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VARIATIONAL CALCULATION OF THERMAL-AVERAGE CROSS SECTIONS

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ABSTRACT

Calculated values of thermal utilization in an infinite medium are in general only as accurate as the neutron energy spectrum used to obtain them. A method of variational calculation of spectra (VARICOS) is outlined here which employs an approximate adjoint (neutron importance) function to obtain improved utilization values with small additional effort.

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VARIATIONAL CALCULATION OF THERMAL-AVERAGE CROSS SECTIONS

J. C. Stewart, N. C. Francis, T. J. Krieger

In the calculation of the thermal utilization of an infinite homogeneous medium it is usually necessary to find the neutron energy spectrum, which depends on the cross sections for energy-exchange scattering and for absorption as functions of energy, as well as on the source present. The resulting flux spectrum is then used to weight the fuel cross section and total capture cross section, and the ratio of these flux-weighted cross sections is the thermal utilization. Similarly, flux-weighted cross sections for other constituents of the medium are sometimes required for the determination of burnout rates.

An accurate flux spectrum, unless absorption is small, requires accurate knowledge of chemical binding effects on the energy-exchange scattering kernel $\sum(E \rightarrow E')$. However, under certain circumstances accurate spectra are superfluous; for example, if the fuel and total-capture cross sections have nearly the same energy dependence the thermal utilization is insensitive to the spectrum. This is another way of saying that the adjoint function, or neutron importance, is nearly constant with neutron energy in this case.

This point can be generalized: if an accurate adjoint (which need not be nearly constant) is known, it is possible to get the thermal utilization and similar integral quantities accurately even though the flux spectrum used is inaccurate. This can be done through the use of variational expressions for the desired integral quantities, containing trial functions which are approximations to the flux and adjoint; the error in such a variational expression is of the order of the product of the flux and

adjoint errors. The straightforward averaging of cross sections over an approximate flux spectrum, as will be seen, is a particular case of the variational expression and results from the insertion of a constant as the adjoint trial function. A very simple improved adjoint can easily be obtained, however, and leads to an improvement in the accuracy of the utilization obtained from a given approximate flux spectrum.

The flux satisfies the integral equation

$$\left[\Sigma_s(E) + \Sigma_a(E)\right]\phi(E) = \int_0^\infty \phi(E')\Sigma(E' \to E)\,dE' + S(E) \tag{1}$$

in the usual notation; upon integration over energy and use of the definition

$$\Sigma_s(E) \equiv \int_0^\infty \Sigma(E \to E')\,dE' \tag{2}$$

a conservation condition is obtained:

$$\int \Sigma_a \phi\, dE = \int S\, dE \tag{3}$$

which equates total capture with total source. The integral of some function F(E) weighted with $\phi(E)$ is desired; expressing this integral in units of the total capture rate in the medium, we have

$$U = \int F \phi\, dE \Big/ \int \Sigma_a \phi\, dE \tag{4}$$

as the desired quantity. When F is the fuel cross section, then, U is the thermal utilization.

We now define g(E), the "adjoint with respect to F", as the solution of the integral equation

$$[\Sigma_s(E)+\Sigma_a(E)]\, g(E) = \int_0^\infty \Sigma(E\to E')\, g(E')\, dE' + F(E) \tag{5}$$

with the physical interpretation that g(E) is the probability that a neutron injected at energy E will be absorbed by the constituent whose cross section is F. In terms of this adjoint, U is just the average of g over the energies at which the source neutrons are injected, i.e.

$$U = \int S g\, dE \Big/ \int S\, dE\ . \tag{6}$$

The detailed-balance property of the scattering kernel may be written

$$M(E)\,\Sigma(E\to E') = M(E')\,\Sigma(E'\to E) \tag{7}$$

where M(E) is the Maxwellian function characteristic of the moderator temperature. This property leads to an adjoint conservation condition

$$\int FM\, dE = \int \Sigma_a M g\, dE \tag{8}$$

which permits us to write (6) in a form independent of normalization:

$$U = \frac{\int FM\, dE}{\int S\, dE} \cdot \frac{\int S g\, dE}{\int \Sigma_a M g\, dE} \tag{9}$$

which may be used as an alternative to (4) if it is g, rather than ϕ, which is known.

