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Number of: Pages 6 Tables 1 Figures 0

Word Count: Text 617 + (No. of figures plus tables) × 150 150 + (No. of lines of equations × 10) 70

Total 837

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COMPUTATION OF ANALYTICAL BOUNDS FOR CROSS SECTION SELF-SHIELDING FACTORS*

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Submitted for Presentation to the American Nuclear Society

San Francisco, California, November 11-16, 1979

*Research sponsored by the Reactor Research and Technology Division, U. S. Department of Energy under contract W-7405-eng-26 with the Union Carbide Corporation.

COMPUTATION OF ANALYTICAL BOUNDS FOR CROSS SECTION SELF-SHIELDING FACTORS

The shielding factor method (SFM) is a frequently used economical procedure for computing the effective multigroup cross sections needed in reactor analysis. While initially developed and employed in codes used by the fast reactor community,[1-4] the method has been receiving increased attention in recent years from the electric utility industry, for applications to power reactors.[4-6] A fundamental problem regarding the method's applicability is to determine the limits of the range of values within which a cross section shielding factor is restricted, and whether these limits are physically meaningful. In a previous paper[7] strict upper and lower bounds for the transport f-factor and for the sum of reaction f-factors were derived and discussed. The purpose of the present work is to present extensions of the methodology of Ref. (7).

Strict upper and lower bounds for individual reaction f-factors have now been derived, allowing for cross section discontinuities (e.g. between the resolved and unresolved regions). The resulting expressions were coded in BRINE, a stand alone module easily incorporable into existing SFM cross section processors. BRINE will be used to check the shielding factors in the multi-purpose ENDF/B-V based VITAMIN-E library,[8] now under production at ORNL.

The computation of analytical bounds for the self-shielding factors involves separate treatments of the resolved and unresolved regions, since the corresponding cross-section representations differ. Moreover, particular care is required in handling those groups where cross section discontinuities, allowed by the ENDF specifications,[9] occur. For illustrative purposes, the methodology for deriving a strict upper bound for a flux-weighted reaction f-factor in the resolved resonance region will now be presented. Complete results covering all possible cases are summarized in Table I.

The reaction self-shielding factor $f_G^{x,r}(\sigma_B,T)$ is defined[1-3] as

$$f_G^{x,r}(\sigma_B,T) = \frac{I_G[C(E)]}{I_G[C(E)\sigma_x^r(E,0)]} \cdot I_G\left[\frac{C(E)\sigma_x^r(E,T)}{\sigma_B + \sigma_t^r(E,T)}\right] \Big/ I_G\left[\frac{C(E)}{\sigma_B + \sigma_t^r(E,T)}\right]. \quad (1)$$

$C(E)$ represents the slowly varying broad energy behavior of the flux. The symbol I_G denotes integration over energy, in group G. The various definite integrals involved are clearly finite. The Diaz-Goldmann-Metcalf inequality[10] applied to a pair of positive real valued functions g and h defined on G, gives:

$$I_G[g^2] \cdot I_G[h^2] \leq \{I_G[g \cdot h]\}^2 \cdot [\tfrac{1}{2} + \tfrac{1}{4}(B^2 + \tfrac{1}{B^2})] \quad (2)$$

where $B^2 = (M_g M_h / m_g m_h)$, and M_g, m_g, M_h and m_h denote Sup g, Inf g, Sup h and Inf h over group G, respectively; M_g and m_g can be taken to be the maximum and minimum values, respectively, attained by the function g in the energy interval (group) G. M_h and m_h can be taken similarly for the function h. Consider now two additional functions $\bar{g}$ and $\bar{h}$, defined on G such that:

$$g(E)h(E) = \bar{g}(E)\bar{h}(E) \qquad \text{for } E \in G \;. \quad (3)$$

Then the Cauchy-Schwarz inequality[10] gives:

$$\{I_G[g \cdot h]\}^2 = \{I_G[\bar{g} \cdot \bar{h}]\}^2 \leq I_G[\bar{g}^2] \cdot I_G[\bar{h}^2] \quad (4)$$

