LA-UR-77-872

CONF-770401--18

TITLE: THE BACKGROUND CROSS SECTION APPROACH TO GENERATING GROUP CONSTANTS FOR SHIELDING CALCULATIONS

AUTHOR(S): R. E. MacFarlane and R. B. Kidman
Theoretical Division
Los Alamos Scientific Laboratory
and
Martin Becker
Rensselaer Polytechinic Institute

SUBMITTED TO:

FIFTH INTERNATIONAL CONFERENCE ON REACTOR SHIELDING

Knoxville, Tennessee

April 18-22,1977

los alamos
scientific laboratory
of the University of California
LOS ALAMOS, NEW MEXICO 87545

An Affirmative Action/Equal Opportunity Employer

Form No. 836
St. No. 2629
1/75

UNITED STATES
ENERGY RESEARCH AND
DEVELOPMENT ADMINISTRATION
CONTRACT W-7405-ENG. 36

THE BACKGROUND CROSS SECTION APPROACH TO GENERATING GROUP CONSTANTS FOR SHIELDING CALCULATIONS *

R. E. MacFarlane and R. B. Kidman
Theoretical Division
Los Alamos Scientific Laboratory, University of California
Los Alamos, New Mexico 87545
and
Martin Becker
Department of Nuclear Engineering
Rensselaer Polytechnic Institute
Troy, New York 12181

ABSTRACT

The background cross section method is evaluated for applications in shielding analysis. It is shown that approximations used in the standard method are inadequate for deep penetration in nearly pure materials and for problems in which elastic removal is important. Three improvements are proposed and tested: buckling iteration to improve leakage calculations, improved elastic removal iteration, and explicit self-shielding of all elements and Legendre orders of the elastic matrix.

INTRODUCTION

The Los Alamos Scientific Laboratory is engaged in the development of the background cross section method[1] as a general purpose approach to the generation of group constants for nuclear analysis. As part of this development program, a systematic effort is being devoted to the identification of limitations to the state of the art in the use of this method, and to the formulation of testing of procedures to deal with these limitations. This paper will concentrate on procedures of importance to shielding, although the overall program is also concerned with fast and thermal reactor analysis.

There are some characteristics of shielding problems which make them particularly sensitive to some of the assumptions previously utilized in the background cross section method. First, the need to deal with penetration of nearly pure materials -- steel, sodium, etc. -- results in situations where background cross sections are small. In such cases, the weighting spectrum becomes more complex and may even become position dependent. Second, shielding problems are relatively more sensitive to resonance scattering than reactor core problems. Accurate self-shielded removal cross sections must be obtained even in the presence of non-asymptotic fluxes. Third, deep penetration and streaming make shielding problems sensitive to anisotropic scattering. Due care must be taken to represent the anisotropy of the weighting flux.

*Work performed under the auspices of the United States ERDA.

Thus, it is quite possible for practices which have been acceptable in other areas (e.g., fast reactor critical analysis[2]) to fail in shielding applications. In this paper, we shall identify how some presently used versions of the background cross section method can lead to difficulty in shielding applications, and we shall indicate how new procedures can remove these difficulties.

THE BACKGROUND CROSS SECTION METHOD

This section will review briefly the logic behind the background cross section method. Consider the definition of the average cross section for group g, material i, and reaction type x:

$$\sigma^{g}_{xi} = \frac{\int_{u_{g-1}}^{u_g} du\,\sigma_{xi}(u)\phi(u)}{\int_{u_{g-1}}^{u_g} du\,\phi(u)} \quad . \tag{1}$$

In the background cross section method as usually applied, the weighting flux has been assumed to be of the form

$$\phi(u) = \frac{\psi(u)}{\sum_t(u)} = \frac{\psi(u)}{N_i\sigma_{ti}(u) + \sum_{j\neq i} N_j\sigma_{tj}(u)} \quad , \tag{2}$$

where $\psi(u)$ is a smooth function of lethargy u (e.g., constant or fission spectrum) and Σ_t is the macroscopic total cross section. This is a smooth collision density assumption and is consistent with the narrow-resonance approximation. It is further assumed that the sum of the total cross section of the other materials can be replaced by an effective background cross section so that Eq. (2) becomes

$$\phi(u) = \frac{\psi(u)}{N_i[\sigma_{ti}(u)+\sigma_0]} \quad . \tag{3}$$

Eq. (1) is evaluated at several temperatures for several specific values (from very small to very large) of σ_0. Self shielding factors are then defined by

$$f^{g}_{xi}(T,\sigma_0) = \frac{\sigma^{g}_{xi}(T,\sigma_0)}{\sigma^{g}_{xi}(\sigma_0=\infty)} \quad , \tag{4}$$

where the denominator is called the infinite dilution cross section. The analyst may determine the f-factor for any particular set of σ_0 and T values by interpolating among the precalculated values. This procedure is the basis for a number of computer codes, including ETOX,[3] ENDRUN,[4] and MINX.[5]

These processing codes are coupled to a number of space-energy collapse codes, including 1DX,[6] TDOWN,[7] and SPHINX.[8] These codes compute the σ_0,s from mixture data and equivalence principles, interpolate for f-factors, compute a flux spectrum, and collapse to a subset group structure. The result is a set of macroscopic space-and-energy self-shielded group constants for subsequent calculations.

