\tau_{0g+1}} + \frac{n'_{p,g-1}}{\tau_{0g}} + \tilde{S}_{0g} \quad (8a)$$

where

$$\tilde{S}_{0g} = S_{0g} - n'_{p,g} v_{p,g} \sum_{T,R} \sigma_{p,g,T,R} n_T + \sum_{p',g' < p,g} n'_{p',g'} v_{p',g'} \sum_{p',g' \rightarrow p,g}^0 \quad (8b)$$

This can be done since for a given particle and group one is solving for the number $n'_{p,g}$, for which by that time its 'predecessors' have already been calculated, these being the numbers of particles $n'_{p',g' < p,g}$.

Assuming azimuthal symmetry so that space is one dimensional, the spatial zone j is integrated over the zone volume. This spatial discretization⁶ allows one to write

$$\frac{\partial n'_{p,g,j}}{\partial t} = \nabla \cdot J'_{p,g,j} - \frac{n'_{p,g,j}}{\tau_{0g+1,j}} + \frac{n'_{p,g-1,j}}{\tau_{0g,j}} + \tilde{S}_{0g,j}, \quad (9a)$$

and

$$\nabla \cdot J'_{p,g,j} = \alpha_{p,g,j,j-1} n_{p,g,j-1} + \alpha_{p,g,j,j} n_{p,g,j} + \alpha_{p,g,j,j+1} n_{p,g,j+1}, \quad (9b)$$

with

$$\alpha_{p,g,j,j+1} \propto \frac{v_{p,g} \bar{\mu}_{p,g,j+1/2}}{\Delta r_{j+1/2}}. \quad (9c)$$

where $\bar{\mu}_{p,g,j+1/2}$ is the arithmetic average of the direction cosine, μ , at each boundary. This analogy also holds for Δr . Note that the j subscript on a quantity denotes its average in the zone j . Eq. (9) can be written in matrix form as

$$\frac{\partial \bar{n}'_g}{\partial t} + A_g(\bar{n}') \bar{n}'_g + T_g \bar{n}'_g = T_{g-1} \bar{n}'_g + \tilde{S}_{0g}, \quad (10)$$

where

$$\bar{n}'_g = \begin{pmatrix} n'_{g,1} \\ n'_{g,2} \\ \bullet \\ \bullet \\ \bullet \\ n'_{g,M} \end{pmatrix}, \quad \bar{\tilde{S}}_{0_g} = \begin{pmatrix} \tilde{S}_{0_g,1} \\ \tilde{S}_{0_g,2} \\ \bullet \\ \bullet \\ \bullet \\ \tilde{S}_{0_g,M} \end{pmatrix}, \quad (11)$$

$$A_g(\bar{N}_g) = \begin{pmatrix} \alpha_{g,1,1} & \alpha_{g,1,2} & & & & \\ \alpha_{g,2,1} & \alpha_{g,2,2} & \alpha_{g,2,3} & & & \\ & \bullet & & \bullet & & \\ & & & & \bullet & \\ & & & & & \bullet \\ & & & & & \alpha_{g,M,M-1} & \alpha_{g,M,M} \end{pmatrix}, \quad (12)$$

$$T_g = \begin{pmatrix} \frac{1}{\tau_{0_g,1}} & & & & & \\ & \frac{1}{\tau_{0_g,2}} & & & & \\ & & \bullet & & & \\ & & & \bullet & & \\ & & & & \bullet & \\ & & & & & \frac{1}{\tau_{0_g,M}} \end{pmatrix}. \quad (13)$$

Define t_n as the present time, t_{n+1} as the time at the end of the time step, and $\Delta t = t_{n+1} - t_n$. Equation (10) is then discretized using the backward Euler technique to yield

$$\frac{\bar{n}_g^{n+1} - \bar{n}_g^n}{\Delta t} + A_g(\bar{n}_g^{n+1})\bar{n}_g^{n+1} + T_g\bar{n}_g^{n+1} = T_{g-1}\bar{n}_{g-1}^{n+1} + \bar{\tilde{S}}_{0_g}^{n+1}. \quad (14)$$

where a superscript n or $n+1$ denotes time centering at t_n or t_{n+1} , respectively. Eq. (14) is a nonlinear equation since the matrix A_g depends on $\bar{n}_g^{n+1}$ and is solved by an approximate iterative Newton's method. For more information on this technique, see reference 5.

V. THE IMPLICIT SOURCE DESCRIPTION

To illustrate the source description in more detail, initially solve Eq. (10) for energetic protons by using the old proton number $n_{p,g=1}$ to calculate the new proton number $n'_{p,g=1}$ for the top-most energy group, $g=1$. For this initial calculation, contributions from the positive scattering summation cannot be included since their amounts are not yet known.

