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A Transformation of the Radiative Transfer Equation Useful for Problems with Steep Source Gradients*

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A simple transformation of the dependent variable in the radiative transfer equation is described which eliminates most numerical solution problems caused by rapidly varying (spatially or temporally) sources. Numerical results for several problems illustrate the improved accuracy obtained with the transformed equation.

The numerical calculation of radiative transfer in two-space dimensions is of interest in connection with problems in such diverse subject areas as astrophysics (e.g., rapidly rotating and pulsating stars, solar active areas), re-entry physics, and meteorology (e.g., "greenhouse" effect due to point source of pollution in a stratified atmosphere). An unpleasant feature of many problems involving transfer of thermal radiation can be a source function which has a large range of variation in a relatively small spatial region, making it necessary to use extremely fine zoning for numerical solutions with standard transport codes. A simple transformation of the dependent variable in the transport equation can be made which eliminates most of the rapidly varying source problem.

Let $I_\nu(\mathbf{R}, \hat{\Omega})$ = radiation intensity at point $\mathbf{R}$ with directions in $d\Omega$, S_ν = source function (isotropic) at $\mathbf{R}$. The steady-state transfer equation can be written [1]

$$(\hat{\Omega} \cdot \nabla + \sigma_\nu^a + \sigma_\nu^s) I_\nu = S_\nu + \int \sigma_\nu^s(\hat{\Omega} \cdot \hat{\Omega}') I_\nu(\hat{\Omega}') \, d\Omega'.$$

Here σ_ν^a = absorption coefficient/cm^3 (includes effect of stimulated emission), σ_ν^s = scattering cross section/cm^3. If the new variable

$$\Psi_\nu = \sigma_\nu^a I_\nu / S_\nu$$

is introduced, the transfer equation becomes

$$\hat{\Omega} \cdot \nabla \Psi + [\sigma^t + \hat{\Omega} \cdot \nabla \log(S/\sigma^a)]\Psi = \sigma^a + \int \sigma^s(\hat{\Omega} \cdot \hat{\Omega}') \, \Psi(\hat{\Omega}') \, d\Omega', \qquad (1)$$

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which still looks like the transport equation, where, however, the total cross section has been replaced by $\sigma^t + \hat{\Omega} \cdot \nabla \log(S/\sigma^a)$, and the source term replaced by σ^a. ($\sigma^t = \sigma^a + \sigma^s$. The subscript ν has been omitted.) A standard transport code with minor modification can be used to solve the transformed equation.

In problems where $S_\nu/\sigma_\nu{}^a$ and I_ν have large ranges of variation and the radiation and source are strongly coupled, Ψ_ν will be much more slowly varying. (The transport equation describes the approach of Ψ_ν to its equilibrium value: $\Psi_\nu \to 1$.) The improved accuracy which results from numerical solution of the transformed equation is due, of course, to the fact that fewer terms of the Taylor expansion are required to represent the slowly varying variable Ψ to within a specified accuracy [2].

Numerical results for Sample 1-*D* problems are described below. The method is not limited to 1-*D* calculations, however. The results demonstrate that it is possible to get reasonably accurate answers for cases with rapidly varying sources using relatively coarse zonings, which would be expected to represent an especially important advantage for calculations in two space dimensions.

The transformation described here can also be applied to "variable Eddington factor" [3] approximations to the transport equation [2].

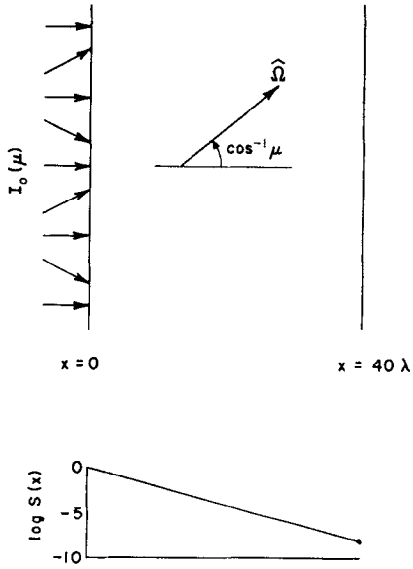

FIG. 1. Problem I. Slab ($0 < x/\lambda < 40$) with isotropic source function $S(x) = \exp(-0.2x/\lambda)$, illuminated on left with angular distribution $I_0(\mu)$ ($0 < \mu$).

