Reply to "Comment on 'Reduction of "Calculational" Uncertainties Due to Approximate Fission-Source Matrices'"

In a recent Note,[1] we proposed a simple scheme for refining transport calculations in codes like ANISN (Ref. 2), DOT (Ref. 3), and XSDRNPM (Ref. 4), which are limited to using only outer-product fission-source matrices, *without* modifying these codes. Unfortunately, Hill's comment[5] misinterprets our Note as a "report on the effect of a single fission-neutron-independent spectrum" (whatever that means . . .) "versus the exact full fission matrix." In this Letter we shall not only clarify a few fine points that Hill might have overlooked, but also describe numerical schemes that we have been successfully using for many years in the *direct* calculation of various eigenvalues using our own S_n code.

The rigorous treatment of the source term in the transport equation calls for a full scattering matrix $\tau^s_{gg'}$ (**S** in Ref. 5) and a full fission matrix $\tau^f_{gg'}$ ($\chi\nu\Sigma_f$ in Ref. 5). The use of full fission-source matrices in neutron transport calculations was indeed reported by Hill et al.[6] in June 1973 and, by the way, also by Wagschal and Yaari[7] even in March 1973. Unfortunately, the use of full fission-source matrices is still rather uncommon, perhaps because Hill et al.[6] concluded that "the use of these fission matrices does not seem warranted." As we emphasize in Ref. 1, even though the effect of the outer-product fission-source matrices is not necessarily that important, it introduces a computational error, which may equal the experimental uncertainty in k_{eff}, and which can be easily substantially reduced or eliminated altogether without having to modify the transport codes.

The rigorous total-source matrix $\tau_{gg'}$ is

$$\tau_{gg'} = \tau^s_{gg'} + \tau^f_{gg'} \quad , \tag{1}$$

and in k_{eff} calculations it is replaced by an effective total-source matrix $\tau^k_{gg'}$, using the k_{eff} eigenvalue k,

$$\tau^k_{gg'} = \tau^s_{gg'} + \frac{1}{k}\tau^f_{gg'} \quad . \tag{2}$$

The Los Alamos National Laboratory codes, ONETRAN (Ref. 8) and TIMEX (Ref. 9), and our own S_n code[7] have an option (default in our case) to correctly treat the full fission-source matrix as in Eq. (2). The values labeled "reference" in Table I of Ref. 1 are therefore quite exact.

Since most commonly used codes are limited to employing outer-product fission-source matrices $(\nu\sigma_f)_{g'}\mathbf{f}_g$ ($\widetilde{\chi\nu\Sigma}_f$ of Ref. 5) only, we proposed to replace the true scattering matrix $\tau^s_{gg'}$ of Eqs. (1) and (2) by a modified scattering matrix $\hat{\tau}^s_{gg'}$ when using these codes. The modified matrix $\hat{\tau}^s_{gg'}$ is[1]

$$\hat{\tau}^s_{gg'} = \tau_{gg'} - (\nu\sigma_f)_{g'}\mathbf{f}_g \quad , \tag{3}$$

and not as implied by Hill[5] in his Eq. (3b). The approximate effective-total-source matrix in codes like ANISN would thus be

$$\hat{\tau}^k_{gg'} = \hat{\tau}^s_{gg'} + \frac{1}{\hat{k}}(\nu\sigma_f)_{g'}\mathbf{f}_g = \tau^s_{gg'} + \tau^f_{gg'} - \left(1 - \frac{1}{\hat{k}}\right)(\nu\sigma_f)_{g'}\mathbf{f}_g \quad , \tag{4}$$

and the difference between the rigorous and approximate effective-total-source matrix is

$$\widehat{\Delta\tau}_{gg'} = \tau^k_{gg'} - \hat{\tau}^k_{gg'} = \left(\frac{1}{k} - 1\right)\tau^f_{gg'} - \left(\frac{1}{\hat{k}} - 1\right)(\nu\sigma_f)_{g'}\mathbf{f}_g \quad . \tag{5}$$