Next, this newly calculated value $n'_{p,g=1}$ is used to calculate the new proton number for the next lower proton group ($g=2$), $n'_{p,g=2}(n'_{p,g=1})$, since $n'_{p,g=1}$ is now known and it appears as a contribution in the positive scattering matrix summation. This procedure is continued using successively the newly calculated proton numbers $n'_{p,g}$ from 1 to g , to calculate proton numbers for the next lower group $g+1$, or $n'_{p,g+1}(n'_{p,1}, n'_{p,2}, \dots, n'_{p,g})$, until all the new proton numbers $n'_{p,g=1,G_p}$ are calculated for all groups, 1 to G_p (G_p is the lowest energy proton group number).

With these newly calculated proton numbers, substitute them (i.e. the proton numbers) in the scattering matrix summation to now calculate the corresponding values for the deuterons, starting with the top deuteron group, or $n'_{p=d,g=1}(n'_{p,1}, n'_{p,2}, \dots, n'_{p,G_p})$. One then works down the deuteron list, from the top group $g=1$ down to the bottom group G_D , again using all the known final numbers, $n'_{p',g'<p,g}$, of protons and deuterons, up to that p,g combination being calculated, in the scattering matrix term, to calculate all of their contributions to the current $n'_{p,g}$.

The foregoing procedure is continued until the sweeps over the main equation for all particles are completed in order: protons, deuterons, tritons, He^3 s, and alphas. In each case, all the known numbers $n'_{p,g}$ from all groups of all the preceding particle species—plus all the groups above the current group of the current particle—are used to make scattering contributions into the current particle group via the scatter matrix summation.

VI. DEPLETIONS AND THE EXPLICIT EQUATION

After the completion of all the particle sweeps for all zones, j , the new number densities $n'_{p,g,j}$ are thereby obtained for all particles and groups. These numbers are subsequently used to deplete the thermal isotopic composition, $C_{T,j}$:

$$\Delta C_{T,j} = -\Delta t \sum_{p=1}^5 \sum_{R=1}^{NR} \sum_{g=1}^{NGPCP(p)} n'_{p,g,j} v_{p,g} \sigma_{p,g,T,R} n_{T,j}, \quad (15)$$

where R is the reaction type index, the summation of which contains the elastic as well as all the possible types of reactions.

The effect of scattering from all the remaining particle-group combinations not covered in the foregoing sweeps is now added in. This contribution is labeled as Eq. (7c) in the main equation, and it will add the scattering contribution to p,g from all those number densities in which p', g' is greater than or equal to p,g, since those values were not yet known during the initial (main) series of sweeps. However, these contributions must now be added explicitly, as stand-alone, add-on equations, since the main sweeps have already been completed.

Thus, we label the finalized values of $n_{p,g}$ as $n''_{p,g}$, which are calculated as add-on corrections to $n'_{p,g}$:

$$\frac{n''_{p,g} - n'_{p,g}}{\Delta t} = \sum_{p',g' \geq p,g} n'_{p',g'} v_{p',g'} \sum^0_{p',g' \rightarrow p,g} \quad (16)$$

After the final sweep of all p,g combinations for all groups of all particles over all zones, each spatial zone is now checked to determine in which energy group and zone the thermal boundary ($3/2 kT_I$) lies, where T_I is the ion temperature. In the groups below thermal, the particles of all species are placed into the thermal sea and the numbers in these corresponding energy groups are zeroed out which conserves all species of particles.

These $n''_{p,g}$ values are then used as the initial values $n_{p,g}$ for the following cycle.

VII. MODIFICATION TO THE CROSS SECTIONS

Charged particle production and interaction matrices are group-split⁷. This technique adjusts the transfer matrix elements so that both particles and energy are conserved. Under group-splitting the particles can only enter or leave the group at the group centered energy, $\bar{E}_g = (E_g + E_{g+1})/2$. This applies not only to particles from nuclear reactions but also to small angle Coulomb scattering wherein energy transfers occur between centered energies of adjacent groups. It was later realized that unless group splitting was extended to a virtual group of zero width at zero energy, energy could not be fully conserved in all cases. This latter technique was not used here. Rather, for another reason, as discussed below, no particles were allowed to transfer to the lowest energies.

