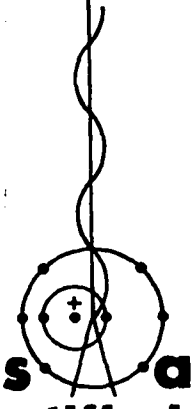
UC-32
Reporting Date: October 1974
Issued: December 1974

Modified Difference Schemes for the Transport Equation Solution

by

Bengt G. Carlson



los alamos
scientific laboratory
of the University of California
LOS ALAMOS, NEW MEXICO 87544

UNITED STATES
ATOMIC ENERGY COMMISSION
CONTRACT W-7405-ENG. 36

Printed in the United States of America. Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road
Springfield, VA 22151
Price: Printed Copy $4.00 Microfiche $2.25

MODIFIED DIFFERENCE SCHEMES FOR THE TRANSPORT EQUATION SOLUTION

by

Bengt G. Carlson

ABSTRACT

This report presents an improved set of numerical methods for solving the neutron transport equation in one or several variables. The revised methods, like earlier S_n-type methods, are based on the multigroup, discrete ordinates reduction of the equation and on simple difference methods with certain iterative techniques for obtaining solutions. The improved set provides reasonable remedies for most of the problems encountered in using codes based on earlier methods, such as oscillating fluxes and ray-effect distortions.

I. INTRODUCTION

This report presents an improved set of methods for solving the neutron transport equation numerically in one or more dimensions. The changes from earlier methods, although not major, have some overall beneficial effects on consistency, accuracy, and generality of procedures and results. The main effects are that smoother solutions are found, accuracy is enhanced in other ways, and time per calculated solution is reduced.

In expectation of smoother, more realistic flux solutions, the count of mesh divisions may be reduced and fewer iterative cycles will complete the calculation. This is partially offset by the fact that some of the newer, more elaborate methods require more calculating time per mesh cell. However, the more elaborate methods are used only when really needed and are activated only for a small fraction of the mesh cells. This fraction depends on cell size and location as well as on particle direction and speed.

The revised methods, like their forerunners, are based on the multigroup, discrete ordinates simplification of the transport equation and on the diamond difference scheme coupled with iterative procedures to effect the numerical solutions. The methods involve, among many other aids, a pseudocharacteristic approach to the equations which also may be developed as an independent, distinct approach to solving the discrete ordinates equations.

The diamond difference relations entail the usual S_n assumption of representing the detailed neutron flux by connected straight line segments. By using this scheme, the solution is generated (usually in a prescribed sequence) mesh cell by mesh cell for each discrete direction in each neutron velocity group. This process assumes a given source distribution at the beginning and a recalculation at the end, thus setting up an iterative cycle.

Assuming that the cells have regular shapes, with d dimensions and 2d sides, the calculations first involve the determination of the mid-cell flux and then d extrapolations across the cell. The latter, based on the d input fluxes and the mid-cell flux, determine the output fluxes. Generally, the extrapolations span time, position with up to three variables, and direction with up to two independent components. In the rectangular geometries, extrapolation in the directional, or angular, variables is not necessary. In the simple curved (r) spherical and (r,z) and (r,θ) cylindrical geometries, only one extrapolation in angle is needed.

The main difficulty with the discrete ordinates, diamond difference approach is the occasional development of oscillations in the calculated flux and of two other types of flux distortions. These are the problems of fluctuations at angles to the main stream, called flux skewing, and of irregular variation of flux known as ray effects.

Flux seesaw evolves because some cell dimensions are too large and because the extrapolations of the unmodified diamond scheme are very stiff. Here the optical dimensions, which depend on the physical interaction cross sections as well as on the cell dimensions, are involved. The obvious solution for flux seesaw (increasing the number of cells) is not always effective, seldom desirable, and probably not possible in practice because of computer time and storage limitations.

Flux skewing develops from extrapolations pivoting about a single mid-cell value of the flux. The flux may be quite smooth in the main flow direction but may, for physical or mathematical reasons, generate fluctuations in one or several of the coordinate directions.

The occurrence of ray effects is associated with the discrete ordinates assumption. In that simplification, isotropic sources are replaced by anisotropic, spoke-like sources emitting neutrons only in specified, usually sparse discrete directions. Therefore, in the presence of isolated or otherwise unevenly distributed sources and in the absence of sufficient natural smoothing by scattering, the calculated flux distributions may show serious distortions unexplainable by the physics of the problem. These distortions are extraneous effects, mainly telltale imprints of the discrete nature of the angular representation.

Oscillations are readily mitigated or eliminated by simple physical arguments that produce approximate lower and upper bounds for the extrapolated fluxes in any given cell. Therefore, the fluxes are first restrained to be positive by very simple means. The main test can be applied to a single, combined extrapolation. If that result goes beyond limits, the straight diamond scheme is replaced by an alternate scheme. Three possibilities are discussed: the "sloping step" schemes that, with slight sacrifice in continuity and differential accuracy, can adjust to specified physical limits. Such difference schemes, which permit flux discontinuities at the input sides of the cell, are much less stiff than the diamond scheme. The diligent use of one of these schemes reduces or prevents the development and propagation of flux oscillations as well as flux skewing. In the latter case, smoothing the outputs can be done in an explicit manner so that the total outflow is conserved.

A possible remedy for ray effects is to increase the number of rays, that is, the order n of the angular representation. This solution is not very attractive because it requires a too large n; therefore too much computing time. Two other, more effective methods are discussed. The first is a very simple remedy based on a particular difference scheme that equates the detailed outflows from a cell to the average outflow. This has a certain consistency with the discrete ordinates assumption, readily solves the equation in the presence of many variables, and smoothes out ray effects in an acceptable manner. This method has the general features of a numerical method of characteristics.

The second method is based on smoothing out the input fluxes before doing the regular calculations for a mesh cell. Here the smoothing is done so that the total inflow is conserved. The degree of smoothing depends on the shape of the cell, but depends more strongly on the angular spread associated with each discrete ray.

Several other difficulties with S_n calculations are discussed in this report, a few are resolved fully, others are resolved partially. Difficulties include getting good accuracy near the origin in spherical geometry, achieving consistency between spherical and cylindrical geometry, practical handling of irregular geometries, and constructing satisfactory two-dimensional quadrature.

Section II discusses plane geometry, modified difference schemes, physical limits, effective optical thickness, and related matters. Section III takes up spherical geometry, the use of combined fluxes, the reduction of two or more dimensions to one, and the correction of the equation for better definition near the origin. Section IV is concerned with cylindrical geometry, its consistency to spherical geometry, the accuracy of two-dimensional quadrature, and the construction of the ES_n quadrature sets. Section V discusses (x,y), (x,y,z), and

(x,y,t) geometry in a general way, alternate difference schemes, two methods for smoothing out ray effects, and, finally, a method for handling split (x,y) cells. Numerical comparisons of methods, and the pseudocharacteristic method as an independent method, will be discussed in future reports.

References 1, 2, and 3 present a general discussion of the discrete ordinates, diamond difference approach.

II. ONE-DIMENSIONAL PLANE GEOMETRY

The transport difference equation for infinite plane (x,μ) geometry is given by

$$\mu(N_{h+\frac{1}{2}} - N_{h-\frac{1}{2}}) + \sigma\Delta N = \Delta S, \tag{1}$$

where all quantities except the output flux $N_{h+\frac{1}{2}}$ and the mid-cell flux N are assumed to be known. Here x denotes position and μ direction, $-1 \le \mu \le 1$. It is also assumed that $\Delta \equiv \Delta x > 0$, that $\sigma \ge 0$, and that μ is discrete valued, $\mu \ne 0$. If μ is negative, then $N_{h-\frac{1}{2}}$, rather than $N_{h+\frac{1}{2}}$, is taken as the unknown output. The cell boundary fluxes $N_{h-\frac{1}{2}}$ and $N_{h+\frac{1}{2}}$ may be identified with $N(x_o)$ and $N(x)$, respectively, where $N(x) = N(x_o + \Delta)$.

