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**Discrete Ordinates Treatment
of Induced Scattering**

by

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ABSTRACT

A transport equation including nonlinear induced scattering effects is written for the photon flux (speed of light times the density). A finite Legendre polynomial expansion is used to represent the scattering transfer probability (differential cross section). A multigroup formulation is derived with appropriate definitions of multigroup coefficients. Treatment of the induced scattering terms (including iterative strategy) in standard discrete ordinates programs is outlined.

I. INTRODUCTION

Photon transport is usually assumed to be described by a linear transport equation. Occasionally, however, photon densities are high enough to require the examination of the nonlinear effects of induced scattering, and discrete ordinates programs for solution of the transport equation are conveniently modified to treat these effects. Because of the nonlinearity, care must be taken to ensure that all appropriate factors are included in coefficients of the nonlinear terms. For example, it is usual to assume that angular integrals are normalized to unity in discrete ordinates programs,¹ and this normalization introduces a factor of 4π into the coefficients of induced scattering. Below, following Watkins,² we trace the derivation of the coefficients involved. We then develop a multigroup formalism for use in conventional multigroup discrete ordinates programs. We also describe an iteration strategy which has been successful in difficult problems, i.e., in problems with high flux levels where induced scattering is important. Section II follows the work of Pomraning³ and Watkins.²

II. TRANSPORT EQUATION WITH INDUCED SCATTERING

Pomraning³ writes (using slightly different notation) the following equation for photon transport including induced effects:

$$\begin{aligned} \frac{1}{c} \frac{\partial I}{\partial t} + \Omega \cdot \nabla I + \sigma_g I(r, \nu, \Omega, t) \\ + \int_0^\infty d\nu' \int_{4\pi} d\Omega' \sigma_g(\nu - \nu', \mu_0) I(1 + \alpha' I) \\ = \int_0^\infty d\nu' \int_{4\pi} d\Omega' \frac{\nu}{\nu'} \sigma_g(\nu' - \nu, \mu_0) I'(1 + \alpha I) \\ + \mathcal{S}(r, \nu, \Omega, t) \end{aligned} \quad (1)$$

In this equation I is the specific intensity which is related to the distribution function f by

$$I(r, \nu, \Omega, t) = ch\nu f(r, \nu, \Omega, t) \quad (2)$$

where $4\pi d\nu d\Omega$ is the number of photons at time t in dr about r , $d\nu$ about ν , and $d\Omega$ about Ω and where c is the speed of light and h is Planck's constant. The quantity $\sigma_g(\nu' - \nu, \mu_0)$ can also depend on r and t as well as on ν' , ν and $\mu_0 = \Omega \cdot \Omega'$, but we omit

these variables for simplicity. The probability that a photon with frequency ν and direction vector Ω scatters into $d\nu$ about ν and $d\Omega$ about Ω while traveling a distance ds is $\sigma_s(\nu' \rightarrow \nu, \mu_0) d\nu d\Omega ds$. Similarly, $\sigma_a(\nu) ds$ represents the photon absorption probability. In neutron transport terminology σ_a is a macroscopic cross section with dimensions of inverse length. $S(r, \nu, \Omega, t)$ is an independent source of photons.

In Eq. (1) we use I' to represent $I(r, \nu', \Omega', t)$. The terms proportional to α and α' , where

$$\alpha = c^2/2h\nu^3 \quad (3)$$

$$\alpha' = c^2/2h\nu'^3$$

are the induced scattering terms. The product αI is the number, n , of photons in an element of phase space. That is, with the momentum $p = h\nu/c$,

$$\begin{aligned} n &= \iiint_{\Delta} d\vec{r} d\nu d\Omega f \\ &= \iiint_{\Delta} d\vec{r} p^2 dp d\Omega f \quad c^3/h^3 \nu^2 \\ &= \frac{c^2}{h} \iiint_{\Delta} d\vec{r} d\vec{p} I/\nu^3 \\ \Delta &= h^3/2 \\ &= \alpha I \end{aligned} \quad (4)$$

where the volume Δ of phase space is $h^3/2$ because there are two polarization states possible.