Using an ANISN-type code without modifying the scattering matrix, the effective-total-source matrix is

$$\tilde{\tau}^k_{gg'} = \tau^s_{gg'} + \frac{1}{\tilde{k}}(\nu\sigma_f)_{g'}\mathbf{f}_g \quad , \tag{6}$$

and the difference between the rigorous and this approximate effective-total-source matrix is

$$\widetilde{\Delta\tau}_{gg'} = \tau^k_{gg'} - \tilde{\tau}^k_{gg'} = \frac{1}{k}\tau^f_{gg'} - \frac{1}{\tilde{k}}(\nu\sigma_f)_{g'}\mathbf{f}_g \quad . \tag{7}$$

It is obvious that $\widehat{\Delta\tau}_{gg'}$ is much smaller than $\widetilde{\Delta\tau}_{gg'}$ even when k is not equal to unity, and that for $k = 1$, $\widehat{\Delta\tau}_{gg'}$ will vanish, whereas $\widetilde{\Delta\tau}_{gg'}$ generally will not vanish.

The decrease of the discrepancy between the rigorous and approximate values of a few integral parameters when using our modified scattering matrix scheme is clearly demonstrated in Table I of Ref. 1.

For other than k_{eff} problems, i.e., other types of eigenvalues or source-driven subcritical systems, $\hat{\tau}_{gg'}$ is indeed *identical* to $\tau_{gg'}$. In such problems $k = \hat{k} = \tilde{k} = 1$, $\widehat{\Delta\tau}_{gg'} = 0$, but $\widetilde{\Delta\tau}_{gg'}$, in general, will not be equal to zero, since the full fission matrix cannot always be factored into $(\nu\sigma_f)_{g'}\mathbf{f}_g$. This is exactly the reason why the ANISN factored-fission-matrix scheme should be replaced by the full fission matrix treatment. However, we have shown[1] that no matter how bad a factorization is used, with our modified scattering matrix, the results are *rigorous* for non-k_{eff} problems and an excellent approximation in k_{eff} problems *without* modifying the ANISN code.

Hill[5] states that to his knowledge, no general S_n transport code can use only the total scattering matrix. What he probably means is the total source matrix. In any case, our S_n code has the option of using only the total source matrix in non-k_{eff} problems. Moreover, we do not use any intermediate eigenvalue, and each primary eigenvalue is being calculated directly. In the following section, we will describe our direct procedure for the calculation of a few eigenvalues.[10]

Several eigenvalue-type representations of the neutron transport equation have been considered. These eigenvalue equations are

$$(\alpha/v + \mathbf{\Omega}\cdot\nabla + \Sigma_t)\phi_\alpha = Q_s[\phi_\alpha] + Q_f[\phi_\alpha] = Q[\phi_\alpha] \quad , \tag{8}$$

$$(\mathbf{\Omega}\cdot\nabla + \Sigma_t)\phi_\gamma = \frac{1}{\gamma}\{Q_s[\phi_\gamma] + Q_f[\phi_\gamma]\} = \frac{1}{\gamma}Q[\phi_\gamma] \quad , \tag{9}$$

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[2] W. W. ENGLE, Jr., "ANISN, A One-Dimensional Discrete Ordinates Transport Code with Anisotropic Scattering," K-1693, Oak Ridge Gaseous Diffusion Plant (1967).

[3] F. R. MYNATT, "DOT—Two Dimensional Discrete Ordinates Transport Code," K-1694, Oak Ridge Gaseous Diffusion Plant (1967).

[4] L. M. PETRIE and N. M. GREENE, "XSDRNPM: AMPX Module with One-Dimensional S_n Capability for Spatial Weighting," Chap. 8, AMPX-II RSIC PSR-63, Radiation Shielding Information Center, Oak Ridge National Laboratory (1978).

[5] T. R. HILL, *Nucl. Sci. Eng.*, **86**, 116 (1984).

[6] T. R. HILL, K. D. LATHROP, and G. HANSEN, *Trans. Am. Nucl. Soc.*, **16**, 329 (1973).