Equation (1) is solved by introducing an auxiliary relation, which defines a difference scheme, in this case a modified diamond difference (MDS) scheme. The auxiliary relation is

$$N_{h+\frac{1}{2}} = (1 + P)N - P\,N_{h-\frac{1}{2}}, \tag{2}$$

which may also be written as

$$N_{h+\frac{1}{2}} - N_{h-\frac{1}{2}} = (1 + P)(N - N_{h-\frac{1}{2}}), \tag{3}$$

or

$$\frac{1}{1+P}\,N_{h+\frac{1}{2}} + \frac{P}{1+P}\,N_{h-\frac{1}{2}} = N. \tag{4}$$

Here P is a parameter, $0 \le P \le 1$, with $P = 1$ in the normal case and is to be determined in other cases. Clearly, the weight multiplying the output flux is greater than or equal to the weight multiplying the input. Equations (3) and (4) with $P = 1$ correspond to the assumption that N is linear in x in the interval $(x_o, x_o + \Delta)$. Reference 4 discusses other possibilities.

The result of substituting Eq. (3) into Eq. (1) and solving for N is

$$N = \frac{(1 + P)N_{h-\frac{1}{2}} + u\,S/\sigma}{1 + P + u}, \tag{5}$$

and also

$$N_{h+\frac{1}{2}} = (1 + P)N - PN_{h-\frac{1}{2}}$$

$$= \frac{(1 + P - uP)N_{h-\frac{1}{2}} + (1 + P)u\,S/\sigma}{1 + P + u}, \tag{6}$$

where u, the apparent optical thickness, is defined by

$$u = \sigma\Delta/|\mu|. \tag{7}$$

If $\sigma = 0$ in Eqs. (5) and (6), then the following replacement is made.

$$u\,S/\sigma \to \Delta S/|\mu|. \tag{8}$$

In the preliminary calculation, which in most cases is also the final one, P is set to unity so that

$$N = \frac{2N_{h-\frac{1}{2}} + u\,S/\sigma}{2 + u}, \tag{9}$$

with the following extrapolation.

$$N_{h+\frac{1}{2}} = 2N - N_{h-\frac{1}{2}}$$

$$= \frac{(2 - u)N_{h-\frac{1}{2}} + 2u\,S/\sigma}{2 + u}. \tag{10}$$

The analytical form of Eq. (1) is a simple differential equation.

$$\mu\frac{\partial N}{\partial x} + \sigma N = S, \tag{11}$$

which is solved by

$$N(x) = N(x_o)\,E(x) + [1 - E(x)]\,S/\sigma, \tag{12}$$

where

$$E(x) = \exp[-\sigma(x - x_o)/|\mu|]. \tag{13}$$

With $x = x_o + \Delta$, Eq. (12) becomes

$$N(x) = N(x_o) \exp(-u) + [1 - \exp(-u)]\, S/\sigma. \quad (14)$$

By averaging the terms in Eq. (12) over the x interval $(x_o, x_o + \Delta)$, the analytical form for the mid-cell flux is obtained.

$$N = N_{h-\frac{1}{2}}(1 - e^{-u})/u + [1 - (1 - e^{-u})/u]\, S/\sigma. \quad (15)$$

Adopting the same notation for Eq. (14), that equation becomes

$$N_{h+\frac{1}{2}} = N_{h-\frac{1}{2}}\, e^{-u} + (1 - e^{-u})\, S/\sigma. \quad (16)$$

The above equations show that N and $N_{h+\frac{1}{2}}$ are weighted averages of $N_{h-\frac{1}{2}}$ and S/σ and that the weights represent penetration probabilities which by nature are positive and sum to unity. Also note that N and $N_{h+\frac{1}{2}}$ are limited by S/σ as u increases. For decaying flux, that is, for

$$S/\sigma < N_{h-\frac{1}{2}}\,, \quad (17)$$

S/σ is a lower limit and

$$S/\sigma < N_{h+\frac{1}{2}} < N < N_{h-\frac{1}{2}}; \quad (18)$$

and for growing flux,

$$S/\sigma \geq N_{h-\frac{1}{2}}\,, \quad (19)$$

S/σ is an upper limit and

$$S/\sigma \geq N_{h+\frac{1}{2}} \geq N \geq N_{h-\frac{1}{2}}\,. \quad (20)$$

By equating coefficients between Eq. (6) and Eq. (16), the exact $1 + P$ is determined.

$$1 + P = u(1 - e^{-u})/(u - 1 + e^{-u}). \quad (21)$$

Examination of this expression readily shows that $1 + P$ is monotonely decreasing, and that

$$1 + P(0) = 2, \qquad 1 + P(\infty) = 1, \quad (22)$$

and, for $u \ll 1$,

$$1 + P \approx u/(u - 1). \quad (23)$$

The approximate coefficients of $N_{h-\frac{1}{2}}$ and S/σ in Eqs. (5) and (6) show the same properties as the exact coefficients in Eqs. (15) and (16) with the notable exception that the probability multiplier of $N_{h-\frac{1}{2}}$ in Eq. (10) can become negative if

$$u > 2, \quad (24)$$

or, as in Eq. (6) for $P \neq 1$, if

$$u > (1 + P)/P. \quad (25)$$

Therefore, extrapolation can lead to violation of the physics of the problem, more specifically of the inequalities in Eqs. (18) and (20). In extreme cases, some remedy in the form of a departure from the normal case of $P = 1$ will become necessary.

It will be convenient later in this section to have available the following approximation to $1 + P$.

$$\begin{cases} 1 + P = 2, & 0 \leq u \leq u_o, \\ 1 + P = (u - u_o + 2)/(u - u_o + 1), & u > u_o, \end{cases} \quad (26)$$

where u_o can be chosen subject to $0 \leq u_o \leq 2$. Here, $1 + P(u_o) = 2$ so that the approximation is continuous. Also, Eq. (23) holds for $u \gg u_o$. Substituting Eq. (26) into Eq. (21) and solving for the exponential, one finds

$$\begin{cases} e^{-u} = (2 - u)/(2 + u), & 0 \leq u \leq u_o, \\ e^{-u} = (2 - u_o)/[(2 - u_o)(1 + u) + u^2], & u > u_o. \end{cases} \quad (27)$$

For $u_o = 1$, the second of these equations becomes

$$e^{-u} = 1/(1 + u + u^2), \quad u > 1. \quad (28)$$

Before discussing the above approximations further, three special MDS schemes will be described: two that are regarded as extremes and one for the many possible compromises.

In the first MDS scheme (Source Limit) one selects the following for $1 + P$.

$$\begin{cases} 1 + P = 2, \ 0 \le u \le 2, \\ 1 + P = u/(u - 1), \ h > 2, \end{cases} \tag{29}$$

that is, Eq. (26) with $u_o = 2$, which guarantees a limited and nonnegative $N_{h+\frac{1}{2}}$. In the straight diamond case of $u \le 2$ in this scheme, N and $N_{h+\frac{1}{2}}$ are obtained from Eqs. (9) and (10), otherwise from

$$N = N_{h-\frac{1}{2}}/u + (1 - 1/u) \ S/\sigma, \tag{30}$$

which derives from Eq. (1) on the basis of

$$N_{h+\frac{1}{2}} = S/\sigma. \tag{31}$$

In practice, these equations are used if $N_{h+\frac{1}{2}}$ from Eq. (10) goes below S/σ in the decay case or goes above S/σ in the growth case. Therefore, Eq. (29) is not needed, and Eqs. (5) and (6) are not used.

