CONF-780329--1

AN ANALYTIC ANGULAR INTEGRATION TECHNIQUE FOR GENERATING MULTIGROUP TRANSFER MATRICES

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*Operated by Union Carbide Corporation under contract W-7405-eng-26 with the U. S. Department of Energy.

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ABSTRACT

Many detailed multigroup transport calculations require group-to-group Legendre transfer coefficients to represent scattering processes in various nuclides. These (fine group) constants must first be generated from the basic data. This paper outlines an alternative technique for generating such data, given the total scattering cross section of a particular nuclide on a pointwise energy basis, $\sigma(E')$, and some information regarding the angular scattering distribution for each initial energy point.

The evaluation of generalized multigroup transfer matrices for transport calculations requires a double integration extending over the primary and secondary energy groups where, for a given initial energy, the integration over the secondary energy group may be replaced by an integral over the possible scattering angles. In the present work, analytic expressions for these angular integrals are derived which are free of truncation error. Differences between the present method (as implemented in ROLAIDS) and other methods (as implemented in MINX and NEWXLACS) will be explored. Of particular interest is the fact that, for hydrogen, the angular integration is shown to simplify to the point that, for many weight functions, the integration over the primary energy group might also be performed analytically. This completely analytic treatment for hydrogen has recently been implemented in NEWXLACS.

Given the Legendre coefficients of the scattering cross section on a point-wise basis, $\sigma_\ell(E'\to E)$, the group-to-group Legendre transfer coefficients are defined as:

$$\sigma_\ell(g'\to g) \equiv (1/\phi_\ell^{g'}) \int_{E^g}^{E^{g-1}} \int_{E^{g'}}^{E^{g'-1}} \phi_\ell(E')\, \sigma_\ell(E'\to E)\, dE'\, dE \qquad (1)$$

where the spatial dependence of each term is understood and $\phi_\ell(E')$ represents the Legendre coefficients of the angular flux distribution at each spatial point. In practice, the higher order terms, $\phi_\ell(E')$, are replaced by an energy dependent weight function $\phi(E')$. In ROLAIDS[1], for example, this would be the (zone averaged) scalar flux resulting from the solution of the integral slowing down equation on a point-wise basis. In other codes, such as XLACS,[2,3] the weight function may be specified by the user. The Legendre coefficients of the point-to-point angular scattering cross section are formally defined as

$$\sigma_\ell(E' \to E) \equiv 2\pi \int_{-1}^{+1} \sigma(E' \to E, \mu_L)\, P_\ell(\mu_L)\, d\mu_L \qquad (2)$$

In the fast and epithermal range, however, there is a unique relationship between the initial and final energies, the exitation energy (Q), the mass of the target nuclide (A), and the cosine of the angle of scatter in the lab system:

$$\mu_L(E', E, Q, A) = \frac{1}{2}\left[(A+1)\sqrt{\frac{E}{E'}} - (A-1)\sqrt{\frac{E'}{E}} + \frac{AQ}{\sqrt{E'E}}\right] \qquad (3)$$

Representing this as a delta function in Eq. (2) yields

$$\sigma_\ell(E' \to E) = \sigma(E' \to E)\, P_\ell[\mu_L(E', E, Q, A)] \qquad (4)$$

and

$$\sigma_\ell(g' \to g) = (1/\phi^{g'}) \int_{E^{g'}}^{E^{g'-1}} \phi(E') \left[\int_{E^g}^{E^{g-1}} P_\ell[\mu_L(E', E, Q, A)]\, \sigma(E' \to E)\, dE\right] dE' \quad . \qquad (5)$$

The accurate evaluation of this expression represents a severe computational burden which must be addressed by any cross section processing code. The present method differs from previous approaches in that it yields an analytic solution for the integral on dE which is free of

truncation error when the scattering function is given by a Legendre expansion in either the center-of-mass (C) or the lab (L) system.