It is now convenient to change from a frequency variable to a dimensionless energy variable and to write our equation in terms of a flux (neutron transport terminology) by letting

$$\phi(r, E, \Omega, t) dE = cf(r, \nu, \Omega, t) d\nu \quad (5)$$

where

$$E = h\nu/m_0 c^2$$

and m_0 is the electron rest mass. Thus,

$$cf = \frac{I}{h\nu} = \frac{\phi dE}{d\nu} = \frac{\phi h}{m_0 c^2} \quad (6)$$

so that

$$I = \frac{h^2 \nu \phi}{m_0 c^2} = hE\phi.$$

Using this relation, we can rewrite Eq. (1) in terms of ϕ :

$$\begin{aligned} \frac{1}{c} \frac{\partial \phi}{\partial t} + \Omega \cdot \nabla \phi + \sigma_a \phi \\ + \int_0^\infty dE' \int_{4\pi} d\Omega' \sigma_s(E \rightarrow E', \mu_0) \phi(1 + \beta \phi'/E'^2) \\ = \int_0^\infty dE' \int_{4\pi} d\Omega' \sigma_s(E' \rightarrow E, \mu_0) \phi'(1 + \beta \phi/E^2) + S. \end{aligned} \quad (7)$$

Here

$$\sigma_s(E' \rightarrow E, \mu_0) dE d\Omega = \sigma_s(\nu' \rightarrow \nu, \mu_0) d\nu d\Omega \quad (8)$$

$$S d\nu d\Omega = S dE d\Omega$$

and

$$\beta = \frac{c^2 h^3}{2(m_0 c^2)^3} \quad (9)$$

Finally, we make one more change of variables. Transport programs like DTF-IV¹ use a normalized quadrature over angles Ω , such that

$$d\Omega = d\Omega'/4\pi. \quad (10)$$

Letting

$$\phi d\Omega = \psi d\Omega' \quad \text{or} \quad \phi = \psi/4\pi \quad (11)$$

and substituting into Eq. (7), we have

$$\begin{aligned} \frac{1}{c} \frac{\partial \psi}{\partial t} + \Omega \cdot \nabla \psi + \sigma_a \psi \\ + \int_0^\infty dE' \int_{4\pi} d\Omega' \hat{\sigma}_s(E \rightarrow E', \mu_0) \psi(1 + \beta \psi'/4\pi E'^2) \\ = \int_0^\infty dE' \int_{4\pi} d\Omega' \hat{\sigma}_s(E' \rightarrow E, \mu_0) \psi'(1 + \beta \psi/4\pi E^2) + Q \end{aligned} \quad (12)$$

where

$$\hat{\sigma}_s d\Omega' = \sigma_s d\Omega \quad (13)$$

$$Q d\Omega' = S d\Omega.$$

III. LEGENDRE POLYNOMIAL EXPANSION OF THE SCATTERING FUNCTION

We now expand the scattering function in a finite sum of Legendre polynomials such that

$$\hat{\sigma}_s(E' \rightarrow E, \mu_0) = \sum_{n=0}^N (2n+1) P_n(\mu_0) \sigma_{sn}(E' \rightarrow E). \quad (14)$$

From Eq. (13) $\hat{\sigma}_s = 4\pi\sigma_s$ so that

$$\sigma_s(E' \rightarrow E, \mu_0) = \sum_{n=0}^N \frac{(2n+1)}{4\pi} P_n(\mu_0) \sigma_{sn}(E' \rightarrow E). \quad (15)$$

The expansion coefficients are found to be, by using the orthogonality of the Legendre polynomials,

$$\begin{aligned} \sigma_{sn}(E' \rightarrow E) &= \int d\omega \hat{\sigma}_s P_n(\mu_0) \\ &= \int d\omega \sigma_s P_n(\mu_0). \end{aligned} \quad (16)$$

If we use the representation $d\omega = d\mu d\varpi/4\pi$, $-1 \leq \mu \leq 1$, $0 \leq \varpi \leq 2\pi$, then the addition theorem lets us write

$$P_n(\mu_0) = \sum_{j=0}^n \frac{(2-\delta_{j0})(n-j)!}{(n+j)!} P_n^j(\mu) P_n^j(\mu') \cos j(\varpi - \varpi') \quad (17)$$

where the P_n^j are associated Legendre functions. We use below the result

$$\int_0^{2\pi} \frac{d\varpi}{2\pi} P_n(\mu_0) = P_n(\mu) P_n(\mu'). \quad (18)$$