In the second MDS scheme (Zero Limit or Zero Fix-Up) more relaxed limits are used. A zero limit is used for decaying flux, and a $2S/\sigma$ limit is used for growing flux. The latter limit is based on a minimum $N_{h-\frac{1}{2}}$ of zero and a maximum N of S/σ, giving a maximum extrapolation to $2S/\sigma$. Recalculation of N gives

$$N = N_{h-\frac{1}{2}}/u + S/\sigma, \tag{32}$$

when

$$N_{h+\frac{1}{2}} = 0, \tag{33}$$

and

$$N = N_{h-\frac{1}{2}}/u + (1 - 2/u) \ S/\sigma, \tag{34}$$

when

$$N_{h+\frac{1}{2}} = 2S/\sigma \tag{35}$$

in the two cases. Again, in practice, no formula for 1 + P is needed and Eqs. (5) and (6) are not used.

It is not generally advisable to use the exact 1 + P given by Eq. (21) in a MDS difference scheme because, first, it applies only to infinite plane geometry and, second, it is based on the assumption that S is independent of N and constant over the cell. In most practical situations, S depends on N through the scattering process or some other process, and if the dependence is strong, which it often is, S tends to vary like the flux across the cell. In this and similar situations there may be considerable cancellation between the $\sigma\Delta N$ and ΔS terms in Eq. (1) so that u is only the apparent thickness, not the effective thickness of the cell which may be much smaller.

Experience indicates that Δx should be chosen so that the effective optical thickness u' of the cell is less than unity at least for cells in the more important subregions of the total mesh. Also, to promote accuracy of the calculated fluxes and of various related functionals that may be of interest (to maintain second-order error terms), it is apparently necessary to keep 1 + P = 2 for all cells which are effectively small, say for x intervals with $u' \le 1$. Equation (26) allows for other possibilities. A suitable formula for u' will be developed below. Here it is noted that u' may be written

$$u' = \sigma'\Delta/|\mu|, \tag{36}$$

where σ' denotes the effective total cross section in units of inverse length.

The third MDS scheme examined here (Reduced Source Limit), which seems to be a good and practical compromise between the first two schemes, is based on the following for 1 + P in the decay case.

$$\begin{cases} 1 + P = 2, \ 0 \le u' \le 1, \\ 1 + P = (u' + 1)/u', \ u' > 1, \end{cases} \tag{37}$$

which is the same as Eq. (26) with u replaced by u' and $u'_o = 1$. As shown later, this scheme implies a lower limit of $\frac{1}{2}S/\sigma$. Therefore in the growth case, a limit of $\frac{3}{2}S/\sigma$ suggests itself. Recalculation in the growth case gives

$$N = N_{h-\frac{1}{2}}/u + (1 - 3/2u)S/\sigma \tag{38}$$

based on Eq. (1) and

$$N_{h+\frac{1}{2}} = \frac{3}{2}S/\sigma. \tag{39}$$

In the decay case, if u' > 1, recalculation is based on Eq. (37) in conjunction with Eqs. (5) and (6).

The effective optical thickness u' is defined here and is computed by setting $uS/\sigma = 0$ in Eq. (9) and solving for u. The result denoted by u' is

$$u' = 2(N_{h-\frac{1}{2}} - N')/N' = u(N' - S/\sigma)/N', \qquad (40)$$

where N' denotes the value of N obtained from Eq. (9) with no change. This reduced u (u') is in essence the answer to the question: What value should be given to u to account for N = N' in the absence of sources? Clearly, from the definition one has

$$0 < u' \leq u, \qquad (41)$$

with u' = u if S = 0. Therefore u' need not be calculated if $u \leq 1$. As can be shown, u' as defined by Eq. (40) tends to be an overestimate of the effective thickness.

Table I gives some comparisons of P by approximations to the "exact" P from Eq. (21).

TABLE I

P FROM FORMULA AS GIVEN

u	Eq. (23)	Eq. (26) $u_o = \frac{1}{2}$	Eq. (26) $u_o = 1$	Eq. (21) Exact
1.0	-	0.6667	1.0000	0.7183
1.5	-	0.5000	0.6667	0.6115
2.0	1.0000	0.4000	0.5000	0.5232
2.5	0.6667	0.3333	0.4000	0.4505
3.0	0.5000	0.2857	0.3333	0.3907
4.0	0.3333	0.2222	0.2500	0.3010
5.0	0.2500	0.1818	0.2000	0.2395

The third MDS scheme guarantees that $N_{h+\frac{1}{2}}$ is positive for large u and u' and implies a number of other properties. To establish a few of these, the following relations are helpful.

$$(u - u')N' = uS/\sigma, \qquad (42)$$

which is implied by Eq. (40), and

$$N_{h-\frac{1}{2}} = (1 + \tfrac{1}{2}u)N' - \tfrac{1}{2}uS/\sigma = (1 + \tfrac{1}{2}u')N', \qquad (43)$$

which follows from Eq. (9) and is simplified by Eq. (42). A corollary of this is that, for u' = 1,

$$N = \frac{2}{3}N_{h-\frac{1}{2}}, \qquad (44)$$

and

$$N_{h+\frac{1}{2}} = \tfrac{1}{2}N = \frac{1}{3}N_{h-\frac{1}{2}}. \qquad (45)$$

Next, Eq. (6) is rewritten, adding and subtracting terms, as follows.

$$N_{h+\frac{1}{2}} = [PN_{h-\frac{1}{2}} + (1 - Pu')N_{h-\frac{1}{2}} - P(u - u')N_{h-\frac{1}{2}} + (1 + P)\, uS/\sigma]/(1 + P + u), \qquad (46)$$

which, after applying Eqs. (42) and (43), becomes

$$N_{h+\frac{1}{2}} = [\, PN_{h-\frac{1}{2}} + (1 - Pu')N_{h-\frac{1}{2}} + u(1 - \tfrac{1}{2}Pu')S/\sigma]/(1 + P + u), \qquad (47)$$

or, assuming that u' < 1 so that P = 1,

$$N_{h+\frac{1}{2}} = [\, (2 - u')N_{h-\frac{1}{2}} + u(1 - \tfrac{1}{2}u')S/\sigma]/(2 + u). \qquad (48)$$

Here, with $N_{h-\frac{1}{2}} > S/\sigma$ and $u' \leq 1$, it is clear that $N_{h+\frac{1}{2}}$ exceeds $\frac{1}{2}S/\sigma$.

If, on the other hand, u' > 1, P is set to 1/u' in accordance with Eq. (37). With this substitution in Eq. (47), one finds

$$N_{h+\frac{1}{2}} = (N_{h-\frac{1}{2}} + \tfrac{1}{2}u'u\, S/\sigma)/(1 + u' + u'u), \qquad (49)$$

which is clearly limited and positive, since on the basis of Eq. (43) and $N' > S/\sigma$,

$$N_{h+\frac{1}{2}} > [(1 + \tfrac{1}{2}u' + \tfrac{1}{2}u'u)\, S/\sigma]/(1 + u' + u'u) > \tfrac{1}{2}S/\sigma. \qquad (50)$$

III. SPHERICAL GEOMETRY

The difference equation for spherical (r,μ) geometry is given by

$$\mu A_{i+\frac{1}{2}}N_{i+\frac{1}{2}} - \mu A_{i-\frac{1}{2}}N_{i-\frac{1}{2}} + (C/w)(\alpha_{m+\frac{1}{2}}N_{m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}}N_{m-\frac{1}{2}}) + \sigma VN = VS, \qquad (51)$$

where

$$A_i = 4\pi r_i^2, \tag{52}$$

$$C = A_{i+\frac{1}{2}} - A_{i-\frac{1}{2}}, \tag{53}$$

$$V_i = (4\pi/3)(r_{i+\frac{1}{2}}^3 - r_{i-\frac{1}{2}}^3), \tag{54}$$

and

$$\alpha_{m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}} = -w\mu, \tag{55}$$

with $\alpha_{\frac{1}{2}} = 0$ and w denoting the weight associated with the direction μ.

