On the Energy Averaging of the Diffusion Coefficient

For several years there has been much discussion on the proper manner in which to energy average the diffusion coefficient for use in multigroup diffusion theory. In particular, the argument has centered around whether one should average the diffusion coefficient or the reciprocal of the diffusion coefficient, i.e., the transport cross section. For example, Weinberg and Wigner[1] and earlier workers have shown that if the flux is separable in space and energy, then the correct procedure is to average the diffusion coefficient with respect to the separable spectrum. On the other hand, Sjostrand[2] has shown, using a separability assumption, that the correct procedure is to average the transport cross section with respect to the separable spectrum. In this note we make a few observations in the hope of shedding some light on this general problem. In particular, we discuss the apparent paradox between the result of Weinberg and Wigner and that of Sjostrand.

If one expands the transport equation in a low-order (P-1) spherical-harmonic series, making use of the transport cross section to account for P-1 scattering, one obtains the simple energy-dependent diffusion approximation, i.e., the conservation equation

$$\vec{\nabla}\cdot\vec{j}(\vec{r},E)+\Sigma(\vec{r},E)\phi(\vec{r},E) = \int_0^\infty dE'\Sigma_s(\vec{r},E'\to E)\phi(\vec{r},E')+ S(\vec{r}), \quad (1)$$

and Fick's law of diffusion

$$\vec{j}(\vec{r},E) = -\frac{1}{3\Sigma_{tr}(\vec{r},E)}\vec{\nabla}\phi(\vec{r},E), \quad (2)$$

where, for simplicity, we have assumed a time-independent problem with no fission. (These assumptions in no way affect the arguments to be made.) In equations 1 and 2,

- $\vec{r}$ is the spatial coordinate,
- E is the energy coordinate,
- $\phi(\vec{r},E)$ is the scalar flux per unit energy,
- $\vec{j}(\vec{r},E)$ is the current per unit energy,
- $\Sigma(\vec{r},E)$ is the macroscopic collision cross section,
- $\Sigma_s(\vec{r},E'\to E)$ is the macroscopic differential-scattering cross section,
- $\Sigma_{tr}(\vec{r},E)$ is the macroscopic transport cross section, and
- $S(\vec{r})$ is the external source.

Integrating the $s(s=s,y,z)$ component of equation 2 over the i^{th} group yields

$$J_s^i(\vec{r}) = -\frac{1}{3}\left[\frac{1}{\Sigma_{tr}(\vec{r})}\right]_i^{\partial\phi/\partial s}\frac{\partial\Phi^i(\vec{r})}{\partial s}, \quad (3)$$

where we have defined the i^{th} group flux and s component of the i^{th} group current as

$$\Phi^i(\vec{r}) \equiv \int_i dE\phi(\vec{r},E), \quad (4)$$

$$J_s^i(\vec{r}) \equiv \int_i dE j_s(\vec{r},E), \quad (5)$$

and

$$\left[\frac{1}{\Sigma_{tr}(\vec{r})}\right]_i^{\partial\phi/\partial s} \equiv \frac{\int_i dE\left(\frac{1}{\Sigma_{tr}(\vec{r},E)}\right)\frac{\partial\phi(\vec{r},E)}{\partial s}}{\int_i dE\frac{\partial\phi(\vec{r},E)}{\partial s}}. \quad (6)$$

Thus we see that we obtain a parallel average of Σ_{tr} with respect to the gradient of the flux. It is emphasized here that no approximations (i.e., separability) have been introduced.

Equally well, equation 2 can be written

$$3\Sigma_{tr}(\vec{r},E)\,\vec{j}(\vec{r},E) + \vec{\nabla}\phi(\vec{r},E) = 0. \quad (7)$$

Integrating the s component of equation 7 over the i^{th} group yields

$$3[\Sigma_{tr}(\vec{r})]_i^{j_s} J_s^i(\vec{r}) + \frac{\partial\Phi^i(\vec{r})}{\partial s} = 0, \quad (8)$$

where we have defined

$$[\Sigma_{tr}(\vec{r})]_i^{j_s} \equiv \frac{\int_i dE\Sigma_{tr}(\vec{r},E)j_s(\vec{r},E)}{\int_i dE j_s(\vec{r},E)}. \quad (9)$$

Equation 9 indicates that one should series average Σ_{tr} with respect to the current. Again no approximations have been made.

Now, comparing equations 3 and 8, we deduce

$$\left[\frac{1}{\Sigma_{tr}(\vec{r})}\right]_i^{\partial\phi/\partial s} = 1/[\Sigma_{tr}(\vec{r})]_i^{j_s}, \quad (10)$$

i.e., the average of the reciprocal of the transport cross section with respect to the gradient of the exact flux solution of equations 1 and 2 is precisely equal to the reciprocal of the average of the transport cross section with respect to the exact current solution of equations 1 and 2. Equation 10 can also directly be shown to be an identity by using equation 2 (Fick's law) in the right side of equation 9 to eliminate $j_s(\vec{r},E)$ in favor of $\frac{\partial\phi(\vec{r},E)}{\partial s}$. The result is just the reciprocal of the right side of equation 6. Thus, if one has available the exact solution of equations 1 and 2, one can either parallel or series average Σ_{tr} according

[1] A. M. WEINBERG and E. P. WIGNER, *The Physical Theory of Neutron Chain Reactors*, p. 514. Univ. of Chicago Press, Chicago, (1958).