We now substitute Eq. (14) into Eq. (12) and assume that ψ is independent of ϖ (thereby restricting ourselves to one-dimensional planar or spherical geometry). We also drop time dependence for simplicity. Using Eq. (18) we find

$$\begin{aligned} &+ \omega \cdot \nabla \psi + \sigma_a \psi + \psi \sum_{n=0}^N (2n+1) P_n(\mu) \int_0^\infty dE' \sigma_{sn}(E \rightarrow E') \int_{-1}^1 \frac{d\mu'}{2} P_n(\mu') (1 + \beta \psi' / 4\pi E'^2) \\ &= (1 + \beta \psi / 4\pi E^2) \sum_{n=0}^N (2n+1) P_n(\mu) \int_0^\infty dE' \sigma_{sn}(E' \rightarrow E) \int_{-1}^1 d\mu' \psi' / 2 + Q. \end{aligned} \quad (19)$$

If we make the expansion

$$\psi = \sum (2n+1) P_n(\mu) \psi_n(\mu) \quad (20)$$

we note that

$$\psi_n = \int \frac{d\mu}{2} \int \frac{d\varpi}{2\pi} \psi = \int \frac{d\mu}{2} \psi \quad (21)$$

because we assumed ψ does not depend on ϖ . Using this notation and simplifying one term on the left of Eq. (19) we have

$$\begin{aligned} &\omega \cdot \nabla \psi + \sigma_a \psi \\ &+ \frac{\beta \psi}{4\pi} \sum_{n=0}^N (2n+1) P_n(\mu) \int_0^\infty dE' \sigma_{sn}(E \rightarrow E') \psi_n' / E'^2 \\ &= \sum_{n=0}^N (2n+1) P_n(\mu) \int_0^\infty dE' \sigma_{sn}(E' \rightarrow E) \psi_n' \\ &+ \frac{\beta \psi}{4\pi} \sum_{n=0}^N (2n+1) P_n(\mu) \int_0^\infty dE' \sigma_{sn}(E' \rightarrow E) \psi_n' / E'^2 \\ &+ Q. \end{aligned} \quad (22)$$

Here,

$$\sigma_t = \sigma_a + \sigma_s \quad (23)$$

and

$$\sigma_s = \int_0^\infty \sigma_{so}(E \rightarrow E') dE'. \quad (24)$$

We have modified the DIFF-IV program¹ to solve the multigroup form of equations like Eq. (22), including cylindrical geometry where the anisotropic scattering terms are more complicated. For completeness, we review in the next section the definition of multigroup constants that should be used.

IV. DEFINITION OF MULTIGROUP CONSTANTS

The nonlinear terms in Eq. (22) require the

definition of extra cross sections. We integrate Eq. (22) over the range ΔE_g ($g = 1, 2, \dots$, IGM with increasing g denoting decreasing E) and define

$$\begin{aligned}
\int_{\Delta E_g} Q dE &= Q_g \\
\int_{\Delta E_g} \psi dE &= \psi_g \\
\int_{\Delta E_g} \sigma_t \psi &= \int_{\Delta E_g} (\sigma_a + \sigma_{sc}) \psi = \sigma_{tg} \psi_g
\end{aligned} \quad (25)$$

In integral terms, we replace the integral from 0 to ∞ by a sum of integrals of E' in the range ΔE_h and define

$$\begin{aligned}
\int_{\Delta E_h} \psi' dE' &= \psi_{nh} \\
\int_{\Delta E_g} dE \int_{\Delta E_h} dE' \sigma_{sn}(E' \rightarrow E) \psi'_n &= \psi_{nh} \sigma_{snh-g}
\end{aligned} \quad (26)$$

$$\int_{\Delta E_g} \frac{dE \psi}{E^2} \int_{\Delta E_h} dE' \sigma_{sn}(E' \rightarrow E) \psi'_n = \psi_g \psi_{nh} \tilde{\sigma}_{snh-g} \quad (27)$$

$$\int_{\Delta E_g} dE \psi \int_{\Delta E_h} dE' \frac{\sigma_{sn}(E' \rightarrow E)}{E^2} \psi'_n = \psi_g \psi_{nh} \bar{\sigma}_{snh-g} \quad (28)$$