The scattering function, $\sigma(E' \rightarrow E)$, represents a distribution over the secondary energy (E) and hence over the scattering angle. Thus,

$$\sigma(E' \rightarrow E)\, dE = \sigma(E')\, f(E', \mu_c)\, 2\pi d\mu_c \tag{6}$$

where μ_c is the cosine of the scattering angle in the center-of-mass system and $f(E', \mu_c)$ is the angular distribution function in that system. A similar expression could certainly have been written for the lab system. Because all scattering processes appear more isotropic in the C system and because most scattering involving the formation of a compound nucleus is in fact isotropic in the C system, the present choice was made. While the present method can easily accomodate anisotropic scattering, it is most easily introduced assuming isotropic elastic scattering in the C system [$f(E', \mu_c) = 1/4\pi$, $Q = 0$]. The integral on dE can then be written as

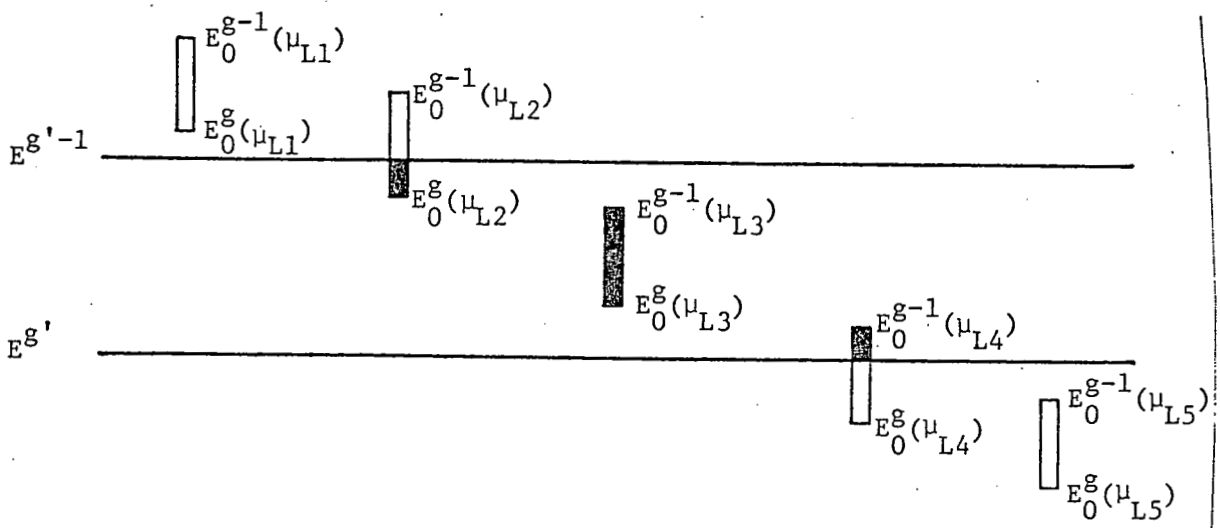
$$\int_{E^g}^{E^{g-1}} P_\ell[\mu_L(E', E, Q, A)]\, \sigma(E' \rightarrow E)\, dE =$$

$$= \frac{1}{2}\, \sigma(E') \int_{\mu_c(E', E_L, Q, A)}^{\mu_c(E', E_U, Q, A)} P_\ell[\mu_L(E', E(\mu_c), Q, A)]\, d\mu_c \tag{7a}$$

$$= \frac{1}{2}\, \sigma(E') \int_{\mu_L(E', E_L, Q, A)}^{\mu_L(E', E_U, Q, A)} P_\ell[\mu_L(E', E, Q, A)] \left| \frac{d\mu_c}{d\mu_L} \right| d\mu_L \tag{7b}$$

$$= \frac{\sigma(E')}{2A} \int_{\mu_L(E', E_L, Q, A)}^{\mu_L(E', E_U, Q, A)} \left\{ 2\mu_L + \sqrt{a^2 + \mu_L^2} + \frac{\mu_L^2}{\sqrt{a^2 + \mu_L^2}} \right\} P_\ell(\mu_L)\, d\mu_L \tag{7c}$$

where E_U and E_L depend on the location of the secondary energy group relative to E' as shown in Fig. 1, and the relationship between μ_c and μ_L is given by



$E_{high}=0$	$E_{high}=E^{g'-1}$	$E_{high}=E_0^{g-1}$	$E_{high}=E_0^{g-1}$	$E_{high}=0$
$E_{low}=0$	$E_{low}=E_0^g$	$E_{low}=E_0^g$	$E_{low}=E^{g'}$	$E_{low}=0$