CROSS SECTION MINIMA AND LEAKAGE

When dilution is small and a deep cross section minimum is encountered, Eq. (3) predicts a very large flux. This high flux weights the low cross section very heavily, leading to a relatively small group cross section. However, in practice, the flux cannot become so large because the long mean-free-path allows many neutrons to escape "out the window," and the appropriate cross section is somewhat larger than that predicted by the usual method.

To analyze this effect further, consider the flux predicted by the B_0 approximation:

$$\phi(u) = \frac{\psi(u)}{B} \tan^{-1} \frac{B}{\Sigma_t(u)} \quad . \tag{5}$$

When the buckling B is small, this reduces to the standard form of Eq. (2) (i.e., the standard method applied in "large" systems). However, when the cross section goes to zero, Eq. (5) gives a finite limit, and reasonable cross sections are obtained. This effect is illustrated in Fig. 1.

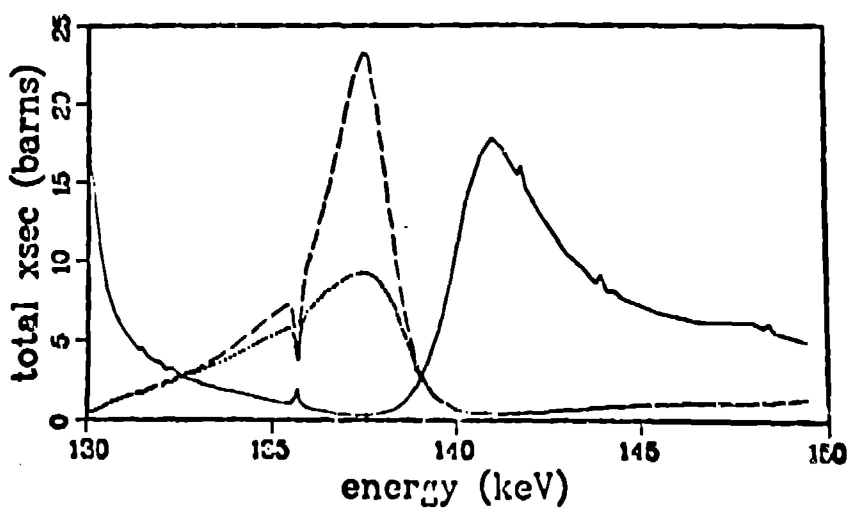

Fig. 1. Effect of "window" on weighting flux for iron; solid curve is flux with standard background assumption, dotted curve is buckled flux.

A rational approximation to this result is obtained by using

$$\sigma(u) = \frac{\psi(u)}{N_1[\sigma_{t1}(u)+\sigma_0+\frac{2B}{N_1\pi}]} \quad . \tag{6}$$

This formulation allows all of the features of the standard method to be used with an effective background cross section given by

$$\sigma_0^{eff} = \sigma_0 + \frac{2B}{N_1\pi} \quad . \tag{7}$$

The problem in shielding applications, where asysmptotic situations do not exist, is the evaluation of the appropriate B value to use in Eq. (7) when B can depend on both energy and position. The solution is to use the flux calculator in the space-energy collapse code to compute B from the calculated flux and leakage. The cross sections are then reshielded using the new values of σ_0, and a new flux calculation is made. The iteration is continued to convergence. This procedure has been implemented in the 1DX code using diffusion theory with

$$B_z^g = \sqrt{\left|\frac{L_z^g}{D_z^g \phi_z^g V_z}\right|} \quad , \tag{8}$$

where L_z^g is the leakage rate from zone z and group g, and V_z is the volume of the zone. Furthermore, D_z^g is the diffusion coefficient given by

$$D_z^g = \frac{\frac{\Sigma_t}{B}\tan^{-1}\left(\frac{B}{\Sigma_t}\right)-1}{B\tan^{-1}\left(\frac{B}{\Sigma_t}\right)\left\{1+\frac{3\Sigma_t\Sigma_{s1}}{B^2}\left[\frac{\Sigma_t}{B}\tan^{-1}\left(\frac{B}{\Sigma_t}\right)-1\right]\right\}} \quad , \tag{9}$$

where Σ_{s1} is the P_1 scattering cross section [Eq. (9) reduces to the conventional $1/3\Sigma_{tr}$ for small B/Σ]. Group and zone indices have been suppressed for clarity.