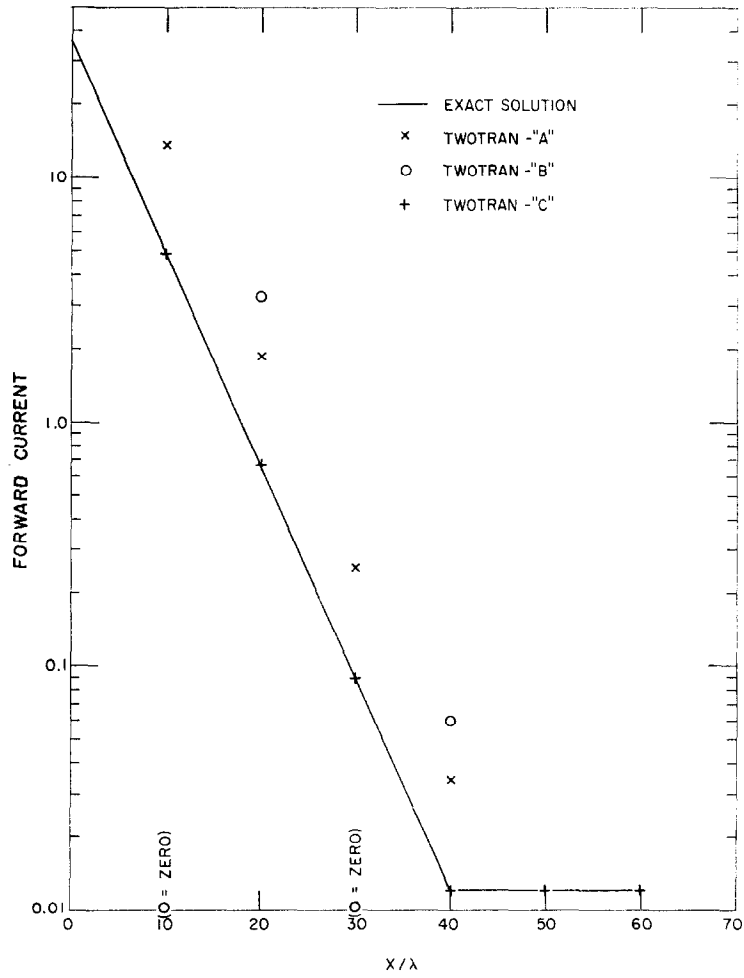

FIG. 2. Problem I. Results of calculations with three versions of TWOTRAN (see text) with $\Delta X = 10\lambda = \Delta Y$ are compared with the exact solution for the forward current,

$$2\pi \int_0^1 \mu I(X, \mu)\, d\mu.$$

(The vacuum region, $40 < x/\lambda < 60$, was also zoned.)

Numerical Results

Problem I featured a slab with constant mean free path for absorption and a distributed source $S = e^{-\alpha x/\lambda}$. ($\lambda = 1/\sigma^a$, $\sigma^s = 0$.) The slab is illuminated on the left with radiation with angular distribution

$$I_0(\mu) = (1 - \alpha\mu)^{-1} \quad (0 < \mu),$$

and radiates into a vacuum on the right (Fig. 1). Figures 2, 3, and 4 show results of calculations of this 1-D problem. Three versions of the X-Y TWOTRAN code developed by Lathrop and Brinkley [4] for numerical solution of the steady-state

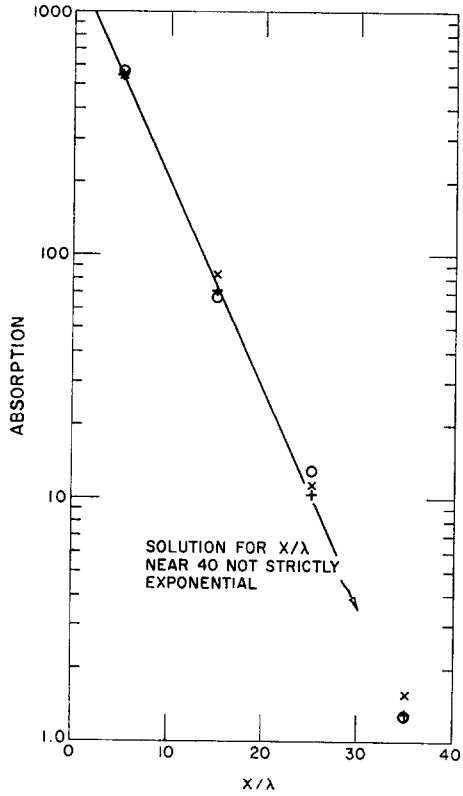

FIG. 3. Problem I.