Here, as in Sec. II, the convenient convention of omitting central subscripts is followed. Therefore, $w = w_m$, $\mu = \mu_m$, $\sigma = \sigma_i$, $S = S_i$, $N_{i+\frac{1}{2}} = N_{m,i+\frac{1}{2}}$, $N_{m-\frac{1}{2}} = N_{m-\frac{1}{2},i}$, $N = N_{mi}$, etc. Note that infinite slab geometry is the special case of Eq. (5) with $A \equiv 1$, hence $C \equiv 0$, and $V = \Delta$. For the quadrature used, the following is assumed.

$$\Sigma_m w_m = 1, \qquad \Sigma_m w_m \mu_m = 0, \tag{56}$$

and

$$\Sigma_m w_m \mu_m^2 = 1/3. \tag{57}$$

In Eq. (56), the second sum should be taken as a consequence of a stronger condition, that of symmetric quadrature. This assumes that if μ_m with weight w_m is in the quadrature set, so is $-\mu_m$ with the same weight. Symmetry here is a customary but not a required condition.

Equation (51) is solved by the methods given in Sec. II by first converting it to an equation which in essentials is equivalent to the equation for plane geometry. To convert, first write Eq. (51) as follows.

$$T(\hat{N}_{h+\frac{1}{2}} - \hat{N}_{h-\frac{1}{2}}) + \sigma V N = VS, \tag{58}$$

where T is the total effective outflow area, the sum of the detailed outflow areas $|\mu|A_{i+\frac{1}{2}}$ and $C\alpha_{m+\frac{1}{2}}/w$, which equals the total effective inflow area, the sum of the inflow areas $|\mu|A_{i-\frac{1}{2}}$ and $C\alpha_{m-\frac{1}{2}}/w$. The equality is a consequence of Eq. (55).

Hence,

$$\begin{aligned} T &\equiv |\mu|A_{i+\frac{1}{2}} + C\alpha_{m+\frac{1}{2}}/w \\ &= |\mu|A_{i-\frac{1}{2}} + C\alpha_{m-\frac{1}{2}}/w \\ &= |\mu|\bar{A} + C\,\bar{\alpha}/w, \end{aligned} \tag{59}$$

where the last quality comes from the definitions

$$\bar{A} \equiv \tfrac{1}{2}(A_{i+\frac{1}{2}} + A_{i-\frac{1}{2}}), \tag{60}$$

and

$$\bar{\alpha} \equiv \tfrac{1}{2}(\alpha_{m+\frac{1}{2}} + \alpha_{m-\frac{1}{2}}). \tag{61}$$

Comparing Eqs. (51) and (58), which are supposed to be equivalent, leads to the following formulas for the total outflow $T\hat{N}_{h+\frac{1}{2}}$ and the total inflow $T\hat{N}_{h-\frac{1}{2}}$.

$$T\hat{N}_{h+\frac{1}{2}} \equiv |\mu|A_{i+\frac{1}{2}}N_{i+\frac{1}{2}} + (C\alpha_{m+\frac{1}{2}}/w)N_{m+\frac{1}{2}} \tag{62}$$

and

$$T\hat{N}_{h-\frac{1}{2}} \equiv |\mu|A_{i-\frac{1}{2}}N_{i-\frac{1}{2}} + (C\alpha_{m-\frac{1}{2}}/w)N_{m-\frac{1}{2}}. \tag{63}$$

Thus $\hat{N}_{h+\frac{1}{2}}$ is a weighted average of the outflows $N_{i+\frac{1}{2}}$ and $N_{m+\frac{1}{2}}$ with the effective outflow areas as weights, and $N_{h-\frac{1}{2}}$ represents a similar average for the inflow sides. In what follows, $N_{h+\frac{1}{2}}$ and $N_{h-\frac{1}{2}}$ will have the meaning of weighted averages using $\bar{A}$ and $\bar{\alpha}$ as weights.

Proceeding with the conversion,

$$T\hat{N}_{h+\frac{1}{2}} = TN_{h+\frac{1}{2}} + \tfrac{1}{2}\mu C(N_{i+\frac{1}{2}} - N_{m+\frac{1}{2}}), \tag{64}$$

where

$$TN_{h+\frac{1}{2}} = |\mu|\bar{A}N_{i+\frac{1}{2}} - (C\bar{\alpha}/w)N_{m+\frac{1}{2}}, \tag{65}$$

likewise

$$T\hat{N}_{h-\frac{1}{2}} = TN_{h-\frac{1}{2}} - \tfrac{1}{2}\mu C(N_{i-\frac{1}{2}} - N_{m-\frac{1}{2}}), \tag{66}$$

with

$$TN_{h-\frac{1}{2}} = |\mu|\bar{A}N_{i-\frac{1}{2}} + (C\bar{\alpha}/w)N_{m-\frac{1}{2}}. \tag{67}$$

Next, introducing and applying the following cross difference relation

$$(N_{i+\frac{1}{2}} - N_{m+\frac{1}{2}}) = P(N_{m-\frac{1}{2}} - N_{i-\frac{1}{2}}), \tag{68}$$

Eq. (64) for $T\hat{N}_{h+\frac{1}{2}}$ becomes

$$T\hat{N}_{h+\frac{1}{2}} = TN_{h+\frac{1}{2}} + P(T\hat{N}_{h-\frac{1}{2}} - TN_{h-\frac{1}{2}}). \tag{69}$$

Therefore, on the basis of the relation in Eq. (68), substituting Eq. (69) in Eq. (58), Eq. (51) is reduced to

$$T[N_{h+\frac{1}{2}} - N_{h-\frac{1}{2}} + (1 - P)(N_{h-\frac{1}{2}} - \hat{N}_{h-\frac{1}{2}})]$$

$$+ \sigma VN = VS. \tag{70}$$

In the normal case, P = 1, Eq. (51) has been reduced to the equation for the plane case with $\Delta T/V$ playing the roll of $|\mu|$. On this basis the apparent cell thickness u can be written

$$u = \sigma V/T. \tag{71}$$

If $P \neq 1$, an extra boundary source $(1 - P)S_o$ is involved.

$$TS_o = T(\hat{N}_{h-\frac{1}{2}} - N_{h-\frac{1}{2}}) = \tfrac{1}{2}\mu C(N_{m-\frac{1}{2}} - N_{i-\frac{1}{2}}), \tag{72}$$

the sign of which cannot be predicted.

