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THE BACKGROUND CROSS SECTION METHOD AS A GENERAL TOOL FOR REACTOR ANALYSIS[*]

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ABSTRACT

The background cross section method (also called the self-shielding method) has been used extensively in fast reactor analysis. More recently it has also become important in thermal power reactor studies. This paper reviews current applications of the method and describes efforts underway at the Los Alamos Scientific Laboratory to improve the accuracy and reliability of the approach and to extend its applicability to graphite moderated systems and shielding problems. Improvements discussed include a method for automatically accounting for energy dependent buckling that resolves long-standing discrepancies in the calculation of iron reflected criticals and which promises to improve deep-penetration calculations in iron, methods for treating intermediate resonance effects, methods for treating double heterogeneity in gas-cooled reactors, the automatic calculation of Levine factors, improved treatments of elastic removal, and improvements in processing codes and formats.

INTRODUCTION

The background cross-section method (also called the shielding factor method and Bondarenko[1] method) is an economical, designer-oriented method for producing the space-and-energy averaged cross sections required for reactor core analysis. In fast reactor calculations, the codes SPHINX,[2] 1DX,[3] and TDOWN[4] are used extensively. More recently, the background cross section method is becoming important in thermal reactor analysis because of the development of EPRI-CELL and EPRI-CPM.[5]

These codes all use the basic structure shown in Fig. 1. First, an evaluated nuclear data file such as ENDF/B (Ref. 6) is processed into a problem-independent library of microscopic cross sections and shielding parameters using a code like NJOY,[7] MINX,[8] or ETOX.[9] Second, the space-energy code produces self-shielded macroscopic cross sections taking due account of composition and geometry, computes the flux in the assembly vs energy and position, and collapses the cross sections for appropriate space regions and coarse energy groups. The iteration shown allows for criticality searches or self-consistent shielding calculations (see below). The final result is a library of macroscopic cross sections ready to use in a large multidimensional calculation.

The five codes mentioned above differ in the type of flux calculation used (integral transport, collision probability method, B_1, diffusion, and S_N) and in the approximations used in the shielding calculation. This paper will discuss the latter, showing how some of the approximations can be improved, thereby extending the range of applicability of the codes, and showing how the methods of the various codes can be merged into a more consistent and convenient system.
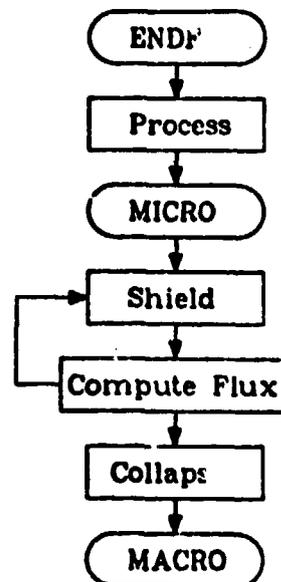
Fig. 1. Basic structure of background method codes.

BACKGROUND METHOD THEORY

The average cross section for group g, material i, and reaction x is defined by

$$\sigma_{xg}^i = \frac{\int_g \sigma_x^i(E)\phi(E)\,dE}{\int_g \phi(E)\,dE} \quad .$$ (1)

Since the flux ϕ is not known, some model flux must be assumed. For example, using the narrow resonance approximation in a large homogeneous system,

$$\phi(E) = \frac{S(E)}{\Sigma_t(E)}$$ (2)

where S(E) is a smooth function of energy representing the scattering and fission sources into E, and Σ_t is the total macroscopic cross section.

In evaluating the numerator of Eq. (1), it is assumed that the important effect is the interaction between a resonance in σ_x and the dip in ϕ caused by that resonance (hence, self-shielding). The reaction rate becomes

$$\int_g \frac{\sigma_x^i(E)}{\sigma_0^i + \sigma_t^i(E)} \, S(E)dE \quad , \tag{3}$$

where

$$\sigma_0^i = \frac{1}{N_i} \sum_{j \neq i} N_j \sigma_t^i \quad , \tag{4}$$

and where N_i is the number density for material i in the mix. It is now further assumed that the "background cross section" σ_0^i is constant in the group. It is this assumption which allows a problem-independent library to be constructed; the processing code simply evaluates Eq. (3) for a range of values of σ_0. The space-energy code determines σ_0 and interpolates for the corresponding self-shielded cross section.