[7] J. J. WAGSCHAL and A. YAARI, "A Systematic Test of the ENDF-B3 Evaluated Cross-Section Library on 'Clean' Critical Assemblies," in "Nuclear Data in Science and Technology II," IAEA-SM-170/19, International Atomic Energy Agency (1973).

[8] T. R. HILL, "ONETRAN: A Discrete Ordinates Finite Element Code for the Solution of the Multigroup Transport Equation," LA-5990-MS, Los Alamos National Laboratory (1975).

[9] T. R. HILL and W. H. REED, "TIMEX: A Time-Dependent Explicit Discrete Ordinates Program for the Solution of the Multigroup Transport Equations with Delayed Neutrons," LA-6201-MS, Los Alamos National Laboratory (1976).

[10] D. G. CACUCI et al., *Nucl. Sci. Eng.*, **81**, 432 (1982).

and

$$\boldsymbol{\Omega}\cdot\nabla\phi_\delta = \frac{1}{\delta}\{Q_s[\phi_\delta] + Q_f[\phi_\delta] - \Sigma_t\phi_\delta\}$$

$$= \frac{1}{\delta}Q[\phi_\delta] - \frac{\Sigma_t}{\delta}\phi_\delta \ . \qquad (10)$$

The quantities appearing (in abbreviated notation) in the above equations are defined as follows:

1. The quantities $\phi(\boldsymbol{r},E,\boldsymbol{\Omega})$ and $\Sigma_t(\boldsymbol{r},E)$ are the (space-, energy-, and angle-dependent) flux and the (space- and energy-dependent) total macroscopic cross section.

2. The quantity

$$Q_s[\phi] \equiv \int_0^\infty dE' \int_{4\pi} d\boldsymbol{\Omega}'\Sigma_s(\boldsymbol{r};E',\boldsymbol{\Omega}'\to E,\boldsymbol{\Omega})\phi(\boldsymbol{r},E',\boldsymbol{\Omega}') \qquad (11)$$

is the scattering source term.

3. The quantity

$$Q_f[\phi] \equiv \int_0^\infty dE' \int_{4\pi} d\boldsymbol{\Omega}'[\chi(E'\to E)\nu(\boldsymbol{r},E')\Sigma_f(\boldsymbol{r},E')/4\pi]$$

$$\times\,\phi(\boldsymbol{r},E',\boldsymbol{\Omega}') \qquad (12)$$

is the fission source term.

Note that both $Q_s[\phi]$ and $Q_f[\phi]$ are linear functionals of the flux ϕ. The eigenvalues α, γ, and δ, which appear in Eqs. (8), (9), and (10), respectively, represent the asymptotic inverse reactor period, the effective collision multiplication factor, and the effective density factor.

Equations (8), (9), and (10) are being solved iteratively. The flux obtained in the $(n-1)$'th iteration, $\phi^{(n-1)}$, is used to calculate the source term for the n'th iteration, $Q[\phi^{(n-1)}]$, and the latest eigenvalue $[\alpha^{(n-1)}, \gamma^{(n-1)}$, and $\delta^{(n-1)}]$ is being used to calculate the flux in the n'th iteration. Equations (8), (9), and (10) can thus be rewritten as

$$[\alpha^{(n-1)}/v + \boldsymbol{\Omega}\cdot\nabla + \Sigma_t]\phi_\alpha^{(n)} = Q[\phi_\alpha^{(n-1)}] \ , \qquad (8')$$

$$(\boldsymbol{\Omega}\cdot\nabla + \Sigma_t)\phi_\gamma^{(n)} = \frac{1}{\gamma^{(n-1)}}Q[\phi_\gamma^{(n-1)}] \ , \qquad (9')$$

and

$$\left[\boldsymbol{\Omega}\cdot\nabla + \frac{\Sigma_t}{\delta^{(n-1)}}\right]\phi_\delta^{(n)} = \frac{1}{\delta^{(n-1)}}Q[\phi_\delta^{(n-1)}] \ . \qquad (10')$$