$$\text{Absorption} = \frac{2\pi}{\lambda} \int_{X - \frac{\Delta X}{2}}^{X + \frac{\Delta X}{2}} dx' \int_{-1}^{-1} I(x', \mu)\, d\mu.$$

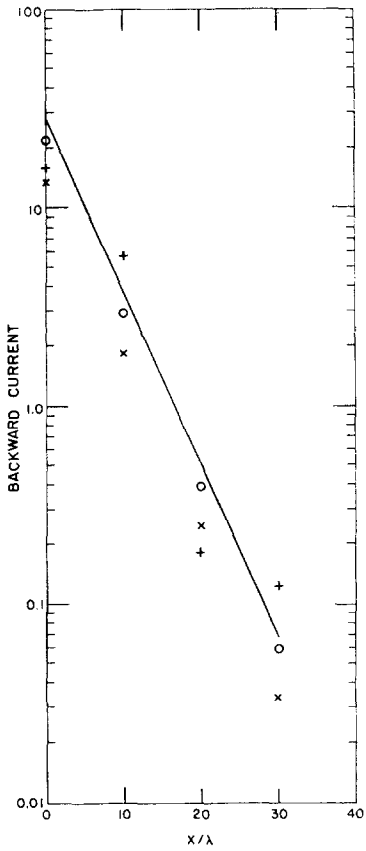

FIG. 4. Problem I. Backward current.

transport equation in two space dimensions were used. In order to run this 1-*D* problem with the 2-*D* code a flat distribution in the y direction was assumed [5]. Results labeled "*A*" were obtained using the standard version of TWOTRAN with the "strictly positive weighted diamond" difference scheme. "*B*" indicates results obtained with the standard version and the "weighted diamond with fix-up" scheme.[1] The latter version of TWOTRAN was modified to solve the transformed Eq. (1) as above ("*C*"). The exact solution of the problem is also shown.

Problem II calculated flow of 11–12 keV photons through a slab of iron ($0 < x < 1.2$ cm) which has a Milne problem-like temperature distribution and a realistic material density distribution ($25 < \sigma^a < 160$ cm^{-1}) (i.e., temperature and density distributions taken from a computation with a standard radiation hydro-

[1] See Appendix for description of TWOTRAN difference schemes.

dynamics code [3] are assumed to be given data). Local thermodynamic equilibrium is assumed, with source function [1]

$$S_\nu(T, \rho) = \sigma_\nu^a B_\nu(T).$$

B_ν = Planck function = $(2h\nu^3/c^2)[\exp(h\nu/T) - 1]^{-1}$. The iron slab is adjacent to an isothermal ($T = 1.3$ keV) scattering region ($\sigma^s = 0.191$ cm^{-1}, -22 cm $< x < 0$) which is also zoned ($\Delta x = 1$ cm) and which has a reflection boundary condition on the left (Fig. 5).

Results for the forward current (Fig. 6) again show a significant improvement in accuracy for the modified TWOTRAN.

Problem II was also computed using a time-dependent 1-D program (ONETRAN code)[6]. In this case the material density distribution is assumed independent of time, and the temperatures and radiation intensities are determined by numerical solution of the time-dependent transfer equation and the coupled energy equation [8]:

$$\begin{aligned}\frac{\partial E_m(T, \rho)}{\partial t} &= c \sum_g \sigma_a{}^g(T, \rho) \int [I^g - B^g(T)]\, d\Omega \\ &= c \sum_g \sigma_a{}^g(T, \rho)[B^g(T) + B_0{}^g] \int (\Psi^g - 1)\, d\Omega.\end{aligned} \tag{2}$$