It is the use of this single σ_0 parameter that characterizes the background cross section method. Improvements to the method can be made by (1) improving the cross sections $\sigma_x(\sigma_0)$ or (2) making better choices for σ_0.

THE BUCKLING ITERATION

As an example of the second approach, consider the problem of the iron energy "windows." As shown in Fig. 2, the flux predicted by Eq. (2) becomes very large when the iron cross section becomes small. This high flux weights the small cross section 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 group-averaged cross section is somewhat larger than that predicted by the simple method.

To analyze this effect further, consider the flux predicted by the B_0 and narrow resonance approximations

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

When $B << \Sigma_t$, this reduces to Eq. (2) (i.e., the large system). However, even when the cross section goes to zero, Eq. (5) gives a finite limit (see Fig. 2). A rational approximation to this result is

$$\phi(E) = \frac{S(E)}{\Sigma_t(E) + \frac{2B}{\pi}} \quad . \tag{6}$$

This allows the standard cross section library to be used with

$$\sigma_0^i \leftarrow \sigma_0^i + \frac{2B}{\pi N_i} \quad . \tag{7}$$

In many problems, B can depend on both energy and position[10] and cannot be simply estimated from the size of the system. The solution is to use the flux calculation in the space-energy code to compute B from the calculated flux and leakage. The iteration path is then used to reshield the cross sections for the new σ_0, compute a new flux, and continue to convergence. This procedure has been tested in the 1DX code using diffusion theory with

$$B_{zg} = \sqrt{\left| \frac{L_{zg}}{D_{zg}\phi_{zg}V_z} \right|} \quad . \tag{8}$$

where L_{zg} is the leakage rate from zone z and group g, V_z is the volume of the zone, and D_{zg} is a special diffusion coefficient chosen to reproduce the buckling-theory current (it reduces to $1/3\Sigma_{tr}$ for small B/Σ_t).

The success of the B-iteration in accounting for the "window" streaming is illustrated by an analysis of the iron-reflected critical assembly 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.

ELASTIC SCATTERING

The existing background method codes are weak in their treatment of elastic scattering. As an illustration, the elastic removal differences between 1DX and MC^2-2 (Ref. 11) for a simple homogeneous problem lead to a difference in k of 0.009. These differences have two sources: removal self-shielding and coarse-flux correction.

Following Bondarenko, the fast reactor codes assume that the shielding factor for removal is the same as that for the elastic cross section. Table 1 shows some actual removal shielding factors computed by NJOY; the standard approximation is clearly deficient. The thermal codes either neglect elastic self-shielding entirely or use the potential cross section as an approximation to the fully shielded cross section. Future background method codes and formats should allow for the use of shielded group-to-group transfer cross sections such as those produced by NJOY.
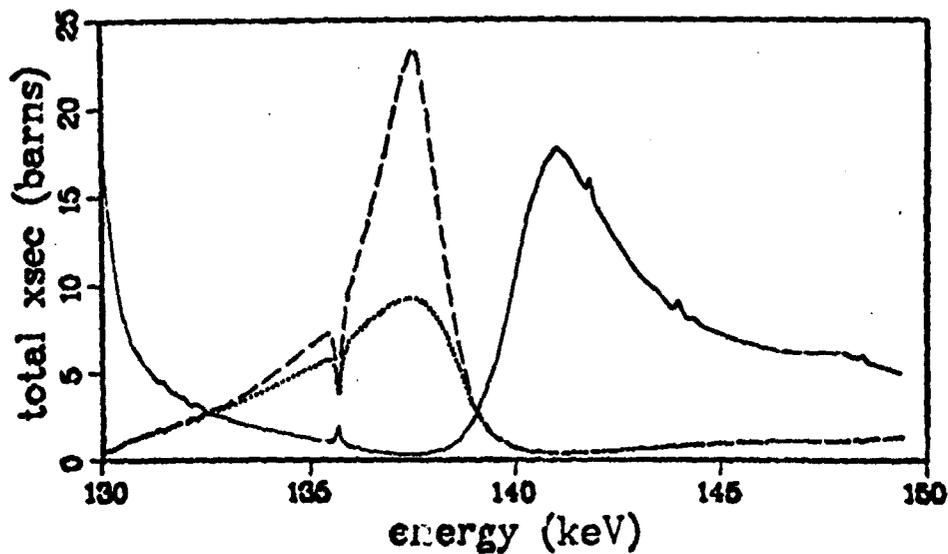
Fig. 2. Flux approximations in a cross section "window" of iron. The solid curve is the scattering cross section, the dashed curve is the infinite medium flux, and the dotted curve if the flux with B_0 approximation leakage.