Fig. 1. Possible Location of an Arbitrary Secondary Energy Group Relative to the Range of Possible Secondary Energies $E' \rightarrow \alpha E'$ and the Limits of Integration that Should be Used in Each Case.

$$\mu_c = \left(\frac{1}{A}\right)\left[\mu_L^2 - 1 + \mu_L\sqrt{a^2 + \mu_L^2}\right], \qquad a^2 = A^2 - 1 \tag{8}$$

Since $P_\ell(\mu_L)$ is simply a polynomial in μ_L, it is necessary only to evaluate integrals of the form:

$$f_n(x) = \int x^n\, dx \qquad n=1,2,3,4,5, \ldots, (\ell+1) \tag{9}$$

$$g_n(x) = \int x^n \sqrt{a^2+x^2}\, dx \qquad n=0,1,2,3,4, \ldots, \ell \tag{10}$$

$$h_n(x) = \int \frac{x^n}{\sqrt{a^2+x^2}}\, dx \qquad n=2,4,5,6,7, \ldots, (\ell+2) \tag{11}$$

The integrals represented by $g_n(x)$ and $h_n(x)$ are less obvious than those represented by $f_n(x)$. They can, however, be evaluated analytically by setting $x = a \tan\theta = a\sqrt{\sec^2\theta - 1}$, using the Binomial theorem to expand integer powers of $(\sec^2\theta - 1)$, and applying a standard reduction formula to integrate powers of $(\sec\theta)$. Defining $r = \sqrt{a^2 + x^2}$ and letting $m = n/2$ for n = even and $m = (n-1)/2$ for n = odd, the results may be written as:

$$g_n(x) = a^{n+2} \sum_{i=0}^{m} (-1)^i \binom{m}{i} \rho_{2(m-i)+3}(x) \qquad n=0,2,4, \ldots, \tag{12}$$

$$g_n(x) = a^{n+2} \sum_{i=0}^{m} \left[\frac{(-1)^i}{2(m-i)+3}\right] \binom{m}{i} \left[\frac{r}{a}\right]^{2(m-i)+3} \qquad n=1,3,5, \ldots, \tag{13}$$

$$h_n(x) = a^n \sum_{i=0}^{m} (-1)^i \binom{m}{i} \rho_{2(m-i)+1}(x) \qquad n=2,4,6, \ldots, \qquad (14)$$

$$h_n(x) = a^n \sum_{i=0}^{m} \left[\frac{(-1)^i}{2(m-i)+1}\right] \binom{m}{i} \left[\frac{r}{a}\right]^{2(m-i)+1} \qquad n=3,5,7, \ldots, \qquad (15)$$

where

$$\rho_j(x) = \left(\frac{1}{j-1}\right)\left(\frac{r}{a}\right)^{j-2}\left(\frac{x}{a}\right) + \left(\frac{j-2}{j-1}\right)\rho_{j-2}(x) \qquad (16)$$

$$\rho_1(x) = \ell n(x+r), \qquad \text{and} \qquad \binom{m}{i} = \frac{m!}{(m-i)!\,i!} \qquad (17a,b)$$

Despite their appearance, these expressions are generally quite simple. For example:

$$\int_{E^g}^{E^{g-1}} P_0(\mu_L)\sigma(E' \rightarrow E)\, dE = \frac{\sigma(E')}{2A}\left[x(1+r) + (1-a^2)\ell n(x+r)\right]\Big|_{x=\mu_L^L}^{x=\mu_L^U} \qquad (18)$$

$$\int_{E^g}^{E^{g-1}} P_l(\mu_L)\sigma(E'\to E)\,dE = \frac{\sigma(E')}{2A}\left[\frac{2}{3}(x^3 + r^3) - a^2 r\right]\Bigg|_{x=\mu_L}^{x=\mu_L^U} \tag{19}$$

Note that these analytic expressions are in closed form, and do not simply represent the first few terms of an infinite series. It is for this reason that the present method has been incorporated in the ROLAIDS cross section processing code.[1]

For anisotropic scattering in the C-system, the angular distribution function $f(E',\mu_c)$ would look like:

$$f(E',\mu_c) = \sum_{k=0}^{ISCT(CM)} \frac{2k+1}{4\pi} f_k(E')\, P_k(\mu_c) \tag{20}$$

and $P_\ell(\mu_L)$ in Eq. (7c) would be replaced by the product $P_k(\mu_c)P_\ell(\mu_L)$. Using Eq. (8) to represent each power of μ_c in $P_k(\mu_c)$, Eq. (7c) could still be written in terms of $f_n(x)$, $g_n(x)$ and $h_n(x)$. Thus, the resulting expressions could again be written in closed form with no truncation error.