Note well that $\tilde{\sigma}_{snh-g} \neq \bar{\sigma}_{snh-g}$ unless special weighting functions are chosen in Eqs. (27) and (28). Using the definitions of Eqs. (25) and (26), we write Eq. (22) in multigroup notation

$$\begin{aligned}
\psi_{ng} \nabla_g + (\sigma_{tg} + \sigma_{out,g}) \psi_g \\
= \sum_{n=0}^N (2n+1) P_n(\mu) \sum_{h=1}^{IGM} \psi_{nh} \sigma_{snh-g} + \sigma_{in,g} \psi_g + Q_g
\end{aligned} \quad (29)$$

where

$$\begin{aligned}
\sigma_{out,g}(\mu, \psi_n) &= \frac{\beta}{4\pi} \sum_{n=0}^N (2n+1) P_n(\mu) \sum_{h=1}^{IGM} \bar{\sigma}_{snh-g} \psi_{nh} \\
\sigma_{in,g}(\mu, \psi_n) &= \frac{\beta}{4\pi} \sum_{n=0}^N (2n+1) P_n(\mu) \sum_{h=1}^{IGM} \tilde{\sigma}_{snh-g} \psi_{nh}
\end{aligned} \quad (30)$$

The definitions of Eqs. (25) through (28) are used in the production of multigroup cross sections. If angularly dependent approximate fluxes are used for weighting, then σ_{tg} as well as $\sigma_{out,g}$ and $\sigma_{in,g}$

depend on μ . (The latter would depend on μ even for $N = 0$.) If the weighting function depends only on energy, i.e., $\psi \approx \psi_n \approx f(E)$ then $\tilde{\sigma}_{snh-g} = \bar{\sigma}_{snh-g}$ and these averages are independent of μ . In the simple case of a constant weight function

$$\tilde{\sigma}_{snh-g} = \bar{\sigma}_{snh-g} = \frac{\int_{\Delta E_g} dE \int_{\Delta E_h} dE' \sigma_{sn}(E' \rightarrow E) / E^2}{\Delta E_g \Delta E_h} \quad (31)$$

V. SOLUTION OF THE DISCRETE ORDINATES EQUATIONS WITH INDUCED SCATTERING

In all that follows, we assume that $\tilde{\sigma}_{snh-g} = \bar{\sigma}_{snh-g}$. That is, we assume only one of these cross section matrices is necessary.

There are several complications introduced by the induced effects.

First, the cross sections σ_{in} and σ_{out} depend on angle. By using a Legendre expansion, we have made it relatively easy to construct the terms of Eq. (30). Nevertheless, it is necessary to introduce additional space and angle dependent arrays to hold $\sigma_{in,g}$ and $\sigma_{out,g}$.

Second, σ_{out} acts as an increment to the total cross section and makes any group optically thicker (increasing truncation error of spatial finite difference schemes), while σ_{in} acts as a scattering source which tends to slow the usual within group iterative process. We alleviate this difficulty by subtracting as much of $\sigma_{in,g} \psi_g$ as we can [i.e., $\min(\sigma_{tg} + \sigma_{in,g}, \sigma_{out,g}) \psi_g$] from each side of Eq. (29).

Third, because σ_{in} and σ_{out} depend on ψ , we have no guarantee that each group is subcritical. That is, the value of $\sigma_{in,g}$ might be so large (because of poor estimates of ψ_{ng}) that a group might be supercritical and the iteration process would diverge. This can be avoided by using angular flux values from a previous outer iteration to calculate that portion of the right side of Eq. (29) due to $\sigma_{in,g}$. In other words, we do not attempt to improve this portion of the source during an inner iteration.

Fourth, if there is a residual term on the right side of Eq. (29), that is, if $\sigma_{out,g} + \sigma_{tg} < \sigma_{in,g}$, we must adjust the system wide rebalance procedures used to accelerate the inner iteration process. In any case, the usual tally of group balance tables

must be adjusted to account for induced scattering. We have added the volume integral of the net source $(\sigma_{in,g} \psi_g - \sigma_{out,g} \psi_g)$ to the usual "inscatter" term after inner iteration in a group is complete.

