Letters to the Editor

On the Factorized Kernel Approach for Solving Multidimensional Neutron Transport Problems

In a recent paper, Bassini et al.[1] have developed the factorized kernel approach for solving neutron transport problems in two and three dimensions. The method involves the expansion of total flux and other higher order spherical harmonic moments of angular flux in terms of Legendre polynomials of the reduced spatial coordinates, x/a, y/b, and z/c where $2a$, $2b$, and $2c$ are the dimensions of the parallelepiped. The method can be viewed as an extension of Carlvik's method[2] for plane geometry, which was shown by Mika and Stankiewicz[3] to be equivalent to the j_N method developed by Asaoka,[4] Kschwendt,[5] and others. It is therefore understandable that the method described in Ref. 1 is closely related to Sahni's work[6] on the integral transform method for multidimensional problems, which was restricted to isotropic scattering. In an attempt to treat the anisotropic scattering, Bassini et al.[1] have generalized Eq. (7) of Ref. 6

$$\frac{\exp(-\Sigma|\boldsymbol{r}-\boldsymbol{r}'|)}{|\boldsymbol{r}-\boldsymbol{r}'|^n} = \frac{\sqrt{\pi}}{2\pi^2}\int_0^\infty \operatorname{erfc}(u\Sigma)du \times \int_{(\infty)} \exp[-k'^2u^2 - i\boldsymbol{k}'\cdot(\boldsymbol{r}-\boldsymbol{r}')]d\boldsymbol{k}' \ , \quad n=2 \ , \tag{1}$$

to the values of $n > 2$. Thus we have the equation[1]

$$\frac{\exp(-\Sigma|\boldsymbol{r}-\boldsymbol{r}'|)}{|\boldsymbol{r}-\boldsymbol{r}'|^n} = \frac{1}{2}\int_0^\infty \frac{i^{(n-2)}\operatorname{erfc}(u\Sigma)}{(u\Sigma)^{n+1}}\, du \exp\left(-\frac{|\boldsymbol{r}-\boldsymbol{r}'|^2}{4u^2}\right) \ , \tag{2}$$

where $i^n\operatorname{erfc}(x)$ is the n'th repeated integral of the function $\operatorname{erfc}(x)$. Equation (1) cannot really be generalized for $n > 2$ because the singularity of the kernel on the left side when $\boldsymbol{r}$ equals $\boldsymbol{r}'$ cannot be integrated, and hence its Fourier transform cannot be defined. Moreover, this generalization is not needed for treating anisotropic scattering because such terms basically arise out of the expansion of the spherical harmonics

$$y_l^m\left(\frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|}\right) \ ,$$

where the argument is a unit vector. This can be seen very clearly if one considers the linearly anisotropic case first.

Let the transfer cross section $\Sigma_s(\boldsymbol{\Omega}' \to \boldsymbol{\Omega})$ be given by

$$\Sigma_s(\boldsymbol{\Omega}' \to \boldsymbol{\Omega}) = \frac{\Sigma_s}{4\pi}(1 + 3b_1\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}') \ . \tag{3}$$

The source-free, stationary, monoenergetic integral transport equation for a single homogeneous convex medium with vacuum boundary conditions gives[1]

$$\psi(\boldsymbol{r},\boldsymbol{\Omega}) = \frac{\lambda}{4\pi}\int_v \frac{\exp(-\Sigma|\boldsymbol{r}-\boldsymbol{r}'|)}{|\boldsymbol{r}-\boldsymbol{r}'|^2}\,\delta_2\left(\boldsymbol{\Omega} - \frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|}\right)d\boldsymbol{r}' \times \int \Sigma_s(\boldsymbol{\Omega}' \to \boldsymbol{\Omega})\,\psi(\boldsymbol{r}',\boldsymbol{\Omega}')d\boldsymbol{\Omega}' \ . \tag{4}$$

This equation must be solved for the criticality of a region v, λ being the eigenvalue. The extension to source problems is relatively simple, but the requirement of a single homogeneous medium, so that the total cross-section Σ is constant, is essential, and the multiregion problems have to be treated through interface boundary conditions.

