

## Letters to the Editors

### Group Averaging of Diffusion Coefficients\*

If one assumes the neutron flux in a reactor to be separable in space and energy, it is simple to show that in the context of the diffusion approximation the correct definition of a group averaged diffusion coefficient is given in terms of the transport mean free path, viz.,

$$D_i \equiv \frac{\langle \lambda_{tr} \rangle_i}{3} \quad (1)$$

The subscript  $i$  denotes the  $i$ th energy group;  $D$  is the diffusion coefficient,  $\Sigma_{tr}$  the transport cross section, and  $\lambda_{tr}$  the transport mean free path. Note that  $\Sigma_{tr i} \neq \langle \Sigma_{tr} \rangle_i$  ( $\Sigma_{tr i} \equiv \frac{1}{3} D_i^{-1}$ )

Equation (1) is inconvenient for practical application because mean free paths combine as the reciprocal of sums of reciprocals. This means that it is not possible to form a group cross-section library of average transport mean free paths for use in various calculations. Rather, each time a reactor's composition is changed the transport mean free path must be re-averaged.<sup>2</sup>

While this difficulty is inherent, there are two alternate definitions of  $D_i$  (or  $\Sigma_{tr i}$ ) which can be combined in elemental fashion and which provide upper and lower limits on the "correct," i.e., Eq. (1), definition of  $\Sigma_{tr i}$ . They are (for an  $N$ -component mixture)

$$\Sigma_{tr i}^a = \sum_{j=1}^N \langle \lambda_i^j \rangle^{-1} \quad (2a)$$

and

$$\Sigma_{tr i}^b = \sum_{j=1}^N \langle \Sigma_{tr}^j \rangle_i \quad (2b)$$

\* A complete description of this work was presented at the Seminar on the Physics of Fast and Intermediate Reactors, sponsored by the International Atomic Energy Agency, Vienna, Austria, August 3-11, 1961, and will appear in the proceedings of that conference under the title "Group Cross Sections for Fast Reactors."

<sup>1</sup> Angular brackets will be used throughout to denote flux-weighted averages, i.e.,

$$\langle X \rangle_i \equiv \frac{\int_i \varphi(E) X(E) dE}{\int_i \varphi(E) dE}$$

where the integration is performed over the  $i$ th energy group.  $\varphi(E)$  represents the neutron flux. An unbracketed, subscripted quantity represents a "group constant".

<sup>2</sup> This problem has been discussed by Petrie, Storm, and Zweifel, *Nuclear Sci. and Eng.* **2**, 728 (1957), in connection with averages in the thermal group.

where the superscript goes over every element in the mixture. In fact, Definition (2a) is commonly used (1). However it is quite simple to prove the following inequality:

$$\Sigma_{tr i}^a \leq \Sigma_{tr i} \leq \Sigma_{tr i}^b \quad (3)$$

To prove inequality (3), we first show that  $\Sigma_{tr i}^b / \Sigma_{tr i} \geq 1$  for a binary mixture whose transport mean free paths are  $\Sigma_1$  and  $\Sigma_2$ . The extension to the general case is trivial, and will not be indicated here.

$$\Sigma_{tr i}^b / \Sigma_{tr i} = \langle \Sigma_1 \rangle + \langle \Sigma_2 \rangle \left\langle \frac{1}{\Sigma_1 + \Sigma_2} \right\rangle \quad (4)$$