Proceeding with the solution, introducing the difference relation

$$N_{h+\frac{1}{2}} - N_{h-\frac{1}{2}} = (1 + P)(N - N_{h-\frac{1}{2}}), \tag{73}$$

which, together with the relation in Eq. (68), implies

$$N_{i+\frac{1}{2}} - N_{i-\frac{1}{2}} = (1 + P)(N - N_{i-\frac{1}{2}}), \tag{74}$$

and

$$N_{m+\frac{1}{2}} - N_{m-\frac{1}{2}} = (1 + P)(N - N_{m-\frac{1}{2}}), \tag{75}$$

one finds upon substitution in Eq. (70) and solving for N that

$$N = \frac{2PN_{h-\frac{1}{2}} + (1 - P)\hat{N}_{h-\frac{1}{2}} + uS/\sigma}{1 + P + u}, \tag{76}$$

which shows that N is positive for all allowed P, $0 \leq P \leq 1$. N can also be written as

$$N = \frac{(1 + P)\, N_{h-\frac{1}{2}} + (1 - P)S_o + uS/\sigma}{1 + P + u}$$

$$= \frac{(1 + P)\, \hat{N}_{h-\frac{1}{2}} - 2PS_o + uS/\sigma}{1 + P + u}. \tag{77}$$

Extrapolating for $N_{h+\frac{1}{2}}$ and $\hat{N}_{h+\frac{1}{2}}$, one obtains

$$N_{h+\frac{1}{2}} = \frac{(1 + P - Pu)N_{h-\frac{1}{2}} + (1 - P^2)S_o + (1 + P)uS/\sigma}{1 + P + u}, \tag{78}$$

and

$$\hat{N}_{h+\frac{1}{2}} = N_{h+\frac{1}{2}} + PS_o$$

$$= \frac{(1 + P + Pu)\hat{N}_{h-\frac{1}{2}} - 2Pu\, N_{h-\frac{1}{2}} + (1 + P)uS/\sigma}{1 + P + u}, \tag{79}$$

which can also be written as

$$\hat{N}_{h+\frac{1}{2}} = \frac{(1 + P - Pu)N_{h-\frac{1}{2}} + (1 + P + Pu)S_o + (1 + P)uS/\sigma}{1 + P + u}$$

$$= \frac{(1 + P - Pu)\hat{N}_{h-\frac{1}{2}} + 2PuS_o + (1 + P)uS/\sigma}{1 + P + u}. \tag{80}$$

In the normal case, for P = 1, Eqs. (76) and (79) reduce to

$$N = \frac{2N_{h-\frac{1}{2}} + uS/\sigma}{2 + u}, \tag{81}$$

and

$$\hat{N}_{h+\frac{1}{2}} = \frac{(2 + u)\hat{N}_{h-\frac{1}{2}} - 2u\, N_{h-\frac{1}{2}} + 2u\, S/\sigma}{2 + u}$$

$$= \frac{(2 - u)\hat{N}_{h-\frac{1}{2}} + 2u\, S_o + 2u\, S/\sigma}{2 + u}. \tag{82}$$

If P values are actually used in the calculations, $P \neq 1$, as happens in the Modified Source Limit Scheme described in Sec. II, then

$$P = 1/u', \quad u' > 1,$$

and Eqs. (76) and (79) may be written

$$N = \frac{2N_{h-\frac{1}{2}} + (u' - 1)\hat{N}_{h-\frac{1}{2}} + u'u\ S/\sigma}{1 + u' + u'u}, \tag{83}$$

and

$$N_{h+\frac{1}{2}} = \frac{(1 + u' + u)\hat{N}_{h-\frac{1}{2}} - 2uN_{h-\frac{1}{2}} + (1 + u')u\ S/\sigma}{1 + u' + u'u}. \tag{84}$$

Here, in the spherical case, it is necessary to compare $\hat{N}_{h+\frac{1}{2}}$ to a lower or an upper limit $L_{h+\frac{1}{2}}$ in all cases including the third MDS scheme because of the presence of the $(1 - P)S_o$ boundary source. This source includes a factor $C = A_{i+\frac{1}{2}} - A_{i-\frac{1}{2}}$, which is significant in size only near the origin. S_o may also be small because a difference between two neighboring fluxes is involved. The limit $L_{h+\frac{1}{2}}$, if a lower limit, equals S/σ, zero, or $\frac{1}{2}S/\sigma$, depending on the limiting method; and, if an upper limit, $L_{h+\frac{1}{2}}$ equals S/σ, $2S/\sigma$, or $\frac{3}{2}S/\sigma$, respectively, in the three methods. In any case, if $N_{h+\frac{1}{2}}$ reaches beyond a limit, one sets

$$N_{i+\frac{1}{2}} = N_{m+\frac{1}{2}} = L_{h+\frac{1}{2}}, \tag{85}$$

and recomputes N from

$$N = (\hat{N}_{h-\frac{1}{2}} - L_{h+\frac{1}{2}})/u + S/\sigma. \tag{86}$$

In the normal case of $\hat{N}_{h+\frac{1}{2}}$ staying within bounds, the individual, or detailed, extrapolations using Eqs. (74) and (75) are performed next. This is done with P = 1 except in the Reduced Limit method where P = 1/u' is used if u' > 1. Because more than one extrapolation is calculated, it is possible, though not very likely, that one of them goes outside bounds. In general, if d is the dimensionality of the cell, as many as d - 1 of the extrapolations can give undesirable results. Here one is dealing with extrapolations at angles to the principal flow. There is, therefore, very little physics to use as a guide beyond insisting that the output fluxes be positive, that is, setting such fluxes to zero if one or more of them becomes negative. The zero limit correction to the problem of flux skewing is, however, quite simple. After computing all the extrapolations each one is tested. If, for example, $N_{i+\frac{1}{2}}$ is negative, one sets $N_{i+\frac{1}{2}} = 0$ after first computing a factor f.

$$f = -N_{i+\frac{1}{2}}/(N_{h+\frac{1}{2}} - N_{i+\frac{1}{2}}). \tag{87}$$

Then all the remaining extrapolations are modified according to

$$N_{s+\frac{1}{2}} + f(N_{h+\frac{1}{2}} - N_{s+\frac{1}{2}}) \to N_{s+\frac{1}{2}}, \tag{88}$$

where s denotes any one of the subscripts. For this example and geometry, s = m only. Clearly, for s = i, Eq. (88) gives zero. This correction scheme conserves particles because the sum of the individual corrections for each discovered negative outflow equals zero.

The auxiliary equations derived from Eq. (51), the balance and net flux equations, are of special interest. They are obtained by multiplying the terms of Eq. (51) by w_m and $3w_m\mu_m$, respectively, then summing over the index m, obtaining two equations in terms of the scalar flux $\bar{N}$ and the current, or net flux, I defined by

$$\bar{N}_i = \Sigma_m w_m N_{mi}, \tag{89}$$

and

$$I_i = \Sigma_m w_m \mu_m N_{mi}. \tag{90}$$

By performing the first sum for the balance equation, one finds

$$A_{i+\frac{1}{2}} I_{i+\frac{1}{2}} - A_{i-\frac{1}{2}} I_{i-\frac{1}{2}} + \sigma V\bar{N} = VS \tag{91}$$

noting that, in the summing, the terms in α vanish due to cross cancellation.

The second sum for the net flux equation depends on the diffusion condition, which is another assumption, valid or nearly valid in many situations, to the effect that N is given to sufficient accuracy by the linear form

$$N = \bar{N} + 3\mu I. \tag{92}$$

From this, one derives in particular that

$$N_{m+\frac{1}{2}} - N_{m-\frac{1}{2}} = 3(\mu_{m+\frac{1}{2}} - \mu_{m-\frac{1}{2}})\, I = 6w_m I, \qquad (93)$$

a result which will be used below.