Substituting Eq. (3) in Eq. (4), one can get two coupled integral equations for total flux $\phi(\boldsymbol{r})$ and current $\boldsymbol{J}(\boldsymbol{r})$, defined as

$$\phi(\boldsymbol{r}) = \int \psi(\boldsymbol{r},\boldsymbol{\Omega})d\boldsymbol{\Omega} \ ,$$
$$\boldsymbol{J}(\boldsymbol{r}) = \int \boldsymbol{\Omega}\psi(\boldsymbol{r},\boldsymbol{\Omega})d\boldsymbol{\Omega} \ . \tag{5}$$

These integral equations are

$$\phi(\boldsymbol{r}) = \frac{\lambda\Sigma_s}{4\pi}\int_v \frac{\exp(-\Sigma|\boldsymbol{r}-\boldsymbol{r}'|)}{|\boldsymbol{r}-\boldsymbol{r}'|^2}\left[\phi(\boldsymbol{r}') + 3b_1\frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|}\cdot\boldsymbol{J}(\boldsymbol{r}')\right]d\boldsymbol{r}' \ , \tag{6}$$

and

$$\boldsymbol{J}(\boldsymbol{r}) = \frac{\lambda\Sigma_s}{4\pi}\int_v \frac{\exp(-\Sigma|\boldsymbol{r}-\boldsymbol{r}'|)}{|\boldsymbol{r}-\boldsymbol{r}'|^2} \times \left\{\phi(\boldsymbol{r}')\frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|} + 3b_1\frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|}\left[\frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|}\cdot\boldsymbol{J}(\boldsymbol{r}')\right]\right\}d\boldsymbol{r}' \ . \tag{7}$$

The essential idea of factorized kernel approach is to cast these equations in a form so that the kernel appears as a product of three functions, each depending on the pair of coordinates (x,x'), (y,y'), and (z,z'). This factorization is much clearer if we work in the k space (the variable for Fourier transform) rather than in the coordinate space $\boldsymbol{r}$. For this purpose we introduce the Fourier representation of the kernels.

[1] A. BASSINI, F. PREMUDA, and W. A. WASSEF, *Nucl. Sci. Eng.*, **71**, 87 (1979).

[2] I. CARLVIK, *Nucl. Sci. Eng.*, **31**, 295 (1968).

[3] J. MIKA and R. STANKIEWICZ, *Nucl. Sci. Eng.*, **36**, 450 (1969).

[4] T. ASAOKA, *J. Nucl. Energy*, **18**, 665 (1964)

[5] H. KSCHWENDT, *Nucl. Sci. Eng.*, **36**, 447 (1969).

[6] D. C. SAHNI, *J. Nucl. Energy*, **26**, 367 (1972).

$$\frac{1}{4\pi}\,\frac{\exp(-\Sigma|\boldsymbol{r}-\boldsymbol{r}'|)}{|\boldsymbol{r}-\boldsymbol{r}'|^2}=\frac{\Sigma}{8\pi^3}\int_{(\infty)}\exp[-i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')]d\boldsymbol{k}'\times\int_0^1\frac{d\mu}{\Sigma^2+k'^2\mu^2}\ , \tag{8}$$

$$\frac{1}{4\pi}\,\frac{\exp(-\Sigma|\boldsymbol{r}-\boldsymbol{r}'|)}{|\boldsymbol{r}-\boldsymbol{r}'|^2}\,\frac{(\boldsymbol{r}-\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}=\frac{1}{8\pi^3}\int_{(\infty)}i\boldsymbol{k}'\exp[-i\boldsymbol{k}'\cdot(\boldsymbol{r}-\boldsymbol{r}')]d\boldsymbol{k}'\int_0^1\frac{\mu^2d\mu}{\Sigma^2+k'^2\mu^2}\ , \tag{9}$$