The success of the B-iteration in accounting for "window" streaming has been illustrated dramatically by an analysis of the iron-reflected ZPR3-54.* Criticality predictions for this assembly have been consistently several percent low with ENDF/B-IV; a standard 1DX analysis gives 0.9532. With the B-iteration, k_{eff} increases to 1.014 (both results include a net correction of + .021 for heterogeneity, dimensionality, and transport). The improvement in k_{eff} implies that the leakage through the reflector is predicted better for shielding purposes. The 1DX total leakage with and without B-iteration are compared in Fig. 2. As expected

*This assembly is used throughout this paper as a shielding problem. The core can be considered to be a source for leakage through the "shield" (reflector); k_{eff} provides an integral measure of how well different methods represent this leakage.

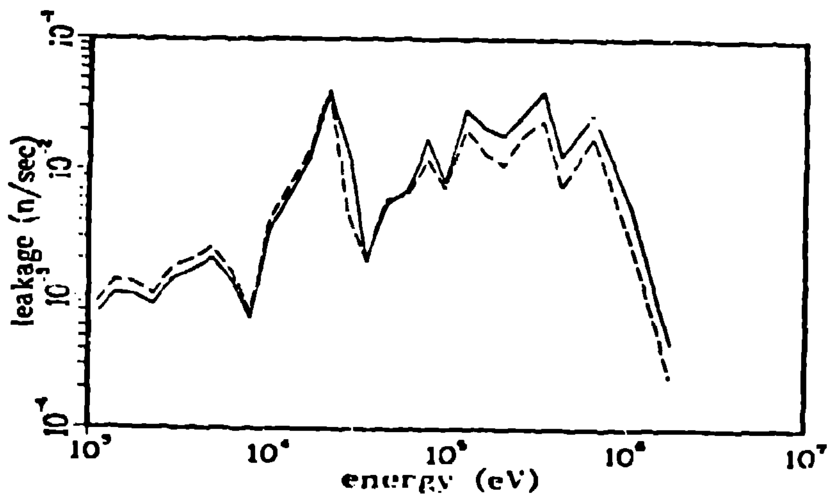

Fig. 2. Total leakage through reflector of ZPR3-54 with (solid) and without (dashed) buckling iteration.

leakage through the "shield" is significantly reduced in the groups containing important resonance minima.

ELASTIC REMOVAL ITERATION

Proper calculation of elastic removal can be particularly important in shielding applications. Shielding calculations frequently involve intermediate mass materials such as iron and sodium for which inelastic scattering is a less influential slowing down mechanism than for the heavy materials found in reactor cores. In addition, such materials (i.e., iron) can have substantial resonance structure in their cross sections.

Formally, the elastic scattering matrix is given by

$$\sigma_{e\ell}^{g\to h} = \frac{\int_{u_{g-1}}^{u_g} du \int_{u_{h-1}}^{u_h} du' \sigma_e(u) p_\ell(u\to u') \phi_\ell(u)}{\int_{u_{g-1}}^{u_g} du \phi_\ell(u)} , \tag{10}$$

where σ_e is the elastic scattering cross section, $p_\ell(u\to u')$ is a Legendre component of the probability of scattering from u to u', and ϕ_ℓ is a Legendre component of the weighting flux.

In the standard background cross section method, the removal from g is approximated by multiplying the group elastic cross section by the logarithmic energy decrement ξ and the flux near the bottom of the group as estimated using the adjacent groups. It has been pointed out[10] that this rather crude approach neglects consideration of the location of resonances within a group. The approach taken in recent cross section libraries[11] has been to evaluate Eq. (10) directly. It still remains to correct for the actual flux at the bottom of the group which may be quite different from the model flux ϕ used in Eq. (10), especially in non-asymptotic shielding problems. Two avenues of improvement have been explored. One is to increase the order of the interpolation on the flux. The other is to retain linear interpolation but to interpolate on a smoother function, the collision density. A combination of the two approaches is also possible. Table 1 gives comparative results.

Table 1. Elastic Removal Correction Factors for Iron in the Reflector of ZPR3-54 for Three Different Methods of Removal Iteration.

Energy Bounds (keV)	Standard Method	High Order Interpolation	Reaction Rate Interpolation
183.2-142.6	.513	.990	1.031
142.6-111.1	1.377	.983	1.093
111.1-86.52	.747	.988	1.010
86.52-67.38	2.561	.982	1.116
67.38-52.48	.758	.977	1.017
52.48-40.87	1.102	.962	.964
40.87-31.83	1.132	1.000	1.153
31.83-24.79	11.414	.996	1.167
24.79-1931	.958	.955	1.001
k_{eff}	0.93221	0.92345	0.92518

It may be observed the k_{eff} (and thus leakage through the "shield") is very sensitive to the removal adjustment. Further in some instances, the standard method led to very large modifications. Actual divergence was observed in a few cases. The improved interpolation procedures have led, in general, to better convergence behavior and more reasonable cross sections.