[2] N. G. SJÖSTRAND, *J. Nucl. Energy, Part A; Reactor Science*, 12, 151-154 (1960).

to equation 6 or equation 9. Both equations give the same result. The multigroup diffusion equations, with these values of the group-average diffusion coefficients, will then yield an exact solution of equations 1 and 2 for the group fluxes and currents.

However, if one has available the exact solution of equations 1 and 2 for $\phi(\vec{r},E)$ and $\vec{j}(\vec{r},E)$, then one can directly compute all the details of the system being studied, and there is no need to consider the multigroup equations. In general, one performs an approximate calculation to obtain the spectrum from which the multigroup constants are obtained. The crudest (and most commonly used) method is to assume that the energy dependence of the flux and current is separable from the spatial dependence. One then performs a zero-dimensional calculation to obtain this energy dependence.

We now come to the apparent paradox between the conclusion of Weinberg and Wigner and that of Sjostrand. The significant point here is that one must define precisely what is meant by space-energy separation. Weinberg and Wigner write

$$\phi(\vec{r},E) = \phi(\vec{r})f(E). \tag{11}$$

From equations 2 and 11, the following proportionalities, in the energy variable, are evident:

$$\vec{\nabla}\phi \sim f(E), \tag{12}$$

$$\vec{j} \sim \frac{f(E)}{\Sigma_{tr}(\vec{r},E)}. \tag{13}$$

We note that the flux and current have different energy dependences. Using equation 12 in equation 6, we deduce that one should parallel average the transport cross section with respect to the flux spectrum, $f(E)$—i.e., one should series average the diffusion coefficient. Using equation 13 in equation 9, we again draw the same conclusion.

Sjostrand assumes that the transport directional flux is separable according to

$$\phi(\vec{r},\vec{\Omega},E) = \phi(\vec{r},\vec{\Omega})g(E). \tag{14}$$

Here, in the energy variable, the proportionalities that follow are

$$\vec{\nabla}\phi \sim g(E), \tag{15}$$

$$\vec{j} \sim g(E). \tag{16}$$

We note that the flux and current have the same energy dependence. Using equation 15 in equation 6, we deduce that one should parallel average Σ_{tr} with respect to $g(E)$, whereas, using equation 16 in equation 9, we deduce that one should series average Σ_{tr} with respect to $g(E)$. Thus with Sjostrand's assumed separability, one is able to arrive at either conclusion. In his paper, Sjostrand arrived at the series average of Σ_{tr}. We conclude that Sjostrand's assumption can only be strictly true if both averaging procedures yield identical results, which in general implies that the transport cross section is energy independent.

We finally come to the question of which averaging procedure should be used in practice. Since the assumption of Weinberg and Wigner always leads to the same conclusion, whereas that of Sjostrand does not, it seems reasonable that, *a priori*, Weinberg and Wigner's scheme should be used, i.e., one should parallel average Σ_{tr}. Moreover, it is clear that Sjostrand's separability assumption is far more restrictive than that of Weinberg and Wigner. Sjostrand assumes that all of the angular modes of the directional flux have a common, separable energy dependence. Weinberg and Wigner merely claim that the zeroth mode (scalar flux) has a separable energy dependence. For example, it is a well known fact that the diffusion-theory solution of the homogeneous bare core (with a negligible extrapolation distance) is indeed separable according to equation 11 for an arbitrary energy dependence of the transport cross section. The corresponding angular flux, truncated to the diffusion-theory approximation, is not separable—i.e., equation 14 does not hold. Said another way: if energy-dependent diffusion theory is assumed to describe the system adequately, then equation 2 immediately indicates that the spectrum of the current must, in general, be different from that of the flux, contrary to equation 14. Thus, Sjostrand's separability assumption is incompatible with energy-dependent diffusion theory. Another argument in favor of the parallel average of Σ_{tr} is that it is obtained by integrating over equation 2, thus preserving the current.

Of course, when the flux is not separable in any sense, it may well be that in certain instances a series average of Σ_{tr} may lead to more accurate results than a parallel average. Which scheme to use in a particular instance will depend upon the problem under consideration and the assumptions used in computing the separable spectrum, as well as the particular quantities of interest from the multigroup solution. Without any *a priori* knowledge of the problem to be solved, however, the 'best strategy' seems to be a parallel average of the transport cross section.