and, finally,

$$\frac{1}{4\pi}\,\frac{\exp(-\Sigma|\boldsymbol{r}-\boldsymbol{r}'|)}{|\boldsymbol{r}-\boldsymbol{r}'|^2}\,\frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|}\,\frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|}=\Sigma\int_{(\infty)}\exp[-i\boldsymbol{k}'\cdot(\boldsymbol{r}-\boldsymbol{r}')]d\boldsymbol{k}'\times\int_0^1\frac{d\mu}{\Sigma^2+k'^2\mu^2}\left(\frac{1-\mu^2}{2}\mathsf{I}+\frac{3\mu^2-1}{2}\,\frac{\boldsymbol{k}'\boldsymbol{k}'}{k'^2}\right)\ . \tag{10}$$

In Eq. (10), I is the unit dyadic. The presence of k'^2 in the denominators in Eqs. (8), (9), and (10) prevents the factorization mentioned earlier. To remove this difficulty, one first effects the transformation $s=\Sigma/\mu$, and then uses the integral representation

$$\frac{1}{s^2+k'^2}=\int_0^\infty\exp[-u^2(s^2+k'^2)]2u\,du\ . \tag{11}$$

For Eq. (10), one also has to use the relation

$$\frac{1}{k'^2(s^2+k'^2)}=\frac{1}{s^2}\left(\frac{1}{k'^2}-\frac{1}{s^2+k'^2}\right)\ . \tag{12}$$

With these transformations we have the following representations for the kernels:

$$\frac{\exp(-\Sigma|\boldsymbol{r}-\boldsymbol{r}'|)}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|^2}=\int_0^\infty\frac{\rho_1(u\Sigma)du}{8\pi^3}\times\int_{(\infty)}\exp[-k'^2u^2-i\boldsymbol{k}'\cdot(\boldsymbol{r}-\boldsymbol{r}')]d\boldsymbol{k}'\ ,$$

$$\rho_1(u\Sigma)=\sqrt{\pi}\,\mathrm{erfc}(u\Sigma)\ , \tag{13}$$

$$\frac{\exp(-|\boldsymbol{r}-\boldsymbol{r}'|)}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|^2}\,\frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|}=\int_0^\infty\rho_2(u\Sigma)\frac{du}{8\pi^3}\int_{(\infty)}\frac{i\boldsymbol{k}'}{\Sigma}d\boldsymbol{k}'\times\exp[-k'^2u^2-i\boldsymbol{k}'\cdot(\boldsymbol{r}-\boldsymbol{r}')]\ ,$$

$$\rho_2(u\Sigma)=2u\Sigma[\exp(-u^2\Sigma^2)-u\Sigma\rho_1(u\Sigma)]\ , \tag{14}$$

and

$$\frac{\exp(-\Sigma|\boldsymbol{r}-\boldsymbol{r}'|)}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|^2}\,\frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|}\,\frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|}=\int_0^\infty[\rho_1(u\Sigma)-\rho_2(u\Sigma)]du\int_{(\infty)}\exp[-k'^2u^2-i\boldsymbol{k}'\cdot(\boldsymbol{r}-\boldsymbol{r}')]\times\frac{d\boldsymbol{k}'}{8\pi^3}\left(\frac{\mathsf{I}}{2}-u^2\Sigma^2\frac{\boldsymbol{k}'}{\Sigma}\frac{\boldsymbol{k}'}{\Sigma}\right)\ . \tag{15}$$