ELASTIC SELF-SHIELDING AND ANISOTROPY

The effects of self-shielding and the anisotropy explicitly represented by "ℓ" in Eq. (10) remain to be considered. In the standard incarnations of the background cross section method, the f-factor for the elastic scattering cross section for group g is used for all other groups h (normally only h + 1) and all Legendre orders ℓ. Considering that total scattering depends on the entire group energy range to some degree while removel depends mostly on the bottom of the group, this approximation is suspect. For this reason, the new NJOY[12] processing code includes the ability to compute self-shielding factors for all elements of the elastic matrix. Some representative examples are given in Table 2.

It has been noted that deep penetration and streaming make shielding problems sensitive to anisotropic scattering. Concern about the use of the same f-factors for all orders of anisotropy is based on the notion that weighting spectra tend to behave as

Table 2. F-factors for Elastic Scattering in Iron for a 50-Group Structure (T=300 K, σ_0 = .1 barn).

Energy Bounds (keV)	P_0 Total	P_0 Removal	P_1 Total
235.2-182.5	.613	.482	.315
182.5-142.6	.635	.355	.383
142.6-111.1	.481	.612	.250
111.1-86.52	.929	.640	.930
86.52-67.38	.396	1.153	.202
67.38-52.48	.936	.665	.877

$$\phi_\ell \propto \frac{1}{\left[\Sigma_t(u)\right]^{\ell+1}} \quad . \tag{11}$$

Table 2 also illustrates this effect.

CONCLUSION

We have identified three improvements to the background cross section method which promise to make it more generally applicable to shielding problems: buckling iteration, improved removal iteration, and improved elastic matrix self-shielding. These improvements, and others, are being included in a new space-energy cross section code based on transport theory under development at the Los Alamos Scientific Laboratory.

REFERENCES

1. I. Bondarenko, Group Constants for Nuclear Reactor Calculations, Consultants Bureau, New York, 1964.

2. E. M. Bohn, R. Maerker, B. A. Magurno, F. J. McCrossen, and R. E. Schenter, eds., Benchmark Testing of ENDF/B-IV, Brookhaven National Laboratory report BNL-NCS-21118 (ENDF-230) (March 1976).

3. R. E. Schenter, J. L. Baker, and R. B. Kidman, ETOX, A Code to Calculate Group Constants for Nuclear Reactor Calculations, Battelle Northwest Laboratories report BNWL-1002 (1969).

4. B. A. Hutchins and L. N. Price, ENDRUN-1, A Computer Code to Generate a Generalized Multigroup Data File from ENDF/B, General Electric Co. report GEAP-13592 (1970).

5. C. R. Weisbin, P. D. Soran, R. E. MacFarlane, D. R. Harris, R. J. LaBauve, J. S. Hendricks, J. E. White, and R. B. Kidman, MINX: A Multigroup Interpretation of Nuclear X-Sections from ENDF/B, Los Alamos Scientific Laboratory report LA-6486-MS (September 1976).

6. R. W. Hardie and W. W. Little, Jr., 1DX, A One-Dimensional Diffusion Code for Generating Effective Nuclear Cross Sections, Battelle Northwest Laboratories report BNWL-954 (1959).

7. C. L. Cowan, B. A. Hutchins, and J. E. Turner, TDOWN-1, A Code to Compute Composition-Dependent Cross-Sections, General Electric Co. report GEAP-13740 (1971).

8. N. C. Paik, W. Davis, M. B. Yarbrough, and D. Petras, Physics Evaluations and Applications Quarterly Progress Report. Westinghouse Corp. report WARD-XS-3045-7 (1974); see also other reports in this series.

9. R. E. MacFarlane and M. Becker, Self-Shielded Cross Sections for Neutron Transport in Iron," Trans. Am. Nucl. Soc. 22, 668 (1975).

10. W. W. Stacey, "The Effect of Wide Scattering Resonances on Neutron Multigroup Cross Sections," Nucl. Sci. Eng. 47, 29 (1972).

11. R. B. Kidman and R. E. MacFarlane, LIB-IV, A Library of Group Constants for Nuclear Reactor Calculations, Los Alamos Scientific Laboratory report LA-6260-MS (March 1976).

12. R. E. MacFarlane and P. M. Boicourt, "NJOY: A Neutron and Photon Cross-Section Processing System," Trans. Am. Nucl. Soc. 22, 720 (1975).