If one is not satisfied with the separability assumption and computes approximate spatially-dependent flux and current spectra, these spectra will not, in general, satisfy equation 2. Thus equations 6 and 9 will yield different results. As the spectra used approach the exact spectra, equation 2 will be satisfied, and in this limit the two averaging schemes will give the same result. (We note that any spectra, no matter how inaccurate, that satisfy equation 2 will force equations 6

and 9 to give the same result.) If equation 2 is not satisfied by the approximate spectra, it seems reasonable to use equation 6 in preference to equation 9, since equation 6, obtained by integrating over equation 2, preserves the current. It is emphasized that if the flux spectrum is spatially dependent, the proper weight function for the parallel averaging procedure, equation 6, is the gradient of the flux, and not the flux itself. For multidimensional problems this will, in general, lead to an anisotropic diffusion coefficient.

For completeness, we show how one can arrive at another averaging scheme often quoted in the literature—that of averaging the reciprocal of the transport cross section in a homogeneous region over the Laplacian of the flux. Using equation 2 in equation 1, we find for the leakage term in a homogeneous region

$$\text{Leakage} = \frac{1}{3\Sigma_{tr}(E)} \nabla^2 \phi(\vec{r}, E). \qquad (17)$$

Equating the integral over energy of equation 17 to the i^{th} group leakage term yields

$$(\text{Leakage})_i = \frac{1}{3}\left[\frac{1}{\Sigma_{tr}(E)}\right]_i^{\nabla^2} \nabla^2 \Phi^i(\vec{r}), \qquad (18)$$

where we have defined

$$\left[\frac{1}{\Sigma_{tr}(E)}\right]_i^{\nabla^2} \equiv \frac{\int_i dE \left(\frac{1}{\Sigma_{tr}(E)}\right) \nabla^2 \phi(\vec{r}, E)}{\int_i dE \nabla^2 \phi(\vec{r}, E)}. \qquad (19)$$

Equation 19 indeed indicates that one should average the reciprocal of the transport cross section over the Laplacian of the flux. We note that this type of average leads to a simpler result than equation 6 in that the group-averaged diffusion coefficient is isotropic. This simplicity is obtained at the expense of accuracy—i.e., equation 19 was derived by integrating over the net leakage term, thus preserving the divergence of the current, whereas equation 6 was derived by integrating over Fick's law, equation 2, thus preserving the current itself. Accordingly, *a priori* one should expect that equation 6, which preserves more detailed quantities, will yield better over-all results than equation 19. If one is only interested in computing the group fluxes, both averaging procedures should be equally accurate since it is only the divergence of the current that enters into the calculation. If, however, one wishes to compute the group currents, then the use of equation 6 should yield more accurate results. It is interesting to note that the group-averaged diffusion coefficient defined by equation 19 is properly a multiplier of the Laplacian in equation 18, even though, in general, equation 19 will lead to a spatially dependent quantity. If equation 6 or equation 9 is used, the diffusion coefficient is acted upon by the divergence operator in computing the net leakage.

It is hoped that the foregoing remarks may be of some help in comparing the bases for the various averaging procedures suggested in the literature.

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Generalizations of Fick's Law

Using the one-velocity Boltzmann equation for slab geometry and a homogeneous isotropic medium, Adler[1] derived a relationship between the net current $J(z)$ and the neutron density $N(z)$,

$$J(z) = -\frac{v}{\Sigma_{tr}} \frac{d}{dz} [\overline{\mu^2}(z) N(z)] \qquad (1)$$

$$\overline{\mu^2}(z) = \frac{\int \mu^2 n(z,\mu) d\mu}{\int n(z,\mu) d\mu} \qquad (2)$$

$$\Sigma_{tr} = \Sigma - \overline{\mu_0} \Sigma_s \qquad (3)$$

where $\overline{\mu^2}(z)$ is the mean square cosine of the angular distribution and $\overline{\mu_0}$ is the mean cosine of the scattering angle. Equation (1) is a one-velocity generalization of Fick's law.

The one-velocity restriction on Equation (1) can be removed by considering the velocity-dependent Boltzmann equation

$$\frac{\partial n}{\partial t} = -v_z \frac{\partial n}{\partial z} - kn + \iiint n(z, v', \underset{\sim}{\omega}', t) v' \Sigma_s(\underset{\sim}{v}' \rightarrow \underset{\sim}{v}) dv' d\omega' \qquad (4)$$

where $n(z, v, \underset{\sim}{\omega}, t) dV dv d\omega$ is the number of neutrons in dV at z whose speeds are in dv at v and whose directions of motion lie in the solid angle $d\omega$ at $\underset{\sim}{\omega}$ at time t. The term $k = v\Sigma$ is the collision rate per neutron. If we assume that the cross section for velocity change $\Sigma_s(\underset{\sim}{v}' \rightarrow \underset{\sim}{v})$ depends only on the initial speed v', the final speed v, and $\underset{\sim}{\omega}' \cdot \underset{\sim}{\omega}$, then

[1] F. ADLER, in *Reactor Handbook*, (H. SOODAK, ed.), AECD-3645, Vol. I, p. 385. United States Atomic Energy Commission (1955); *Reactor Handbook* (H. SOODAK, ed.), Vol. III, Part A, p. 140. Interscience Publishers, New York (1962).