The present method as described above is to be advocated whenever the angular scattering function is known in the C-system. If, on the other hand, it is specified as an expansion in the L-system such that

$$\tilde{f}(E',\mu_L) = \sum_{k=0}^{ISCT(LAB)} \frac{2k+1}{4\pi} \tilde{f}_k(E')\, P_k(\mu_L) \tag{21}$$

it would be more expedient to write the scattering function as

$$\sigma(E'\to E)\,dE = \sigma(E')\,\tilde{f}(E',\mu_L)\,2\pi d\mu_L \tag{22}$$

and substitute Eqs. (21) and (22) directly into Eq. (5) where the integration in the L-system would involve only the product $P_k(\mu_L)P_\ell(\mu_L)$. Such terms represent simple polynominals in μ_L and are easily integrated.[4] To take advantage of this simplicity, the MINX code[5] uses Amster's transformation[6] to convert C-system expansions to L-system expansions prior to performing the integration. Note, however, that even the simplist function in the C-system [$f(E',\mu_c) = 1/4\pi$] requires an infinite number of Legendre terms in the L-system. In practice, the L-system expansion must be truncated, leaving some residual error not found in the present method.

For comparison purposes, it should be noted that NEWXLACS[7] uses a numerical quadrature to perform the angular integration in the evaluation of $\sigma_\ell(g'\to g)$.[8,9,10] To be more precise, it calculates $\sigma_\ell(g'\to g)$ as

$$\sigma_\ell(g'\to g) \doteq (2\pi/\phi^{g'}) \sum_{n=1}^{N} w_n P_\ell(\mu_{Ln}) \int_{E^{g'}}^{E^{g'-1}} \phi(E')\,\sigma(E')\,\tilde{f}(E',\mu_{Ln})\,\varepsilon(\mu_{Ln})\,dE' \qquad (23)$$

where $\varepsilon(\mu_{Ln}) = 1$ if $\mu_L(E',E_L,Q,A) \le \mu_{Ln} \le \mu_L(E',E_U,Q,A)$ for $E^{g'} \le E' \le E^{g'-1}$, and $\varepsilon(\mu_{Ln}) = 0$ otherwise. The integration over E' is then done semi-analytically. The power of the method is that it is extremely fast and reasonably accurate in most cases. It is, however, an approximate method. Its chief weakness is that one must use higher order quadratures to obtain fairly accurate results as the group structure becomes finer. For light nuclides this method may also leave holes in the multigroup transfer matrices which should physically not be present. Numerical experiments do, however, indicate the approximation to be quite good for heavy nuclides, and adequate for all nuclides but hydrogen. In all cases, the accuracy of the approximation may be increased by increasing N.

To be perfectly rigorous in the case of hydrogen, one should account for the fact that the atomic mass ratio (A) is less than unity. The radicals in Eq. (7c) would then become $\sqrt{\mu_L^2 - b^2}$ where $b^2 = 1 - A^2$. A substitution of the form $\mu_L = b \sec\theta$ would then allow Eq. (7c) to be written in terms of $\rho_j(x)$. This exact treatment, however, would represent an unnecessary degree of accuracy in most cases.

A most interesting and extremely useful simplification of Eq. (7c) results in the case of hydrogen where one is willing to make the A = 1 approximation. In that case, the bracketted quantity in Eq. (7c) simplifies to $4\mu_L$, Eq. (3) simplifies to $\mu_L = \sqrt{E/E'}$, and Eq. (5) becomes

$$\sigma_\ell(g'\to g) = \left(\frac{2}{\phi^{g'}}\right) \int_{E^{g'}}^{E^{g'-1}} \phi(E')\sigma(E') \left[\int_{\mu_L=\sqrt{E_L/E'}}^{\mu_L=\sqrt{E_U/E'}} \mu_L\, P_\ell(\mu_L)\, d\mu_L \right] dE' \qquad (24)$$