An approximate equation of state for iron under these conditions was used:

$$E_m(T, \rho) = 0.112 \rho T^{1.125}. \tag{3}$$

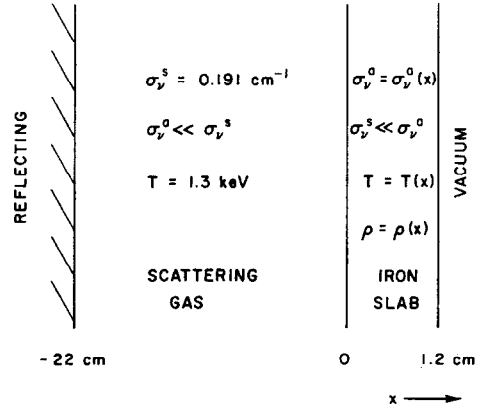

FIG. 5. Problem II. A slab of hot mainly scattering gas is bounded on the left by a perfect reflector and on the right by an optically thick iron slab. A Milne problem-like temperature distribution $T(x)$ and realistic density distribution $\rho(x)$ with corresponding absorption coefficient $\sigma_\nu^a(x)$ are assumed in the iron.

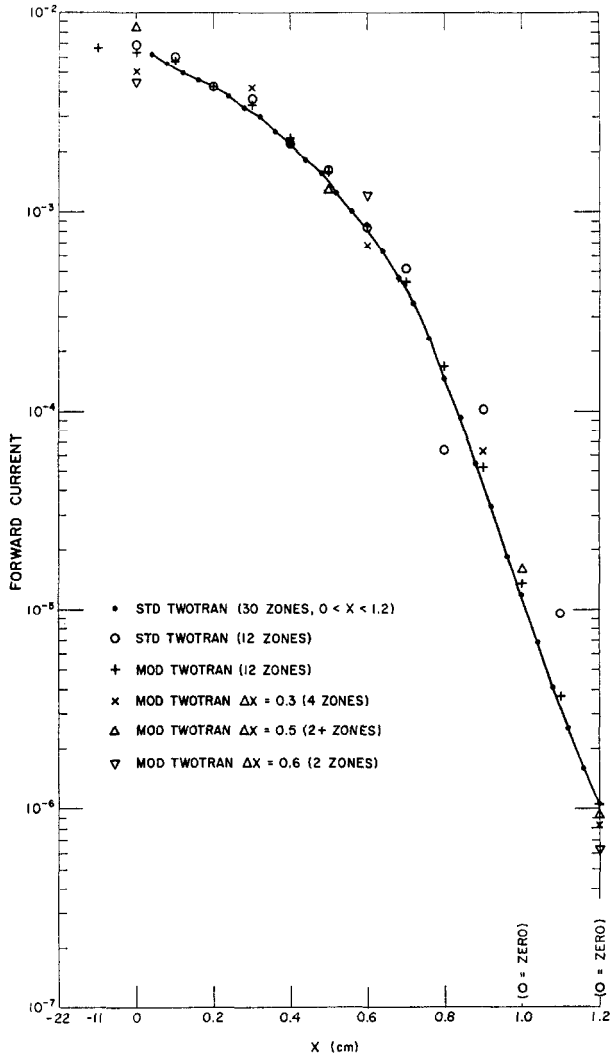

FIG. 6. Forward current for Problem II ($11 < h\nu < 12$ keV), calculated by standard ("weighted diamond with fix-up") and modified versions of TWOTRAN (S_6).

Sixteen photon energy groups were used. Only the penetration of the iron was calculated. It is assumed that the initially cold slab is illuminated on the left with radiation uniformly distributed in forward directions, corresponding to fixed temperature T_0. A straightforward Newton iteration procedure was used to solve Eqs. (2) and (3) for the new value of T.

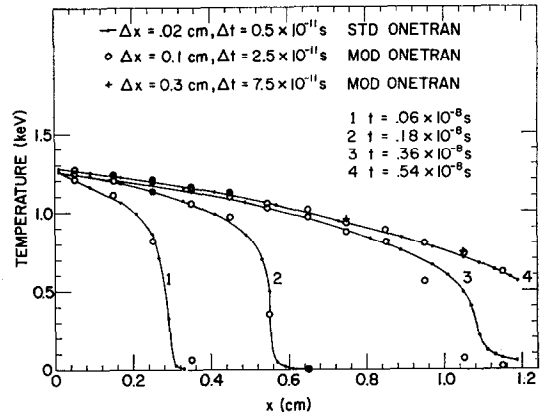

FIG. 7. Penetration of 1.2-cm iron slab by thermal radiation wave, as calculated by standard and modified versions of ONETRAN program (S_8).