Fifth, if upscattering is present, for example due to scattering from relativistic electrons, then the nonlinear terms affect an outer iteration convergence acceleration procedure that is normally used. The balance equation corresponding to Eq. (29) is

$$\begin{aligned} \nabla \cdot \psi_{lg} + \sigma_{tg} \psi_{og} + \frac{\beta}{4\pi} \sum_{n=0}^N (2n+1) \psi_{ng} \sum_{h=1}^{IGM} \tilde{\sigma}_{sng \rightarrow h} \psi_{nh} \\ = \sum_{h=1}^{IGM} \psi_h \sigma_{soh \rightarrow g} + \frac{\beta}{4\pi} \sum_{n=0}^N (2n+1) \psi_{ng} \sum_{h=1}^{IGM} \tilde{\sigma}_{snh \rightarrow g} \psi_{nh} \\ + Q_{og} \end{aligned} \quad (32)$$

When Eq. (32) is summed over groups, the induced terms and the scattering cross section cancel giving

$$\sum_g (\nabla \cdot \psi_{lg} + \sigma_{ag} \psi_{og}) = \sum_g Q_{og} \quad (33)$$

which is the same as the result in the absence of induced scattering. Thus a single upscattering iteration acceleration factor can still be calculated from

$$\text{factor} = \frac{\text{Total Source}}{\text{Total Leakage} + \text{Total Absorption}} \quad (34)$$

The outer iteration upscattering acceleration process in DTF-IV¹ is easily modified to use this factor. (The process now used in the code creates an equivalent factor when there is no induced scattering, but does not work when induced scattering is present.) To use Eq. (34) in DTF-IV it is essential to insure that the σ_{ag} that is input is the same as that implied by input values of σ_{tg} and $\sigma_{sog \rightarrow h}$. We recommend changing the program to generate σ_{ag} from

$$\sigma_{ag} = \sigma_{tg} - \sum_{h=1}^{IGM} \sigma_{sog \rightarrow h} \quad (35)$$

We summarize some of the points made above by tracing the iterative processes of DTF-IV. Inner

iterations are those in which $\sigma_{in,g}$, $\sigma_{out,g}$ and all those ψ_{hn} , $h \neq g$, are assumed known. Then, the equation

$$\begin{aligned} \omega_g \nabla \psi_g^{(k)} + (\sigma_{tg} + \sigma_{out,g} - \tau_g) \psi_g^{(k)} \\ = \sum_{n=0}^N (2n+1) P_n(\mu) \psi_{gn}^{(k-1)} \sigma_{sng \rightarrow g} \\ + (\sigma_{in,g} - \tau) \psi_g^{(k-1)} + \tilde{Q}_g \end{aligned} \quad (36)$$

is solved. Here

$$\tilde{Q}_g = Q_g + \sum_{n=0}^N \sum_{h \neq g}^{IGM} (2n+1) P_n(\mu) \psi_{hn} \sigma_{snh \rightarrow g} \quad (37)$$

$$\tau_g = \text{minimum of } (\sigma_{tg} + \sigma_{out,g}, \sigma_{in,g}) \quad (38)$$

and k is an iteration subscript.* As remarked above, if $\sigma_{in,g} - \tau > 0$ we may, depending on how much leakage the group has, be forced to fix $\psi_g^{(k-1)}$ by using values of ψ from a previous outer iteration. An alternative is to limit the number of inner iterations sharply, to one or two per group.

Outer iterations involve the updating of $\tilde{Q}_g$, $\sigma_{in,g}$ and $\sigma_{out,g}$. Before the inner iterations in each group, latest flux values are used to compute these quantities. After a pass through all groups, all fluxes are modified by the factor computed from Eq. (34).

The above procedures have worked well even in a problem in which the magnitude of Q_g was accidentally made several orders of magnitude larger than it should have been, thereby making the induced scattering effects much more important than they should have been.

References

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*We do not need to consider the portion of σ_{in} and σ_{out} that depends on ψ_g , because with $\bar{\sigma} = \bar{\sigma}$, the terms with $h=g$ in Eq. (30) are equal. In actual calculation, we omit these terms.