Choosing now

$$h^2(E) \equiv \frac{C(E)\sigma_x^r(E,T)}{\sigma_B + \sigma_t^r(E,T)}, \quad \bar{h}^2 \equiv \frac{C(E)}{\sigma_B + \sigma_t^r(E,T)}, \text{ and } g^2(E) \equiv C(E) \quad (5)$$

forces $\overline{g}^2(E)$ to be equal to $C(E)\sigma_x^r(E,T)$, and yields the following strict upper bound for $f_G^{x,r}(\sigma_B,T)$:

$$f_G^{x,r}(\sigma_B,T) \leq \frac{I_G[C(E)\sigma_x^r(E,T)]}{I_G[C(E)\sigma_x^r(E,0)]} \cdot [\tfrac{1}{2} + \tfrac{1}{4}(B^2 + \frac{1}{B^2})] \quad . \tag{6}$$

The strict lower bound for $f_G^{x,r}(\sigma_B,T)$ is derived similarly, leading to

$$f_G^{x,r}(\sigma_B,T) \geq \frac{I_G[C(E)\sigma_x^r(E,T)]}{I_G[C(E)\sigma_x^r(E,0)]} \cdot [\tfrac{1}{2} + \tfrac{1}{4}(B^2 + \frac{1}{B^2})]^{-1} \tag{7}$$

Discontinuities in cross sections at a finite number of points E_b^k in a given group G may occur, as specified by the ENDF procedures.[9] In this case Lebesgue-Stieltjes integrable extensions of the functions g, h, $\overline{g}$, and $\overline{h}$ can readily be constructed. The methodology outlined in Eqs. (2-7) is then directly applicable to the "extended" g and h functions. However extra care needs be excercised when evaluating M_g, m_g, M_h, and m_h since cross section discontinuities may introduce additional "jump" constants. This is shown in Table I.

Important conclusions from this study include:

(1) A general methodology for computing strict upper and lower bounds for self-shielding factors has been developed.

(2) The complete range of self-shielding factors computed by cross section processing codes was addressed, and ENDF/B specified cross section discontinuities were taken into account.

(3) Initial results obtained with data from a preliminary ENDF/B-V file confirm the necessity of replacing any arbitrarily imposed bounds on the shielding factors (e.g. $f_x \leq 1$ forced within some older generation codes[2]) by analytically derived bounds.

(4) The stand alone module BRINE will provide SFM users with a practical tool to check the f-factors.

Table 1. Summary of Analytical Bounds Satisfied by Cross Section Self Shielding Factors