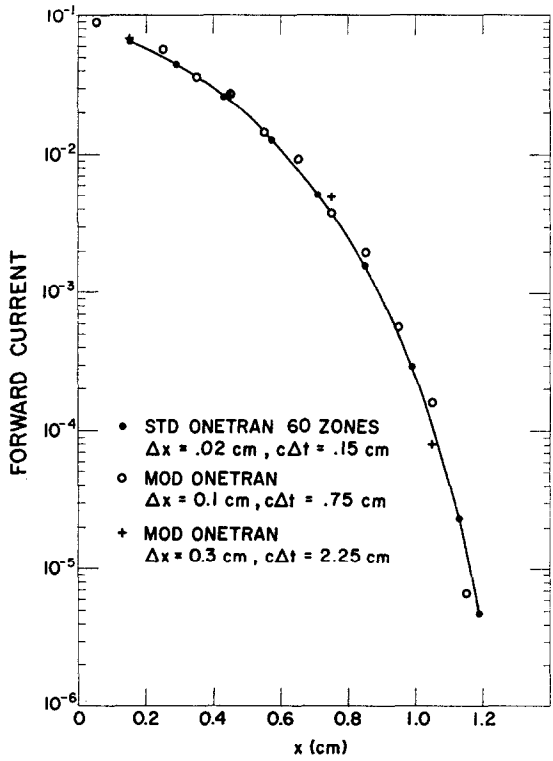

FIG. 8. Problem II. Forward current for photon group 10 ($10 < h\nu < 14$ keV) at $t = 0.54 \times 10^{-8}s$ (~steady-state) as calculated by standard and modified versions of ONETRAN.

Figure 7 shows the approach to the steady-state temperature distribution, as calculated, using ONETRAN with an explicit difference scheme [7, 8]. (The steady-state temperature distribution differs slightly from that assumed for the TWOTRAN calculation described above.) Figure 8 shows the steady-state forward current for the group $10 < h\nu < 14$keV. Figures 7–9 show results obtained with the standard version of ONETRAN ($\Delta x = 0.02$ cm, 60 zones, $c\Delta t = 0.15$ cm) and also with a version modified to integrate the transformed Eq. (1) with time derivative terms added [8] ($\Delta x = 0.1$, 12 zones, $c\Delta t = 0.75$; $\Delta x = 0.3$, 4 zones, $c\Delta t = 2.25$). It was found that runs with the standard version using $\Delta x = 0.1$ cm, $c\Delta t = 0.75$ cm, and $\Delta x = 0.3$ cm, $c\Delta t = 2.25$ cm, became unstable after 50 and 30 cycles, respectively. With 4 zones the rate of penetration calculated with the modified version is too fast. The first ONETRAN run (60 zones, standard version) required 2120 sec of central-processor time on the *CDC*-6600 computer (1080 problem cycles, including data loading, print-out and tape-dump times). The second run (12 zones, modified version) required 134 seconds CP time for 216 problem cycles. The time for the first run could have been reduced somewhat if the

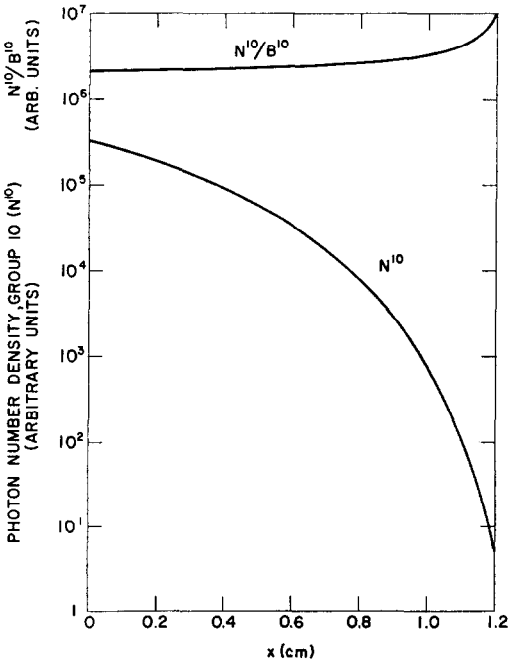

FIG. 9. Problem II. The lower curve is the photon number density $N^{10}(x) = \int_{-1}^{1} I^{10}(x, \mu)d\mu$ for group 10 ($10 < h\nu < 14$ keV) in the iron slab. The upper curve slows the more slowly-varying variable $N^{10}(x)/B^{10}[T(x)]$.

numerical integration had been cut off at the temperature wave front (i.e., instead of carrying all 60 zones each cycle).