However, by appealing to the Schwartz inequality (2), one can show that for sufficiently well behaved functions  $f$  and  $\varphi$ ,

$$\langle f \rangle \langle 1/f \rangle = \frac{\int f(E) \varphi(E) dE \int \{1/f(E)\} \varphi(E) dE}{\left[ \int \varphi(E) dE \right]^2} \geq 1 \quad (5)$$

which proves half of inequality (3). The other half may be proved by writing  $\Sigma_{tr i}^a - \Sigma_{tr i} = \delta$  and showing that  $\delta \leq 0$ . The expression for  $\delta$  can be expressed as the ratio of two quantities, the denominator of which is always positive, and can thus be ignored. The numerator,  $\delta'$ , is given by:

$$\delta' = \left\langle \frac{\Sigma_1 + \Sigma_2}{\Sigma_1 \Sigma_2} \right\rangle \left\langle \frac{1}{\Sigma_1 + \Sigma_2} \right\rangle - \left\langle \frac{1}{\Sigma_1} \right\rangle \left\langle \frac{1}{\Sigma_2} \right\rangle \quad (6)$$

which can be rewritten in the form:

$$\delta' = \frac{1}{2} \iint dE dE' \varphi(E) \varphi(E') \left\{ \frac{\Sigma_1 + \Sigma_2}{\Sigma_1 \Sigma_2} \frac{1}{\Sigma_1' + \Sigma_2'} + \frac{\Sigma_1' + \Sigma_2'}{\Sigma_1' \Sigma_2'} \frac{1}{\Sigma_1 + \Sigma_2} - \frac{1}{\Sigma_1 \Sigma_2'} - \frac{1}{\Sigma_1' \Sigma_2} \right\} \quad (7)$$

where  $\Sigma'$  means  $\Sigma(E')$ . After a little algebraic manipulation,

<sup>3</sup> The proof of Eq. (5) follows from the Schwartz inequality

$$\left( \int gh dE \right)^2 \leq \int g^2 dE \int h^2 dE$$

which holds for functions  $h$  and  $g$  which are *normed* (i.e., the integrals of  $h^2$  and  $g^2$  must exist and be positive). Letting  $g = \sqrt{\varphi/f}$  and  $h = \sqrt{\varphi f}$ , Eq. (5) follows. The condition that  $g$  and  $h$  be normed will clearly be met in any practical reactor core because fluxes and cross sections are positive, nonsingular functions of energy.

Eq. (7) becomes:

$$\delta' = -\frac{1}{2} \iint dE dE' \varphi(E) \varphi(E') \frac{(\Sigma_2 \Sigma_1' - \Sigma_1 \Sigma_2')^2}{\Sigma_1 \Sigma_2 \Sigma_1' \Sigma_2' (\Sigma_1 + \Sigma_2) (\Sigma_1' + \Sigma_2')} \leq 0 \quad (8)$$

This completes the proof of (3).

Another useful result is that a limit can be placed upon the difference between the extremes of (3). Defining

$$\epsilon = \frac{\Sigma_{tr i}^b - \Sigma_{tr i}^a}{\Sigma_{tr i}^a} = \frac{\sum_{j=1}^N \langle \Sigma_j \rangle - \langle 1/\Sigma_j \rangle^{-1}}{\sum_{j=1}^N \langle 1/\Sigma_j \rangle^{-1}}$$

we see that  $\epsilon$  can be written in the form:

$$\epsilon = \frac{\sum_{j=1}^N \langle 1/\Sigma_j \rangle^{-1} \{ \langle \sigma_j \rangle \langle 1/\sigma_j \rangle - 1 \}}{\sum_{j=1}^N \langle 1/\Sigma_j \rangle^{-1}} \quad (9)$$

from which it follows that:

$$[\langle \sigma_j \rangle \langle 1/\sigma_j \rangle - 1]_{\min} \leq \epsilon \leq [\langle \sigma_j \rangle \langle 1/\sigma_j \rangle - 1]_{\max} \quad (10)$$

where  $[\dots]_{\min}$  means that value of the bracketed quantity for that element in the mixture which makes the quantity a minimum and  $[\dots]_{\max}$  has an analogous definition.