Table 1. Comparison of Shielding Factors
for Elastic Removal (FR) with Factors
for the Elastic Cross Section (FE)

Energy Range	Iron		U-238	
	FE	FR	FE	FR
111-143 keV	0.835	0.994		
86.5-111	0.983	0.895		
67.4-86.5	0.734	1.158		
52.5-67.4	0.987	0.918		
40.9-52.5	0.997	0.981		
31.8-40.9	0.977	0.850		
24.5-31.8	0.576	1.782		
⋮				
167-275 eV			0.247	1.121
101-167			0.223	0.036
61.4-101			0.275	1.078
37.3-61.4			0.884	0.376
22.6-37.3			0.085	0.948
13.7-22.6			0.179	1.095

The second source of error arises from the difference between the actual variation of the flux across the group and the variation assumed by the processing code. It is conventional to use $S(E) = 1/E$ in the resonance range. However, in a fast reactor, a function like E or E^2 would be more typical below 1 keV. Since most of the removal comes from the bottom of the group for all but the lightest isotopes, the removal rate using the 1/E-weighted cross section will be too large in this energy range.

This problem would be less severe if a better initial guess for $S(E)$ were used. However, $S(E)$ varies from problem to problem, so many different cross section libraries would be required. The problem can also be mitigated by using finer energy groups. This choice has the disadvantages of library bulk and increased computation time. For these reasons, the existing fast reactor background method codes attempt to correct the removal cross section using information about the flux in the adjacent groups. Since the flux depends on the removal cross section, an iteration is required to obtain the correction.

A number of different methods of making the correction have been used. The original 1DX code uses $\sigma_r = \xi\sigma_e$ and uses linear interpolation on the removal rate $\xi\sigma_e\phi$ to estimate the flux near the bottom of the group. This method neglected the effects of resonances and the iteration sometimes diverged. See the third column of Table 2. Later, computed removal cross sections from MINX became available (column 4 of Table 2). They can be corrected by interpolating on the total collision rate $\Sigma_t\phi$ which should be a smooth function of energy for narrow resonances. The results are in column 5. Further refinements in the method are being explored; however, the problem illustrated in Table 2 will ultimately require more groups to reduce the size of the correction and give smoother data for interpolation.

WIDE AND INTERMEDIATE RESONANCES

For thermal reactors, the narrow resonance approximation is no longer accurate enough below 200-300 eV. In the method originally developed for WIMS,[12] Eq. (2) is solved in detail for an infinite homogeneous mixture of the heavy fuel (σ_f) with varying amounts of hydrogen (σ_m) using a point-energy or super-fine-group integral transport code such as RABBLE.[13] This detailed flux can then be used to compute effective multigroup cross sections vs $\sigma_0 = N_m\sigma_m/N_f$.

The NJOY code uses a simpler variation of this approach. For isotropic scattering in the center-of-mass frame, Eq. (2) can be written

$$[\sigma_f(E)+\sigma_0] \phi(E) = \int_E^{E/\alpha_m} \frac{\sigma_0}{(1-\alpha_m)E'} \phi(E')dE' + \int_E^{E/\alpha_f} \frac{\sigma_{sf}(E')}{(1-\alpha_f)E'} \phi(E)dE', \quad (9)$$

where α is the maximum fractional energy change in scattering, and σ_f is the fuel scattering cross section. In an asymptotic thermal system, it is a good approximation to use $\phi(E') = 1/E'$ in the first integral, giving the result σ_0/E independent of moderator mass. The solution to Eq. (9) then depends on the single parameter σ_0 as required for the background cross section method.

Since this approximation to Eq. (9) only requires data over a limited energy range above each E, it is practical to solve it by iteration using detailed pointwise cross sections. The solution proceeds from low energy to high. Above some specified cutoff energy, the narrow resonance result is used. Table 3 compares cross sections obtained with the flux computed in this way with cross sections computed with the narrow resonance approximation flux. Differences as large as 25% such as those seen here can have an important effect in a thermal system.