APPENDIX: Difference Schemes Used by TWOTRAN and ONETRAN Codes

I. TWOTRAN difference schemes. The following outline description is condensed from Ref. [4].

The differenced form of the two dimensional (x, y) Boltzmann equation is

$$[\mu(\psi_R - \psi_L)/\Delta x] + [\eta(\psi_T - \psi_B)/\Delta y] + \sigma\psi(\mu, \eta) = S(\mu, \eta). \qquad \text{(A-1)}$$

In this equation ψ_R, ψ_L, ψ_T, ψ_B, and ψ denote, respectively, the particle flux on the right boundary, left boundary, top boundary, bottom boundary and within a space cell Δx long and Δy high. The direction cosines μ and η are the x and y components of the direction of particle motion, σ is the total macroscopic interaction cross section, and S is the total source of particles in the system. Depending on the signs of μ and η, the flux is known on some two adjacent boundaries of the cell and must be determined within the cell and on the other two boundaries. Two equations in addition to Eq. (A-1) are required for this determination. Suppose μ and η are positive and that ψ_L and ψ_B are known. We then use the equations

$$\begin{aligned} \psi &= a\psi_R + (1 - a)\,\psi_L \\ &= b\psi_T + (1 - b)\,\psi_B \end{aligned}$$

to complete the solution. In these equations, if $a = b = 1/2$ we have the Diamond relations, and if $a = b = 1$ we have the step difference scheme. If $a = 1/2$ then the relation is accurate to order $(\Delta x)^2$, but if $a = 1$ then the truncation error is of order Δx. The difficulty with the Diamond scheme is that, while accurate with respect to truncation error, it does not guarantee that ψ will be positive.

However, if μ, η, Δx, Δy and σ are given, then it is possible to pick a and b such that all coefficients are positive; and this is what is done in the TWOTRAN program. The optimum solution for a and b, in which a and b are greater than but as close as possible to one-half and in which both coefficients are positive, is an interesting problem in nonlinear programming. In TWOTRAN, values are obtained from the approximate solutions

$$1 - a = \mu\Delta y/(2\eta\Delta x + \sigma\Delta x\Delta y), \qquad 1 - b = \eta\Delta x/(2\mu\Delta y + \sigma\Delta y\Delta x),$$

subject to the further restriction that a and b be greater than or equal to one-half.

In the Diamond scheme, extrapolations of the form $\psi_{i+1/2} = 2\psi - \psi_{i-1/2}$ can

lead to negative values for fluxes. When sources are positive, we attempt to prevent negative fluxes by using a "set-flux-to-zero-and-correct" recipe. The logic of the set-to-zero fixup is as follows: If any one flux is negative, it is set to zero and the cell-centered flux ψ is recomputed assuming that particular flux is zero. If this ψ should be negative, the fixup attempt is aborted. If not, the other two fluxes are re-extrapolated. If either one of these is negative, ψ is recomputed assuming two fluxes are negative. If this ψ is positive, the remaining flux is extrapolated. If it should be negative, then ψ is recomputed assuming all three boundary fluxes are zero (provided the total cross section is not zero). If any center ψ is negative (implying a negative source or boundary flux) or if any fixup leads to a division by zero (e.g., in voids), the fixup attempt is aborted. One cannot exclude negative sources because the finite Legendre polynomial expansion of anisotropic scattering may produce negative numbers in particular directions.