The detailed-balance property (7) also gives an alternative physical significance to g: when the source S in (1) is replaced by FM, the resulting flux is Mg. This fictitious flux, since it is fed by a source concentrated around thermal energies, will typically resemble a Maxwellian function much more closely than the actual flux ϕ fed by the high-energy source S.

A variational expression for U can be derived most easily after using the conservation conditions to render (1) and (5) homogeneous; U then appears as an eigenvalue. The variational expression,

$$U = \frac{\int S g \, dE \cdot \int F \phi \, dE}{\int S \, dE \cdot \left\{ \int \phi(E) \left[\Sigma_s(E) + \Sigma_a(E) \right] g(E) \, dE - \iint \phi(E') \Sigma(E' \to E) g(E) \, dE' \, dE \right\}} \quad (10)$$

is stationary with respect to arbitrary independent variations of ϕ and g about the exact solutions of (1) and (5), and hence (as mentioned before) departs from the exact value of U only by a quantity of the order of $\Delta\phi \cdot \Delta g$. Like (4) and (9), (10) is independent of the normalization of ϕ and g.

Note that since ϕ and g are independent trial functions, the sign of the error in (10) is indeterminate; this is a consequence of the non-self-adjointness of the thermalization process.

The previous expressions for U, (4) and (9), can be recovered from (10) by inserting g = const. or ϕ = M respectively; in either case the scattering terms in the denominator of (10) cancel. Both of these trial functions are good in the limit of small absorption, when the correct U is just the ratio of Maxwellian averages; g = const. is also, of course, correct in the degenerate case F/Σ_a = const., even for strong absorption.

In general, for a given approximate ϕ, (10) may be expected to give a better value for U than (4), provided only that an adjoint trial function is used which is better than a constant. We note from (5) that in the limit of strong absorption relative to scattering $g = F/\Sigma_a$, and accordingly adopt as the adjoint trial function

$$g = F/\Sigma_a + B \tag{11}$$

where B is a variational parameter, independent of energy. (This form of g does not require any information about the scattering kernel.) As a trial function for ϕ we may use a linear combination of a Maxwellian function and some function H(E) which has the appropriate slowing-down behavior ($\sim 1/E$) at high energy. Thus

$$\phi = M + AH \tag{12}$$

where A is another variational parameter. A and B may now be determined by invoking the stationary property of (10):

$$\frac{\partial U}{\partial A} = \frac{\partial U}{\partial B} = 0 \tag{13}$$

when A and B have their optimum values. U is next evaluated for this pair of values of A and B. When this procedure is carried out under the additional (physically reasonable) assumption $F/\Sigma_a = 0$ at source energies, a simple result for U is obtained:

$$\frac{1}{U} = (1-\beta)\frac{\int \Sigma_a M\, dE}{\int FM\, dE} + \beta \frac{\int \Sigma_a H\, dE}{\int FH\, dE} \tag{14}$$

where β is a generalized hardening parameter:

$$\beta = \frac{\int F H \, dE}{\iint (F/\Sigma_a)_E \left[H(E')\Sigma(E' \to E) - H(E)\Sigma(E \to E') \right] dE \, dE'} \qquad (15)$$

and $\beta = 1$ represents a "fully hardened" case in which the absorption is so large relative to scattering that the Maxwellian part of the flux spectrum has disappeared. For large absorption, of course, the trial function H should itself depend on the absorption-to-scattering ratio; an appropriate H for such cases is a solution found by neglecting scattering processes in which the neutron gains energy (i.e., by assuming zero moderator temperature).

The adjoint trial function (11) may be replaced, if desired, by a more sophisticated form. One method of getting approximate solutions to (1) or (5) lies in expanding the kernel in terms of its moments, terminating after a couple of terms, and solving the resulting differential equation.[1] Such an expression should be more successful for g than for ϕ, since generally the adjoint is more nearly constant with energy than the ratio of the flux to the Maxwellian is. One precaution must be observed: if a "consistent" approximation scheme such as an expansion in powers of μ (= neutron mass/moderator mass) is used, the kernel must be expanded to higher order when evaluating (10) than when obtaining ϕ and g, in order to reap the benefit inherent in the use of (10) rather than (4) or (9).

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(1) Hurwitz, Nelkin, and Habetler, Nuc. Sci. & Eng. 1, 280 (1956)