HETEROGENEITY

In order to treat the heterogeneous configurations used in actual reactor cores, use is made of the well-known equivalence relations[14] between heterogeneous and homogeneous systems. The theory is usually developed for an infinite lattice of two regions (fuel and moderator). Assuming that the resonances in the fuel are narrow and isolated, that the moderator is a pure scatterer, that the flux is spatially flat and recovers to 1/E between resonances in both regions, and that the fuel escape probability can be represented by the rational expression

$$P_f = \frac{\Sigma_e}{\Sigma_f + \Sigma_e} \, , \tag{10}$$

it is found that the heterogeneous system is equivalent to a homogeneous mixture of the fuel and moderator with the moderator cross section changed to Σ_e. Thus, the background method cross sections can be used with $\sigma_0^f = \Sigma_e/N_f$.

Although the assumptions made in obtaining this result are reasonable for calculating resonance absorption in water moderated reactors, they are certainly weak in other energy ranges and for faster systems. Some of these restrictions can be loosened by further analysis. Nevertheless, σ_0 is the only parameter available to the background method, and the validity of the equivalence relations must be assumed. In the end, they are checked against more detailed calculations (e.g., Monte-Carlo) and appropriate parameters are adjusted if necessary. Two such parameters are the Levine geometry factor and the effective cross section used in computing the Dancoff correction for interference between the fuel regions. Methods for obtaining improved estimates for such factors must be developed (especially for fast reactors) allowing for complexities such as multiple regions,[15] non-asymptotic flux, and overlapping resonances.

**Table 2. Comparison of Several Approximate
Elastic Removal Calculations with MC^2-2
Results for Iron in a Fast Reactor Mix**

Upper Energy Bound	MC^2-2 Value (b)	Original 1DX (Δ%)	Uncorrected (Δ%)	Collision Rate (Δ%)
67.4 keV	0.1802	71.7	-30.3	- 4.8
40.9	0.3968	5.6	15.3	5.5
24.8	0.2114	248.3	-63.4	0.7
15.0	0.1284	16.1	13.9	12.4
9.12	0.3872	19.3	15.1	9.2
5.53	0.3877	25.5	5.3	9.4
3.35	0.2089	17.1	45.9	29.4
.2.03	1.3256	-10.3	-29.3	-31.7
1.23	0.5950	- 3.5	3.2	- 4.1
749 eV	0.5536	0.2	9.6	- 2.2
454	0.5195	0.3	18.0	- 1.9
275	0.6279	-16.3	12.1	- 0.5
167	0.5389	5.1	49.9	5.3
101	0.3042	76.1	167.4	76.6

**Table 3. Comparison of Cross Sections
Using Computed Flux to Narrow
Resonance (NR) Cross Sections
for ^{238}U at 100 b Background**

Energy Range	Computed Absorption	NR Absorption
4-9.88 eV	11.75 b	11.78 b
9.88-15.97	0.4518	0.4509
15.97-27.7	8.614	7.729
27.7-48.1	6.012	4.713
48.1-75.5	2.796	2.285
75.5-149	3.178	2.737
149-367	1.955	1.760

Table 4. Resolved Resonance Absorption (4-17.6 eV) in ^{232}Th for an HTGR Design

Temperature (K)	MICROX (Nordheim)	1DX (background)
300	6.76 b	6.72 b
800	8.12	8.03
1200	8.78	8.65

As an example, consider reactors where graphite coated fuel grains are assembled into fuel rods. This results in a "double heterogeneity". It has been shown,[16] that the additional contribution of the grain self-shielding can be allowed for using a modified Levine factor in the standard background cross section method. The modification depends on the size of the grains and on the Dancoff factor for grain-to-grain interference. Comparison of the result of the background method calculations using a modified version of 1DX with General Atomic results using the MICROX[17] code (Nordheim method) in Table 4 shows good agreement.

CODES AND FORMATS

The background method codes share the self-shielding methodology, and thus require similar nuclear data. To lessen the confusion associated with many different libraries and to add new data types needed for code improvements (e.g., elastic matrix self-shielding), Los Alamos and Oak Ridge are developing a new flexible and comprehensive interface called MATXS. It is hoped that this new interface file, together with recent advances in the theory such as those discussed here, will provide the nucleus for a new background method code suitable for fast reactor, therma' reactor, shielding, and fusion applications.

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