The new estimates for the eigenvalues are derived from

$$\alpha^{(n)} = \alpha^{(n-1)} + \frac{S[\phi_\alpha^{(n)}] - S[\phi_\alpha^{(n-1)}]}{W[\phi_\alpha^{(n)}]} \ , \qquad (13)$$

$$\gamma^{(n)} = \gamma^{(n-1)}\frac{S[\phi_\gamma^{(n)}]}{S[\phi_\gamma^{(n-1)}]} \ , \qquad (14)$$

and

$$\delta^{(n)} = \delta^{(n-1)}\frac{S[\phi_\delta^{(n)}] - T[\phi_\delta^{(n)}]}{S[\phi_\delta^{(n-1)}] - T[\phi_\delta^{(n)}]} \ . \qquad (15)$$

The quantities appearing (in abbreviated notation) in the preceding equations are defined as follows:

1. $S[\phi^{(n)}]$ is essentially the integral over phase space of the total source term $Q[\phi^{(n)}]$
2. $W[\phi_\alpha^{(n)}]$ is the integral over phase space of $1/v$ times the flux $\phi_\alpha^{(n)}(\boldsymbol{r},E,\boldsymbol{\Omega})$
3. $T[\phi_\delta^{(n)}]$ is the integral over phase space of Σ_t times the flux.

In conclusion, we are grateful to Dr. Hill for his comments that provided an opportunity to stress once again what is rigorous and what is a very good approximation. We are also pleased to be able to introduce the algorithms for the direct evaluation of various eigenvalues. It is a pity that Hill did not make any comment on the closing remarks of Ref. 1.

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Propagation of Knowledge Regarding Conservation During Doppler Broadening

Canfield[1] in 1967 and later Cullen[2] in 1973 demonstrated that the area under the cross-section curve is not conserved and that the only conservation law associated with Doppler broadening is the integral of the reaction rate per incident neutron over all phase space. It was also emphasized by Cullen[2] that "the concept of conservation of area under the curve being conserved has propagated into the literature and become part of the folklore of nuclear engineering." Cullen and Weisbin[3] present an interpretation of the Doppler broadening equations in Eqs. (13) through (19). On pp. 209-211 they explicitly discuss the psi-chi method and its limitations, and Table III on p. 210 contains a concise summary of conservation laws for the exact and various approximations to the Doppler broadening equation.

In this Letter we point out that the books very recently published have not taken note of these facts published a decade ago and they continue to erroneously propagate the concept of conservation of area during Doppler broadening. For instance Waltar and Reynolds[4] state, ". . . infinite dilute group cross section is unaffected by Doppler broadening." Ash[5] makes the same error by stating that "the average cross section over the resonance region stays constant" (independent of temperature). In Ref. 6, a research monograph, it is stated by Rowlands on p. 57 that the total area under the resonance curve is constant when the temperature changes. In the same monograph,[6] James and de Saussure state on p. 136, "It can be shown that Doppler broadening conserves the 'area' under a resonance."

The author of the present Letter sincerely hopes that at

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[2]D. E. CULLEN, *Nucl. Sci. Eng.*, **52**, 498 (1973).

[3]D. E. CULLEN and C. R. WEISBIN, *Nucl. Sci. Eng.*, **60**, 199 (1976).

[4]A. E. WALTAR and A. B. REYNOLDS, *Fast Breeder Reactors*, p. 166, Pergamon Press (1981).

[5]M. ASH, *Nuclear Reactor Kinetics*, 2nd Ed., McGraw-Hill Book Company (1979).

[6]J. L. ROWLANDS, "Fission Cross Section Requirements for the Nuclear Energy Programme," p. 57, and G. D. JAMES and G. de SAUSSURE, "Measurements of Fission Cross Sections," p. 89, *Nuclear Fission and Neutron-Induced Fission Cross Sections*, A. MICHAUDON, Ed., Pergamon Press (1981).