The kernels in Eqs. (13), (14), and (15) are now in the factorized form. On taking the Fourier transforms of Eqs. (6) and (7) over the volume, v, one gets

$$\phi(\boldsymbol{k})=\lambda\Sigma_s\int_0^\infty du\int_{(\infty)}\Delta_v(\boldsymbol{k}-\boldsymbol{k}')\exp(-k'^2u^2)d\boldsymbol{k}'\times\left[\rho_1(u\Sigma)\phi(\boldsymbol{k}')+3b_1\rho_2(u\Sigma)\frac{i\boldsymbol{k}'}{\Sigma}\cdot\boldsymbol{J}(k')\right]\ , \tag{16}$$

and

$$\boldsymbol{J}(\boldsymbol{k}')=\lambda\Sigma_s\int_0^\infty du\int_{(\infty)}\Delta_v(\boldsymbol{k}-\boldsymbol{k}')\exp(-k'^2u^2)d\boldsymbol{k}'\times\left[\rho_2(u\Sigma)\frac{i\boldsymbol{k}'}{\Sigma}\phi(\boldsymbol{k}')+3b_1\rho_3(u\Sigma)\boldsymbol{J}(\boldsymbol{k}')-3b_1\rho_4(u\Sigma)\frac{\boldsymbol{k}'}{\Sigma}\,\frac{\boldsymbol{k}'\cdot\boldsymbol{J}(\boldsymbol{k}')}{\Sigma}\right]\ , \tag{17}$$

where the function

$$\Delta_v(\boldsymbol{k}-\boldsymbol{k}')=\frac{1}{8\pi^3}\int_v\exp[i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}]d\boldsymbol{r}'\ , \tag{18}$$

has been shown to be factorizable for a rectangular parallelepiped and a finite cylinder,[6] while

$$\rho_3(u\Sigma)=\frac{1}{2}[\rho_1(u\Sigma)-\rho_2(u\Sigma)]\ ,$$

$$\rho_4(u\Sigma)=2u^2\Sigma^2\rho_3(u\Sigma)\ . \tag{19}$$

It should be remarked that the integration over u in Eqs. (16) and (17) can be carried out by the Gaussian quadrature coefficients generated for the non-negative weight functions ρ_1, ρ_2, ρ_3, and ρ_4, respectively. Bassini et al.[1] have mentioned the improved techniques for generating the quadrature coefficients. We have also, in more recent work, followed techniques[7] similar to those given by Stroud.[8]

It should also be noted that for the criticality problem (though some of the remarks are true in general) of a rectangular parallelepiped of dimensions $-a \leqslant x \leqslant a$; $-b \leqslant y \leqslant b$; $-c \leqslant z \leqslant c$, the flux $\phi(\boldsymbol{k})$ has to be expanded in even order spherical Bessel functions, corresponding to even order Legendre polynomials of x/a, y/b, and z/c. The current $J_x(\boldsymbol{k})$ will involve odd order spherical Bessel functions of k_x and even order for k_y and k_z. Similar remarks hold for $J_y(\boldsymbol{k})$ and $J_z(\boldsymbol{k})$. After substituting such expansions in Eqs. (16) and (17), one obtains the matrix equations for the determination of expansion coefficients. The matrix elements of these equations, apart from an integration over u, can be evaluated analytically, though it involves intricate mathematical manipulations. In fact, the potential of this method for treating the anisotropic scattering was noted much earlier,[9] but it was also realized that to carry out the determination of matrix elements requires real courage. To this end the authors of Ref. 1 have made a very useful and significant contribution.

D. C. Sahni

Theoretical Reactor Physics Section
Bhabha Atomic Research Centre
Bombay 400 085
India

October 24, 1979

[7]D. C. SAHNI, *First National Convention Applied Numerical Analysis*, Bangalore, India, June 23-24, 1977, p. 189, India Institute of Science (1977).

[8]A. H. STROUD, *Gaussian Quadrature Formulas*, Englewood Cliffs, Prentice-Hall, Inc., Englewood Cliffs, New Jersey (1966).

[9]D. C. SAHNI, *Proc. Indo-Soviet Seminar on Fast Reactors*, Kalpakkam, India, December 6-8, 1972, CONF-721237, p. 417 (1973).