The microscopic cross-sections $\sigma_{p,g,T,R}$ include large angle Coulomb scattering together with the nuclear plus interference elastic, as well as any known reaction cross sections. Since the Coulomb cross section varies as $1/E^2$, it becomes very large at low energies--up into the thousands of barns. To avoid destabilizing the solution of the equations with such large cross sections, it appeared sensible to zero out arbitrarily the large angle Coulomb cross section below a cut-off energy, set at $E_{\min} = 0.5$ MeV. In addition, the nuclear plus interference elastic cross section goes to zero at low energy so it was also zeroed out. This technique affects the interaction transfer matrices, the total, large angle Coulomb, the nuclear plus interference cross sections, as well as the energy deposition terms for these low energies. These deleted cross sections are easily compensated for by adjusting the Coulomb logarithm, L_I , for ion-ion collisions.

In particular, when large angle Coulomb scattering is implemented along with the nuclear elastic and reaction scattering cross sections, a reduction of L_I is necessary to compensate for the more explicit and external treatment of the energetic ions undergoing large angle Coulomb scattering. L_I can be expressed⁸ as

$$L_I = \ell n \left[\sin \left(\frac{\theta_c}{2} \right) / \sin \left(\frac{\theta_{\min}}{2} \right) \right], \quad (17)$$

where θ_c is the center of mass cut off angle between large and small angle Coulomb scattering, and $\theta_{\min}$ is the minimum scattering angle corresponding to the maximum impact parameter. The angle $\theta_{\min}$ is related to the impact parameter by $\cos \theta_{\min} = 1 - \frac{2}{1 + \Lambda^2}$, where Λ is the ratio of the maximum impact parameter (usually the Debye length) to the minimum impact parameter. The ion Coulomb logarithm can then be written as

$$L_I = \ell n (1 + \Lambda^2)^{1/2} + \ell n \sin \left(\frac{\theta_c}{2} \right). \quad (18)$$

The second term--always negative or zero--contains the necessary correction when the large angle Coulomb scattering is handled explicitly by including such cross sections in the general scattering tables. Thus, when the large angle Coulomb cross sections below $E_{\min} = 0.5$ MeV are arbitrarily zeroed out, θ_c is set to 180° for those energy groups below $E_{\min}$, which nullifies the correction to L_I .

VIII. ENERGY AND MOMENTUM DEPOSITION

Both energy and momentum are deposited from nuclear reactions as well as from small angle Coulomb events. Energy deposition will first be discussed. We then show how it is modified through momentum deposition.

For the nuclear component⁷, the production data files include the average total available energy coefficient for particle p in group g on target T, defined by

$$\langle E\sigma \rangle_{p,g,T_{\text{total}}} = \langle E\sigma \rangle_{p,g,T} + \langle Q\sigma \rangle_{p,g,T} \quad (19)$$

The first term on the right hand side is the particle energy in group g and the second term is the energy production. The data files also contain the corresponding average energy coefficient into the outgoing particle field, y_0 , $\langle E\sigma \rangle_{p,g,T,y_0}$. Note that these coefficients are integrated over the energy in the group and summed over all reactions. At generation time, the local energy deposition coefficient is calculated by

$$\langle E\sigma \rangle_{p,g,T_{\text{loc}}} = \langle E\sigma \rangle_{p,g,T_{\text{total}}} - \sum_{y_0} \langle E\sigma \rangle_{p,g,T,y_0} \quad (20)$$

Here the summation over outgoing particles is only over those particles which are actually being transported in the specific calculation. At the end of the time step, the energy deposition per volume is obtained from

$$\Delta E_{\text{loc}} = \Delta t \sum_{p,g,T} n_{p,g} v_{p,g} \langle E\sigma \rangle_{p,g,T_{\text{loc}}} n_T \quad (21)$$

For Coulomb scattering, energy deposition is developed exactly as in Section 3 of ref. 1. For particle p in group g, one considers the time variation of the energy within group g,

$$\frac{\partial Q_{p,g}}{\partial t} = \int_{E_{g+1}}^{E_g} E \frac{\partial n_p(E)}{\partial t} dE \quad (22)$$

The particle density, $n_p(E)$, is taken from the infinite media solution, Eq. (10) of ref. 1, without the space derivative. An integration by parts is performed yielding leakage (in energy) into and out of the group and a deposition integral. Using the steady state solution for the integrand of this deposition integral, and employing the definition of τ_g , Eq. (12) of ref. 1, yields the deposition term. Since particles only enter and leave the group at the group centered energies, the energies in the final expression are then shifted to these group centered values.