An interesting application of these results involves the definition of  $\delta D$ , the perturbation in the diffusion coefficient to be used in the calculation of a reactivity coefficient. We consider the unperturbed system to have a transport cross section  $\Sigma_{tr}^0 = a/E^{1/2}$ , where  $a$  is a constant, and introduce a constant perturbation  $\Sigma_{tr}' = 0.1 a$ . Calculating over an energy group, between limits of 1 and 2 Mev, and assuming for convenience a flux spectrum proportional to  $E^{-1}$ , the following results are obtained:

$$\delta D = -0.043 a^{-1}$$

$$\delta D_a = -0.042 a^{-1}$$

$$\delta D_b = -0.041 a^{-1}$$

The quantity  $\delta D$  was calculated exactly while  $\delta D_a$  and  $\delta D_b$  were obtained from (2a) and (2b) respectively. The expression for  $\delta D$ , given in a report (unpublished) describing the AIM-6 Multigroup Diffusion Equation Code,  $\delta D = -D_0^2 \delta (1/D)$  gives a result of  $0.038 a^{-1}$ , which is about 12% too low.

#### REFERENCES

1. Reactor physics constants. ANL-5800 (1958).
2. A. C. ZAAANEN, "Linear Analysis." Interscience, New York, 1953.

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## Recursion Method for Calculating the Spatial Distribution of Resonance Absorptions

Suppose that the angular and energy distribution of neutrons is known at the surface of a slab which has a single level Breit-Wigner resonance absorption cross section and a constant scattering cross section. We wish to calculate the spatial distribution of these neutrons absorbed in their first collision within the slab.

Since the Breit-Wigner formula is symmetric about the resonance energy, only the symmetric part of the energy dependence of the surface flux will be relevant; let us assume that by some means this symmetric part has been expressed in powers of

$$\psi(x) \equiv (1 + x^2)^{-1}, \quad (1)$$

where  $x \equiv 2(E - E_0)/\Gamma$  in terms of the resonance energy  $E_0$  and half width  $\Gamma$  (a formulation for calculating these components directly from the transport equation is currently being attempted).

The angular dependence of each term can now be expanded in powers of  $\mu$ , the cosine of the angle between the direction of flight and the normal to the slab. For each resulting component of the vector flux,  $\mu^n \psi^n$ , the absorption rate at a distance  $z$  within the slab is proportional to

$$A_{ln}(z) = \frac{1}{\pi} \int_0^1 d\mu \mu^l \int_{-\infty}^{\infty} dx [\psi(x)]^{n+1} \cdot \exp -\frac{z}{\mu} [\Sigma_0 \psi(x) + \Sigma_s], \quad (2)$$

where  $\Sigma_0 \psi$  and  $\Sigma_s$  are the macroscopic absorption and scattering cross sections. Of most interest is  $A_{00}$ , the absorption rate of a thin resonance when the surface flux is isotropic; this case has been treated asymptotically (1) for zero  $\Sigma_s$ .

Rather than seeking closed form approximations, let us consider what would be practical for accurate numerical calculations. Since evaluating  $A_{ln}(z)$  for all values of  $l$ ,  $n$ , and  $z$  by any direct method certainly appears to be a prodigious task, it would seem worthwhile to search for simple relations between adjacent values: what is needed is a differential equation in the continuous variable  $z$  and recursion formulas in the discrete indices  $l$  and  $n$ .

Thus, let us first consider  $A_{l0}$ . By letting  $t$  in Eq. (2) of ref. 2, p. 172 equal  $2\psi - 1$ , one finds that our integral over  $x$  equals  $\pi f(t\rho)$ , where  $f(\xi) \equiv e^{-(1+\alpha)\xi} I_0(\xi)$ ,  $\alpha \equiv 2\Sigma_s/\Sigma_0$ ,  $t \equiv 1/\mu$ ,  $\rho \equiv \Sigma_0 z/2$ , and  $I_0$  is a modified Bessel function (a relationship that has also been used by several authors previously). Changing the variable of integration from  $\mu$  to  $t$  gives

$$A_{l0}(\rho) = \int_1^{\infty} f(t\rho) \frac{dt}{t^{l+2}}. \quad (3)$$

Therefore,