Before substituting Eq. (92) into Eq. (51) and performing the multiplications and summations, Eq. (51) is rewritten as

$$\mu\bar{A}(N_{i+\frac{1}{2}} - N_{i-\frac{1}{2}}) + \tfrac{1}{2}\mu C(N_{i+\frac{1}{2}} + N_{i-\frac{1}{2}})$$

$$+ (C/w)[\bar{\alpha}(N_{m+\frac{1}{2}} - N_{m-\frac{1}{2}}) - w\mu(N_{m+\frac{1}{2}} + N_{m-\frac{1}{2}})]$$

$$+ \sigma VN = VS, \qquad (94)$$

where $\bar{A}$ and V may be written

$$\bar{A} = \tfrac{1}{2}(A_{i+\frac{1}{2}} + A_{i-\frac{1}{2}}) = 2\pi(r_{i+\frac{1}{2}}^2 + r_{i-\frac{1}{2}}^2), \qquad (95)$$

and

$$V = 4\pi\Delta\,\frac{1}{3}(r_{i+\frac{1}{2}}^2 + r_{i+\frac{1}{2}}\, r_{i-\frac{1}{2}} + r_{i-\frac{1}{2}}^2). \qquad (96)$$

From the difference schemes [Eqs. (74) and (75)] for small intervals, it follows that

$$N_{i+\frac{1}{2}} + N_{i-\frac{1}{2}} = N_{m+\frac{1}{2}} + N_{m-\frac{1}{2}}, \qquad (97)$$

so that Eq. (94) simplifies to

$$\mu\bar{A}(N_{i+\frac{1}{2}} - N_{i-\frac{1}{2}}) + (C\bar{\alpha}/w)(N_{m+\frac{1}{2}} - N_{m-\frac{1}{2}})$$

$$+ \sigma VN = VS. \qquad (98)$$

Therefore, for the net flux equation, making use of Eqs. (93) and (98), one obtains

$$\bar{A}(\bar{N}_{i+\frac{1}{2}} - \bar{N}_{i-\frac{1}{2}}) + \sigma VI = 0. \qquad (99)$$

If all the above steps are done analytically by using derivatives and integrations rather than differences and numerical quadratures, one discovers that Eq. (99) is not correct unless $\bar{A} = V/\Delta$. This relation clearly holds for plane geometry, and also, as seen in the next section, for cylindrical geometry. It does not hold for spherical geometry as seen when comparing Eqs. (95) and (96).

There are several remedies for the defect in Eq. (98). The simplest of these is based on the following replacements.

$$\begin{cases} \sigma\Delta\bar{A}/V \to \sigma \\ S/\sigma + (\Delta\bar{A}/V - 1)\bar{N} \to S/\sigma, \end{cases} \qquad (100)$$

which leave the balance equation unchanged and correct the net flux equation. By good fortune the correction to S/σ in Eq. (100) is positive. It has the physical effect of increasing the scattering cross section near the origin, especially in the cell next to the origin. The total effect of the correction decreases as the number of intervals in the system increases. Table II gives some data for the size of the correction near the origin in the case of equal r intervals. The asymptotic behavior, shown in the last column, is given by $\Delta\bar{A}/V \sim 1 + 2/3(2i-1)^2$.

TABLE II

TABLE OF $\Delta\bar{A}/V$

i	$\Delta\bar{A}/V$	Approx. $\Delta\bar{A}/V$
1	1.5000	1.6667
2	1.0714	1.0741
3	1.0263	1.0267
4	1.0135	1.0136
5	1.0082	1.0082

A different, perhaps better method for dealing with the defect in Eq. (99) has been developed by Grant[5] on the basis of truncation error analysis. (Also, see Ref. 6.) In essence that method sets $P = 1$ in Eq. (75) for the $N_{m+\frac{1}{2}}$ extrapolation, but determines P in Eq. (74) for the other extrapolation so that $\bar{A}$ in the net flux equation [Eq. (99)] becomes V/Δ, which also resolves the problem. According to this, $1 + P$ is found to be $C/(A_{i+\frac{1}{2}} - V/\Delta)$ for positive μ, $C/(V/\Delta - A_{i-\frac{1}{2}})$ for negative μ. Grant's method was not used here because it conflicts with two aims in this report: to maintain equal weights in the extrapolations and to hold $P = 1$ for all sufficiently small cells.

IV. THE CYLINDRICAL CASE AND UNIT SPHERE QUADRATURE

The difference equation in the (r,μ,ξ) cylindrical case is given by

$$\mu A_{i+\frac{1}{2}} N_{i+\frac{1}{2}} - \mu A_{i-\frac{1}{2}} N_{i-\frac{1}{2}} + (C/w)(\alpha_{m+\frac{1}{2}} N_{m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}} N_{m-\frac{1}{2}}) + \sigma V N = VS, \tag{101}$$

which is formally identical to the spherical equation [Eq. (51)]. There are, however, some notable differences. First, for area and volume elements,

$$A_i = 2\pi r_i, \tag{102}$$

$$C = A_{i-\frac{1}{2}} - A_{i-\frac{1}{2}} = 2\pi\Delta, \tag{103}$$

$$V_i = \pi(r_{i+\frac{1}{2}}^2 - r_{i-\frac{1}{2}}^2) = 2\pi\bar{r}\Delta, \tag{104}$$

where

$$\Delta \equiv \Delta r = (r_{i+\frac{1}{2}} - r_{i-\frac{1}{2}}), \tag{105}$$

and

$$\bar{r} = \tfrac{1}{2}(r_{i+\frac{1}{2}} + r_{i-\frac{1}{2}}). \tag{106}$$

Therefore,

$$C/V = 1/\bar{r}. \tag{107}$$

Because

$$\bar{A} = \tfrac{1}{2}(A_{i+\frac{1}{2}} + A_{i-\frac{1}{2}}) = 2\pi\bar{r} \tag{108}$$

in this geometry, it follows that $\Delta\bar{A}/V = 1.0$ and that the replacements [Eq. (100)] have no effect for cylinders.

Second, a ξ-level indicator ℓ is omitted in Eq. (101), $\ell = 1,2,\ldots,\frac{1}{2}n$, $\xi_\ell < \xi_{\ell+1}$, where ℓ is attached to w, μ, and α, as well as to the N quantities. Here n is the order of quadrature, $n = 2,4,\ldots$. The basic quadrature procedure is, however, to put $n - 2\ell + 3$ quadrature points on level ℓ, where the levels span two octants on the surface of the unit sphere, and to arrange the total of $n(n + 4)/4$ points in a single sequence, $m = 1,2,\ldots,M$, where

$$M = n(n + 4)/4. \tag{109}$$

Of the M points, $\frac{1}{2}n$ are special points with negative μ and $w = 0$, also with

$$\alpha_{m+\frac{1}{2}} = \alpha_{m-\frac{1}{2}} = \bar{\alpha} = 0, \tag{110}$$

which are needed for the initial flux extrapolation in the μ direction, one for each ξ level. The remaining regular points ($w_m \neq 0$) are divided equally between the two octants, $n(n + 2)/8$ points on each, one octant having negative and the other positive μ.

Associated with μ is the direction cosine ξ and the third cosine μ satisfying

$$\mu^2 + \mu^2 + \xi^2 = 1. \tag{111}$$

For the sake of stable calculations with respect to round-off errors, the sequencing is always in the direction of increasing μ for each ξ level. It is also in the direction of decreasing r if μ is negative, and increasing r if μ is positive. The special points are placed at $m = m_\ell = 1, n + 2, 2n + 1,\ldots, M - 2$.

The cylindrical α coefficients obey the recursion formula

$$\alpha_{m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}} = -w\mu, \tag{112}$$

that is, the same formula as for spheres [Eq. (55)], except that they are generated separately for each ξ level starting with

$$\alpha_{m_\ell+\frac{1}{2}} = \alpha_{m_\ell-\frac{1}{2}} = \bar{\alpha}_{m_\ell} = 0. \tag{113}$$

Here, in the limit of $w \to w_{m_\ell} = 0$, one may write

$$(\alpha_{m_\ell+\frac{1}{2}} - \alpha_{m_\ell-\frac{1}{2}})/w_{m_\ell} \to -\mu_{m_\ell}. \tag{114}$$

The sequencing for the spherical equations is a special case of the above with $m = 1,2,\ldots,M$, and $M = n + 1$, where w represents level weights, that is, sums of point weights by level, rather than by point

weights. There is only one special point in this case: $w_1 = 0$, $\mu_1 = -1.0$, with $\alpha_{3/2} = \alpha_{\frac{1}{2}} = \bar{\alpha}_1 = 0$.