Defining $a_{\ell,n}$ as the coefficients of μ_L^n in $P_\ell(\mu_L)$, it becomes convenient to describe $\sigma_\ell(g' \to g)$ as

$$\sigma_\ell(g' \to g) = \sum_{n=0}^{\ell} a_{\ell,n}\, \sigma_{\ell,n}\,(g' \to g) \tag{25}$$

The terms $\sigma_{\ell,n}(g' \to g)$ can then be written as

$$\sigma_{\ell,n}\,(g' \to g) = \left(\frac{1}{p\phi^{g'}}\right)\left[\left(E^{g-1}\right)^p - \left(E^g\right)^p\right]\beta_p^{g'} \qquad \text{for } g' < g \tag{26}$$

$$\sigma_{\ell,n}(g' \to g) = \left(\frac{1}{p\phi^{g'}}\right)\left[\beta_0^{g'} - \left(E^g\right)^p\,\beta_p^{g'}\right] \qquad \text{for } g' = g \tag{27}$$

where $p = (n+2)/2$ and

$$\beta_p^{g'} = \int_{E^{g'}}^{E^{g'-1}} \phi(E')\sigma(E')[E']^{-p}\, dE' \tag{28}$$

In the case of hydrogen, the piecewise continuous ENDF specification for $\sigma(E')$ is always of the form

$$\sigma(E') = a\,[E']^b \tag{29}$$

for 10^{-5} ev $\leq E' \leq$ 20 Mev. As long as $\phi(E')$ is represented in a piecewise continuous fashion by one of the five ENDF interpolation formulas, the integral in Eq. (28) may be evaluated analytically. Assuming, for example, that the weight function is $1/E'$, Eq. (28) yields

$$\beta_p^{g'} = \int_{E^{g'}}^{E^{g'-1}} a[E']^{b-p-1}\, dE' = \left(\frac{a}{b-p}\right)[E']^{b-p}\Bigg|_{E^{g'}}^{E^{g'-1}} \tag{30}$$

This completely analytic treatment for hydrogen has recently been implemented in NEWXLACS.[11] Because of the analytic treatment and the A = 1 approximation, a full down-scattering matrix is generated with no holes.

REFERENCES

1. R. M. Westfall, "Theory and Validation of ROLAIDS: AMPX Module for Treating Resonance Shielding in Multiregion Geometries," UCCND/CSD/INF-65 (to be published).

2. N. M. Greene et. al., "XLACS: A Program to Produce Weighted Multigroup Cross Sections from ENDF/B Data," ORNL/TM-3646 (1972).

3. N. M. Greene et. al., "AMPX: A Modular Code System for Generating Coupled Multigroup Neutron-Gamma Libraries from ENDF/B," ORNL/TM-3706 (1976).

4. C. R. Weisbin et. al., "A New Procedure for the Determination of Neutron Multigroup Transfer Matrices," Nucl. Sci. & Eng. 45, pp. 329 (1974).

5. D. R. Harris et. al., "MINX, A Modular Code System for Processing Multigroup Cross Sections from Nuclear Data in ENDF/B Format," LA-UR-1766 (1973).

6. H. J. Amster, "Slowing Down in a Uniform Medium," Naval Research Physics Handbook, Vol I (1964).

7. W. E. Ford, III and B. R. Diggs, "AMPX Newsletter - No. 2," UCC-ND Internal Correspondence, December 16, 1977.

8. N. M. Greene, "Anisotropic Inelastic Scattering Matrices from ENDF Data," Trans. Am. Nucl. Soc., 17 (2), 549 (1973).

9. N. M. Greene and J. L. Lucius, "Simple and Efficient Schemes for Processing ENDF/B Scattering Data," Trans. Am. Nucl. Soc., 27, (2), 395 (1977).

10. J. A. Bucholz, "A Method of Generating Multigroup Transfer Matricies Using an Analytic Angular Integration Free of Truncation Error," ORNL/NUREG/CSD-8 (1978).

11. J. A. Bucholz, "A Completely Analytic Scattering Treatment for Hydrogen Presently Available in NEWXLACS," UCC-ND Internal Correspondence, February 28, 1978.