Besides depositing energy locally, charged particles also give an impulse to the media through momentum deposition. Consider a given zone, j . The zonal kinetic energy is $E_j = P_j^2 / 2M_j$. The change of the zone kinetic energy due to a change in zone momentum is then $dE_j = P_j dP_j / M_j = u_j dP_j$, where u_j is the zone speed. Charged particle momentum can therefore change the zonal kinetic energy. The rate of this change of the zone kinetic energy due to momentum deposition by charged particles slowing down is⁹

$$\dot{S}_{ke_g} = u \dot{P}_{dep_g} , \quad (23)$$

where $\dot{P}_{dep_g}$ is the momentum deposition rate. This kinetic energy change is not available for local deposition and must be subtracted from the local energy deposition. The momentum density for particle p in group g is defined by

$$\bar{P}_{p,g} = m_p \bar{J}_{p,g} , \quad (24)$$

where m_p is the mass and $\bar{J}_{p,g}$ is the current for particle p . The rate of change of the momentum density in group g for both nuclear reactions and small angle Coulomb scattering is given by

$$\frac{\partial \bar{J}_{p,g}}{\partial t} = \int_{E_{g+1}}^{E_g} \frac{\partial \bar{J}_p(E)}{\partial t} dE . \quad (25)$$

The term $\frac{\partial \bar{J}_p(E)}{\partial t}$ for nuclear scattering is given by the infinite media P1 equation (with no Coulomb terms). This equation has no source term from other particle fields since the P1 transfer matrices are not available for charged particles. This yields leakage (in energy) into and out of the group and a deposition term. This deposition term involves the group absorption cross section, i.e., the cross section for removing particles from the specific particle field without

introducing new particles into other particle fields. In addition, if other particles are produced, then the split between momentum leakage (in energy) and deposition has to be determined on a reaction by reaction basis. This is not possible since there are no momentum deposition terms as per the energy deposition defined by Eq. (19) - (20). Thus an approximation is used which employs the group transport cross section.

For Coulomb scattering, an analogous procedure is used as described for the energy deposition. The infinite media P₁ equation, Eq. (5) of ref. 1, but without the space derivative, is used in Eq. (25). The term involving $\Sigma_{c,p}(E)J_p(E)v$ is neglected during the development but introduced again at the end. Again, the energies in the final expression are shifted to the group centered values.

We note that there is no particle balance or global energy conservation explicitly incorporated in the solution of the transport equations. Global energy conservation and particle number balance occur simply as an outcome of the energy and momentum deposition equations and the various source and depletion reactions.

Finally, we would like to acknowledge the help of George B. Zimmerman for his suggestions which provided the basic solution algorithm to the transport equation. This was the procedure described in sections III-VI wherein the multigroup equations are solved by partial solutions first to the implicit terms followed by an explicit calculation in an iterative fashion for each energy group and charged particle type.

References:

1. E. G. Corman, W. E. Loewe, G. E. Cooper, A. M. Winslow, *Nuclear Fusion* **15**, 377 (1975).
2. M. R. Dorr, J. F. Painter, and S. T. Perkins, *Nucl. Sci. Eng.*, **94**, 157 (1986).
3. K. Przybylski and J. Ligou, *Nucl. Sci. Eng.* **81**, 92 (1982)
4. cf., for example, J. J. Duderstadt, W. R. Martin, Transport Theory, pg. 221, John Wiley & Sons, New York, N. Y. (1979)
5. C. D. Levermore, G. C. Pomraning, *Astrophysical Journal*, **248**, 321 (1981)
6. M. R. Dorr, "Reformulation of the Charged Particle Package," Private Communication (4/3/90).
7. R. J. Howerton, et. al., "OMEGA: A CRAY 1 Executive Code for LLNL Nuclear Data Libraries," UCRL-50400, Vol. 25, Ch. VI and VII (1983). See also S. T. Perkins, "Energy Deposition for NDFYi Charged Particles," PD-189, Internal LLNL memo (1992).
8. I. P. Shkarofsky, T. W. Johnston, and M. P. Bachynski, The Particle Kinetics of Plasmas, Addison-Wesley Publ. Co., Reading, Mass., (1966). Eq. (17) is derived from the results leading up to Eq. (7-19) of this ref. but with no approximations. See also S. T. Perkins, "Definition of Terms in the Multigroup P₁ Equations," PD-70, Internal LLNL memo (1982).
9. S. T. Perkins, "Energy, Momentum, and Isotope Terms Calculated from Solution of the Multigroup P₁ Equations," PD-71, Internal LLNL memo (1982). See also S. T. Perkins, "The Local Momentum Deposition Rate from Nuclear Reactions for Charged Particles, Revisited," MC-19, Internal LLNL memo (1994).

Technical Information Department · Lawrence Livermore National Laboratory
University of California · Livermore, California 94551