For cylindrical geometry, two sequencing procedures will be considered. In the first method, proceed as described above using the following formula for the special μ's.

$$\mu_{m_\ell} = -\sqrt{1 - \xi_{m_\ell+1}^2} \ . \tag{115}$$

In the second method, to obtain extrapolations that are consistent with the spherical case (explained below), use only one special point -- the same point as for spheres. Thus, $m = 1,2,\ldots,M$, where

$$M = n(n + 2)/4 + 1 \tag{116}$$

with the first regular points for successive levels located at $m = 2, n + 2, n,\ldots,M - 1$.

For the first level, the first extrapolation in μ is done in the regular manner using the fluxes obtained for the $m = 1$ point. For the succeeding levels, the first extrapolation is done using the result of the first extrapolation on the previous level.

The second scheme is consistent with the scheme for spheres in that it can readily be reduced to a one-dimensional scheme. The reduction is immediate if all the μ directions on a given μ level are equal and if the corresponding level weight is equated to the sum of the point weights on that μ level. Under these circumstances, solutions to spherical, and also infinite plane, problems would be independent of the dimensionality of the quadrature used. In specific cases, the μ directions on a given μ level are generally almost equal and occasionally are equal.

In practice one can let a root-mean-square relation hold between the direction cosine for a given level and the individual direction cosines on that level. If the point weights on a level are unequal, one replaces an unweighted mean by a weighted mean. The principal objective here is to preserve the condition in Eq. (57), whether one expands a one-dimensional set to two-dimensional use or reduces a two-dimensional set to one-dimensional use.

The curvature coefficeint C_m in Eq. (51) for spheres, which goes with the angular difference terms in that equation, may for a special value of m, $m = s$ omitting a factor approximately equal to $2/\bar{r}$, be written

$$C_s = (2\mu_s/w_s)\alpha_{s-\frac{1}{2}} = (2\mu_s/w_s)\Sigma_m - w_m\mu_m \ , \tag{117}$$

where s is the index of the smallest positive μ, so that $\alpha_{s-\frac{1}{2}}$ is the maximum α, and where the sum is over those m for which μ_m is negative. Analytically $C_s = \frac{1}{2}$ should hold, but generally the quadrature sets used supply this value only in the limit of large n.

If, for example, Gauss P_{n-1} quadrature is used, say for $n = 4$, 8, and 16, one finds that $2C_s = 1.087$, 1.023, and 1.006, respectively. These departures from the true value of 1.0 are regarded as rather large. By using specially constructed quadratures, such as ES_n (discussed below), which assume that

$$\mu_s = w_s, \tag{118}$$

that is, the smallest positive μ is the midpoint μ of the interval, the situation is considerably improved. For ES_n quadrature, $n = 4$, 8, and 16, one finds $2C_s = 1.032$, 1.011, and 1.003, respectively. In one instance, for a particular value of n, $n = 4$, the improvement can be readily demonstrated. This is the case of the extrapolation length z_o, where for $n = 4$ the formula z_o is

$$z_o = \mu_1 + \mu_2 - \sqrt{3}\ \mu_1\mu_2 \ . \tag{119}$$

Using this for P_{n-1} and ES_n quadratures, each of which has two positive values of μ for $n = 4$ (μ_1 and μ_2), one finds $z_o = 0.6940$ and 0.7061, respectively, compared to the exact value of 0.710446.

In the cylindrical case, assuming Eq. (118), one can establish that

$$C_s = 2\Sigma_m - w_m\,\mu_m \approx w_s\,\mu_s^2/\mu_s \tag{120}$$

should hold for each level. The first teat of the quadrature is that the sum of $2C_s$ over the levels should approach unity as n approaches infinity. Good agreement is not expected for low n here because the right-hand side of Eq. (120) is only approximate. Performing the test using data from ES_n, $n = 2$, 4, 8, and 16, one finds 0.5774, 0.8889, 0.9655, and

0.9924, respectively, and for the sequence n = 6, 12, and 24, one finds 0.9420, 0.9849, and 0.9978. All of which seems satisfactory.

The second test of the two-dimensional quadrature is to compute and examine the differences (multiplied by 2) between the left-hand and right-hand sides of Eq. (120). Computing these for each level by using ES_n, one obtains, for n = 4, the values of 0.032 and 0.111, and for n = 8 the values 0.006, 0.009, 0.011, and 0.019. For higher n, however, one does not obtain as good agreement. For ES_n with n = 16, for example, the differences are 0.011, 0.019, -0.004, -0.015, -0.003, -0.001, 0.001, and 0.003. These seem too large, perhaps by a factor of 2 to 4. The results are not good for EQ_n either, a more carefully constructed quadrature set. In this case, for n = 16, the differences are 0.034, 0.020, 0.000, -0.008, -0.008, -0.032, 0.001, and 0.003. For tables of EQ_n, see Ref. 7.

The second test may be a more sensitive test because it involves a division by μ's, the smallest μ magnitude, in the subtraction term. Nevertheless, one should not exclude the possibility that in some cylindrical problems the angular flux may fail to converge to the right limit as n and the number of r intervals will increase. The improper convergence may be limited to a region near the center of the cylinder where the effect of the geometry curvature is large. For the scalar flux, averages of fluxes over large regions, eigenvalues of the problem, etc., proper convergence is more likely since there will be a tendency for errors to cancel. The remedy for the defect in quadrature hinted at above is, of course, to construct better quadrature sets, perhaps based on conditions such as Eq. (120) with equality sign for all but a few of the highest ξ levels.

The remainder of this section will describe the ES_n quadrature set, a basic easily constructed one-dimensional set which then is expanded to a two-dimensional and "triangular" set, for arbitrary n. It is based on the following assumptions.

(a) Equal point weights, normalized to unity on the octant, given by

$$w_m \equiv p = 8/n(n + 2), \tag{121}$$

$m = 1,2,\ldots,M$, with

$$M = n(n + 2)/8, \tag{122}$$

and μ, η, and ξ subject to

$$\mu_m^2 + \eta_m^2 + \xi_m^2 = 1.0 \tag{123}$$

and positive on the principal octant.

(b) Triangular arrangement of points on the surface of the octant, specified by (μ_m, η_m, ξ_m) triplets, on $\frac{1}{2}n$ levels, n = 2, 4,..., with $\frac{1}{2}n - \ell + 1$ points on level ℓ for a total of M points, M given by Eq. (122).

(c) Permutation symmetry, so that if (μ_m, η_m, ξ_m) is a point in the set so are all points obtained by the possible permutations of the components μ_m, η_m, and ξ_m which may number 1, 3, or 6 depending on how many, if any, of the components are equal.

(d) Extension to 2, 4, or 8 octants, depending on the requirements of the problem, by reflection of the principal M points into the other octants with the appropriate renormalization of weights and sign changes of the components.

The one-dimensional sets are constructed first. Here the level weights w_ℓ are given by

$$w_\ell = (\tfrac{1}{2}n - \ell + 1)p, \tag{124}$$

where p = 1/M, the lower μ-interval boundaries are given by

$$\mu_{\ell-\frac{1}{2}} = 1.0 - (\tfrac{1}{2}n - \ell + 1)(\tfrac{1}{2}n - \ell + 2)p, \tag{125}$$

and the midpoint μ's by

$$\bar{\mu}_\ell = 1.0 - \tfrac{1}{2}(\tfrac{1}{2}n - \ell + 1)^2 p. \tag{126}$$

From the above one can deduce

$$\Sigma_\ell \, w_\ell \, \bar{\mu}_\ell = \tfrac{1}{2}, \tag{127}$$

and, after considerably more algebra,

$$\Sigma_\ell \, w_\ell \, \mu_\ell^2 = (1 - p/4)/3. \tag{128}$$

The one-dimensional ES_n sets are based on Eq. (124) for level weights and on

$$\mu_\ell = R \, \mu_{\ell-\frac{1}{2}} + \bar{\mu}_\ell \tag{129}$$

for level cosines where R is determined so that Eq. (57) is satisfied. A formula for R can be derived.