Shielding Factor Type	Resolved Region or Smooth Cross Sections	Unresolved Region Cross Sections	Group Containing A Cross Section Discontinuity e.g. the Resolved/Unresolved Boundary
Reaction Flux-Weighted	U.B. $= [N_G^{x,r}]^2 \; A_G^{x,r}$ L.B. $= \frac{1}{[N_G^{x,r}]^2} A_G^{x,r}$ $A_G^{x,r} = \frac{I_G[C(E)\sigma_x^r(E,T)]}{I_G[C(E)\sigma_x^r(E,0)]}$ $g_+^2 \equiv C(E)$ $\quad g_-^2 \equiv C(E)\sigma_x^r(E,T)$ $h_+^2 \equiv \frac{C(E)\sigma_x^r(E,T)}{\sigma_B + \sigma_t^r(E,T)}$ $\quad h_-^2 \equiv \frac{C(E)}{\sigma_B + \sigma_t^r(E,T)}$ $\left[\tilde{B}_G^{x,r}\right]^2 = \frac{\phi M}{\phi m}\left[\frac{\Sigma_M^{x,r}}{\Sigma_m^{x,r}}\right]^{\frac{1}{2}}\left[\frac{\sigma_B + \Sigma_M^{t_r}}{\sigma_B + \Sigma_M^{t_r}}\right]^{\frac{1}{2}}$	U.B. $= [N_G^{x,u}]^2 \; A_G^{x,u}$ L.B. $= \frac{1}{[N_G^{x,u}]^2} A_G^{x,u}$ $A_G^{x,u} = \frac{I_G[C(E)\,\overline{\sigma}_x(E,\sigma_B,T)]}{I_G[C(E)\,\overline{\sigma}_x^{\infty}(E)]}$ $g_+^2 \equiv C(E)$ $\quad g_-^2 \equiv C(E)\,\overline{\sigma}_x(E,\sigma_B,T)$ $h_+^2 \equiv \frac{C(E)\overline{\sigma}_x(E,\sigma_B,T)}{\sigma_B + \overline{\sigma}_{t,0}(E,\sigma_B,T)}$ $\quad h_-^2 \equiv \frac{C(E)}{\sigma_B + \overline{\sigma}_{t,0}(E,\sigma_B,T)}$ $\left[\tilde{B}_G^{x,u}\right]^2 = \frac{\phi M}{\phi m}\left[\frac{\Sigma_M^{x,u}}{\Sigma_m^{x,u}}\right]^{\frac{1}{2}}\left[\frac{\sigma_B + \Sigma_M^{t_0}}{\sigma_B + \Sigma_M^{t_0}}\right]^{\frac{1}{2}}$	U.B. $= [N_{\tilde{G}}^{x}]^2 \; A_{\tilde{G}}^{x}$ L.B. $= \frac{1}{[N_{\tilde{G}}^{x}]^2} A_{\tilde{G}}^{x}$ $A_{\tilde{G}}^{x} = \frac{I_r[C(E)\sigma_x^r(E,T)] + I_u[C(E)\,\overline{\sigma}_x(E,\sigma_B,T)]}{I_r[C(E)\sigma_x^r(E,0)] + I_u[C(E)\sigma_x^{\infty}(E)]}$ $\tilde{B}_{\tilde{G}}^{x\;2} = \frac{\tilde{M}_g}{\tilde{m}_g}\frac{\tilde{M}_h}{\tilde{m}_h}$ $\tilde{M}_g = \mathrm{Sup}[\tilde{M}_g^r, \tilde{M}_g^u, M_g^{jump}]$, etc. . . . $\tilde{M}_g^r = [\phi_M^r \Sigma_M^{x,r}]^{\frac{1}{2}}$ $\phi_M^r = \mathrm{Sup}_{E\epsilon\Delta_r}[\sqrt{C(E)}]$ $M_g^{jump} = [\phi_b \Sigma_M^{x,b}]^{\frac{1}{2}}$ $\Sigma_M^{x,b} = \mathrm{Sup}\{\sigma_x^r(E_b - 0,T),\, \overline{\sigma}_x(E_b + 0,\sigma_B,T)$ etc. . . .
Total Current-Weighted	Derived in Ref. 7	Derived in Ref. 7	U.B. $= A_{\tilde{G}}^{t_1}$ L.B. $= \frac{1}{\left[N_{\tilde{G}}^{t_1}\right]^2} A_{\tilde{G}}^{t_1}$ $A_{\tilde{G}}^{t_1} = \frac{I_r[C(E)\sigma_t^r(E,T)] + I_u[C(E)\overline{\sigma}_{t,1}(E,\sigma_B,T)]}{I_r[C(E)\sigma_t^r(E,0)] + I_u[C(E)\overline{\sigma}_{t,1}^{\infty}(E)]}$ $\left[\tilde{B}_{\tilde{G}}^{t_1}\right]^2$ derived as above. Note that: $h_+^2 \equiv \frac{C(E)\overline{\sigma}_{t,1}(E,\sigma_B,T)}{[\sigma_B + \overline{\sigma}_{t,0}(E,\sigma_B,T)][\sigma_B + \overline{\sigma}_{t,1}(E,\sigma_B,T)]}$

Notes: 1. For computational efficiency BRINE allows optional use of $\tilde{B}^2$ (see table) instead of B^2, $[N^2 = \frac{1}{2} + \frac{1}{4}(B^2 + \frac{1}{B^2})]$.

2. Notations are self-explanatory: $\Sigma_M^{x,r} = \mathrm{Sup}_E[\sigma_x^r(E,T)]$ for $E\epsilon\Delta_r \cap G$, etc. $(g_+^2, h_+^2) \equiv$ functions used in deriving the upper bound.

3. U.B. = upper bound; L.B. = lower bound.

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