II. ONETRAN difference scheme. The following description is condensed from Ref. [6].

The following difference approximation to the g-th number of the set of [multigroup] equations [in slab geometry] is used by the ONETRAN code:

$$\frac{1}{v}\left(\frac{\psi^{j+1}-\psi^{j}}{\Delta t}\right)+\mu_m\frac{\psi^{j+1}_{i+1/2}-\psi^{j+1}_{i-1/2}}{\Delta x}+\sigma_i\psi^{j+1}=S^{j}_{m,i}\,,$$

where group and some cell-centered subscripts have been deleted. The notation used above is as follows:

v = group velocity
Δt = time step size
μ_m = quadrature points
w_m = quadrature weights
σ_i = total cross section
$S^{j}_{m,i}$ = scattering and fission sources computed from fluxes at j-th time level

In order to solve Eqs. (10) for ψ^{j+1} given ψ^{j}, it is necessary to make some assumption concerning the shape of the flux over a mesh cell. The "diamond" relations are used in ONETRAN; these relations are given by

$$\psi^{j+1}=\tfrac{1}{2}(\psi^{j+1}_{i+1/2}+\psi^{j+1}_{i-1/2})=\tfrac{1}{2}(\psi^{j+1}_{m+1/2}+\psi^{j+1}_{m-1/2}). \tag{13}$$

If the above relations are used to eliminate $\psi^{j+1}_{i+1/2}$ and $\psi^{j+1}_{m+1/2}$ in Eq. (10), the following equation is obtained:

$$\left(\frac{1}{v\Delta t}+2\frac{\mu_m}{\Delta x}+\sigma_i\right)\psi^{j+1}=2\frac{\mu_m}{\Delta x}\psi^{j+1}_{i-1/2}+\frac{1}{v\Delta t}\psi^{j}+S^{j}_{m,i}\,.$$

The above equation is used to determine ψ^{j+1} from $\psi^{j+1}_{i-1/2}$, $\psi^{j+1}_{m-1/2}$, and ψ^{j} for directions such that $\mu_m > 0$. When $\mu_m < 0$ a similar equation is used to determine ψ^{j+1} from $\psi^{j+1}_{i+1/2}$, $\psi^{j+1}_{m-1/2}$, and ψ^{j}. The diamond difference relations are then used to obtain the cell edge fluxes $\psi^{j+1}_{m+1/2}$ and $\psi^{j+1}_{i+1/2}$ for $\mu_m > 0$ and $\psi^{j+1}_{m+1/2}$ and $\psi^{j+1}_{i-1/2}$ for $\mu_m < 0$.

As is well known, use of a diamond relation such as

$$\psi_{i+1/2} = 2\psi_i - \psi_{i-1/2}$$

may give rise to negative fluxes. This is quite likely to occur whenever

$$(\sigma_i + (1/v\Delta t))\,\Delta X_i$$

is large. In order to prevent negative fluxes, a set to zero fixup is used. The cell edge fluxes $\psi^{j+1}_{i+1/2}$ ($\psi^{j+1}_{i-1/2}$ for $\mu_m < 0$) are tested immediately after computation and are set to zero if negative. The cell-centered flux ψ^{j+1} is then recomputed from Eqs. (10) and (13b) with $\psi^{j+1}_{i+1/2} = 0$ ($\psi^{j+1}_{i-1/2} = 0$ for $\mu_m < 0$) in order to preserve neutron balance. The cell edge flux $\psi^{j+1}_{m+1/2}$ is not tested for positivity, since in practice it is rarely negative.

Acknowledgments

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References

1. S. Chandrasekhar, *Radiative Transfer*, (1950).
2. The method would not be expected to be advantageous for problems in which scattering dominates.
3. "The VERA Code," Defense Atomic Support Agency Report No. 2135, 1968.
4. K. D. Lathrop and F. W. Brinkley, AEC Report LA-4432, 1970; K. D. Lathrop, AEC Report LA-4058, 1969.
5. Specular reflection was used as a boundary condition in the transverse direction.
6. W. H. Reed, AEC Report LA-4800, 1972.
7. Numerical experiments indicated that the difference equations are stable for $c\Delta t \gtrsim 7.5\,\Delta x$. See Appendix for description of ONETRAN difference scheme.
8. For the calculation of penetration into initially cold material or into a vacuum it was found convenient to augment the variables I^g and B^g by a (positive) constant $B_0{}^g$, so that the variable ψ^g becomes $(I^g + B_0{}^g)/(B^g + B_0{}^g)$. The value of $B_0{}^g$ can be taken to correspond to some average temperature. The values of B^g at the boundary points were obtained by extrapolation from interior points.