Variational Calculations of Lattice Self-Shielding

Recently Bengston (1) has derived a method for handling one-velocity lattice self-shielding problems, based on the Serber-Wilson procedure of using the exact transport equation to obtain boundary conditions on diffusion-theory solutions. In his test case, an alternating fuel-moderator lattice of fairly thin slabs, the method gave accuracy comparable with that of the much more laborious double-P_3 method. It is the purpose of this letter to present a variational method which yields extremely accurate results with brief hand calculation in problems of this type.

The variational determination of self-shielding factors for lattices and isolated slabs was suggested by Hurwitz (2) and developed by Francis, Stewart, and Bohl (3). In their papers, the method is developed in greater detail and generality than we shall use here; in this letter we confine ourselves to the analysis of two-component lattices with the simplest possible trial function.

We start from the one-velocity, one-dimensional Boltzmann equation for a periodic lattice with isotropic scattering and sources, written as an integral equation for the scalar flux ψ:

$$\psi(x) = \int_0^b G_b(|x - x'|)[p(x')\psi(x') + S(x')]\,dx' \tag{1}$$

$$G_b(|x - x'|) = \frac{1}{2}\sum_{n=-\infty}^{+\infty} E_1(|x - x' + nb|) \tag{2}$$

where distances are measured in total mean free paths, p is the ratio of scattering to total cross section, b is the lattice period, and S is the source density, which we take as unity in the moderator and zero in the fuel. We symmetrize Eq. (1) by introducing

$$f(x) = \frac{1}{\sqrt{p(x)}}[p(x)\psi(x) + S(x)] \tag{3}$$

$$K(x) = S(x)/\sqrt{p(x)} \tag{4}$$

$$H(x, x') = \delta(x - x') - \sqrt{p(x)}G_b(|x - x'|)\sqrt{p(x')} \tag{5}$$

so that

$$\int_0^b H(x, x')f(x')\,dx' = K(x). \tag{6}$$

We require the average value of the flux in the moderator, which is simply related to the integral $\int_0^b K(x)f(x)\,dx$. A variational expression J for the reciprocal of this integral is

$$J = \frac{\int_0^b \int_0^b f_t(x)H(x, x')f_t(x')\,dx\,dx'}{\left[\int_0^b K(x)f_t(x)\,dx\right]^2} \tag{7}$$

where $f_t(x)$ is a trial function. Owing to the symmetry of $H(x, x')$, first-order deviations of $f_t(x)$ from the rigorous solution of (6) generate only second-order errors in J. Furthermore, it is readily shown that these errors are always positive, so the best trial function is that which gives the smallest value of J. Inserting a trial function which is constant within each slab, minimizing J with respect to the ratio of the constants, and eliminating the source density through neutron conservation, we obtain a variational upper bound for the ratio R of average fuel flux to average moderator flux:

$$R = \left[(1 - p_f) \frac{\xi_f Q_{mm}}{\xi_m Q_{mf}} + p_f \right]^{-1} \tag{8}$$

in which ξ_f and ξ_m are the fuel and moderator slab thicknesses ($\xi_f + \xi_m = b$), and the Q's are first collision probabilities; e.g., Q_{mf} is the probability that a neutron introduced uniformly and isotropically into a moderator slab will make its first collision in one of the fuel slabs.

Equation (8) can be derived more physically from multiple scattering arguments, but the above derivation demonstrates that it is an upper bound good through first order in the trial function error. Note that R is independent of moderator absorption in this approximation. Equation (8) is actually exact when the scattering vanishes everywhere, and breaks down only when one or both of the slabs is thick and scatters strongly.

The computation of the Q's which are functions of ξ_f and ξ_m, is facilitated by the conservation and reciprocity relations

$$Q_{mm} + Q_{mf} = 1 \tag{9}$$

$$Q_{ff} + Q_{fm} = 1 \tag{10}$$

$$\xi_m Q_{mf} = \xi_f Q_{fm} . \tag{11}$$

The Q's are found by integrating the kernel $G_b(| x - x' |)$ over the slab of destination and averaging over the slab of origin. Thus

$$\xi_m Q_{mf} = \frac{1}{2} - E_3(\xi) - \sum_{n=1}^{\infty} [E_3(nb + \xi) + E_3(nb - \xi) - 2E_3(nb)] \tag{12}$$

where ξ is either ξ_m or ξ_f. If either one is small, it is convenient to expand the nth term in the sum about nb, giving

$$\xi_m Q_{mf} = \frac{1}{2} - E_3(\xi) - 2 \sum_{k=1}^{\infty} \frac{\xi^{2k}}{(2k)!} \sum_{n=1}^{\infty} E_{3-2k}(nb) \tag{13}$$

where $E_{3-2k}(y)$ denotes the $(2k)$th derivative of $E_3(y)$. When neither ξ_f nor ξ_m is small, the sum in (12) converges rapidly.

We have computed, using the above procedure, the flux ratio R in the test case given

TABLE I

Method	R
Double-P_1	0.857
Double-P_2	0.814
Double-P_3	0.791
Serber-Wilson-Bengston	0.79
Variational	0.7848
Exact	0.7843

by Bengston:

$$\xi_f = 0.295 \qquad \xi_m = 0.1504$$

$$p_f = 0 \qquad p_m = 1$$

with the result given in Table I. We also list the results quoted by Bengston, as well as an "exact" value. The latter was computed using a transport code (TRANVAR) based on the variational method, which essentially performs the calculation using a much more flexible trial function (*4*).

It is worth noting that the computational labor required in the variational method [evaluation of (12), (9), and (8)] is less than in the SWB method, while the accuracy greatly surpasses that of the double-P_3 method in this case.

Since the variational result is the exact R for a problem with no scattering, we see that for this range of ξ_m the influence of moderator scattering on R is confined to the fourth decimal place. For thicker moderator slabs, the average probability that a scattered neutron will reach the fuel begins to depart from the corresponding average probability for a source neutron. The flux ratio then becomes sensitive to the moderator flux shape and the constant-trial function approximation is less accurate. In such cases a hyperbolic cosine can appropriately be used as part of the moderator trial function.

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