Table III gives computed values for R for n = 4, 6, ..., 32.

TABLE III

VALUES OF THE SCALE FACTOR R VERSUS n

n	R	n	R
4	0.0728757	20	0.0024709
6	0.0287804	22	0.0020428
8	0.0157065	24	0.0017172
10	0.0099458	26	0.0014638
12	0.0068776	28	0.0012627
14	0.0050444	30	0.0011004
16	0.0038600	32	0.0009675
18	0.0030498		

By construction, the second moment $\overline{M}_2$ is exact and equal to 1/3. The fourth moment $\overline{M}_4$, which should equal 1/5, converges rather rapidly to that value, the errors decreasing about as $0.135/n^2$. The higher moments, say up to $\overline{M}_n$, converge at about the same rate.

The two-dimensional ES_n sets are derived from the one-dimensional set making use of the general ES_n assumptions given above and from the following specific rules.

(a) For each point in the triangular arrangement, the formula

$$\mu_m^2 + \eta_m^2 + \xi_2^2 = 1.0 \tag{130}$$

should be satisfied, from which Eq. (57) follows as a corollary.

(b) The root-mean-square relation between μ_ℓ and individual μ's on a given level should hold. This relation is automatically satisfied for the highest two levels, hence for all levels for n = 2 and 4.

(c) The maximum number of unequal μ's on level ℓ to be $\ell + 1$ with $\mu_{\ell,k+1} = \mu_{\ell,k}$, $k = \ell + 1, \ell + 2, \ldots$ until the symmetry requirements overrule.

(d) Additional equating of μ's on specific levels starting with, and going downward from, level $\frac{1}{2}n - 2$ to the extent necessary to determine all points. Thus for n = 12, 14, and 16, $\mu_{\frac{1}{2}n-2,2} = \mu_{\frac{1}{2}n-2,1}$, for n = 16 also $\mu_{\frac{1}{2}n-3,1}$.

Table IV gives the ES_n quadrature sets. The values of $\mu_{\ell k}$, k fixed and ℓ varying, are read diagonally downward. For tables and discussion of other quadrature sets, see Refs. 7 and 8.

V. TWO- AND THREE-RECTANGULAR VARIABLES

The transport difference equation for plane (x, y,z) geometry is written as follows.

$$\mu A(N_{i+\frac{1}{2}} - N_{i-\frac{1}{2}}) + \eta B(N_{j+\frac{1}{2}} - N_{j-\frac{1}{2}}) + \xi C(N_{k+\frac{1}{2}} - N_{k-\frac{1}{2}}) + \sigma VN = VS, \tag{131}$$

where

$$A = \Delta y \Delta z, \tag{132}$$

$$B = \Delta x \Delta z, \tag{133}$$

$$C = \Delta x \Delta y, \tag{134}$$

and

$$V = \Delta x \Delta y \Delta z. \tag{135}$$

If the third difference represents time variation, Δz is replaced by Δt and ξ by unit. The neutron velocity $v = v_g$ enters where v is discrete valued and depends on the velocity group. In this case of time-dependent (x,y) geometry, one can also write

$$A = \Delta y, \tag{136}$$

$$B = \Delta x, \tag{137}$$

$$C = V/v\Delta t, \tag{138}$$

and

$$V = \Delta x \Delta y. \tag{139}$$

For stationary (x,y) geometry, the time-dependent or $v = \infty$ case, C = 0.

Here, as explained in Sec. III, $N_{i+\frac{1}{2}}$ is an abbreviation for $N_{g,i+\frac{1}{2},j,k}$, denoting the number of particles of velocity v_g with stream, per second per unit area, in the direction (μ_m, η_m, ξ_m) at the cell surface specified by ($i + \frac{1}{2}$, j, k). Therefore, $\mu AN_{i+\frac{1}{2}}$ represents the total inflow across that cell surface. This and other terms with a cell edge (half-integer) subscript stand for surface average of flux, whereas σVN and VS represent volume averages.

TABLE IV

ES_n QUADRATURE SETS

ℓ	1	2	3	4	5	6	7	8
n=2								
w_ℓ	1.0000000							
μ_ℓ	0.5773503							
$\mu_{\ell 1}$	0.5773503							
n=4								
w_ℓ	0.6666667	0.3333333						
μ_ℓ	0.3333333	0.8819171						
$\mu_{\ell 1}$	0.3333333							
$\mu_{\ell 2}$	0.3333333	0.8819171						
n=6								
w_ℓ	0.5000000	0.3333333	0.1666667					
μ_ℓ	0.2500000	0.6810569	0.9406503					
$\mu_{\ell 1}$	0.2399760							
$\mu_{\ell 2}$	0.2689295	0.6810569	0.9406503					
$\mu_{\ell 3}$	0.2399760	0.6810569						
n=8								
w_ℓ	0.4000000	0.3000000	0.2000000	0.1000000				
μ_ℓ	0.2000000	0.5562826	0.8109946	0.9641359				
$\mu_{\ell 1}$	0.1876726							
$\mu_{\ell 2}$	0.2116104	0.5454437	0.8109946					
$\mu_{\ell 3}$	0.2116104	0.5773503	0.8109946	0.9641359				
$\mu_{\ell 4}$	0.1876726	0.5454437						
n=10								
w_ℓ	0.3333333	0.2666667	0.2000000	0.1333333	0.0666667			
μ_ℓ	0.1666667	0.4699819	0.7059675	0.8746233	0.9759494			
$\mu_{\ell 1}$	0.1541474							
$\mu_{\ell 2}$	0.1745146	0.4523038	0.6962559					
$\mu_{\ell 3}$	0.1745146	0.4870187	0.7250004	0.8746233	0.9759494			
$\mu_{\ell 4}$	0.1745146	0.4870187	0.6962559	0.8746233				
$\mu_{\ell 5}$	0.1541474	0.4523038						
n=12								
w_ℓ	0.2857143	0.2380952	0.1904762	0.1428571	0.0952381	0.0476191		
μ_ℓ	0.1428751	0.4067269	0.6226502	0.7906269	0.9106570	0.9827406		
$\mu_{\ell 1}$	0.1308070							
$\mu_{\ell 2}$	0.1485160	0.3855474	0.5940136					
$\mu_{\ell 3}$	0.1485160	0.4329602	0.6500264	0.7906269	0.9106570			
$\mu_{\ell 4}$	0.1485160	0.3936131	0.6500264	0.7906269	0.9106570	0.9827406		
$\mu_{\ell 5}$	0.1485160	0.4329602	0.5940136	0.7906269				
$\mu_{\ell 6}$	0.1308070	0.3855474						

TABLE IV (cont)

ℓ	1	2	3	4	5	6	7	8
n=14								
w_ℓ	0.2500000	0.2142857	0.1785714	0.1428571	0.1071429	0.0714286	0.0357143	
μ_ℓ	0.1250000	0.3584040	0.5559135	0.7176286	0.8432492	0.9330754	0.9870071	
$\mu_{\ell 1}$	0.1136154							
$\mu_{\ell 2}$	0.1292734	0.3356467						
$\mu_{\ell 3}$	0.1292734	0.3800860	0.5217463					
$\mu_{\ell 4}$	0.1292734	0.3581007	0.5776795	0.7001734				
$\mu_{\ell 5}$	0.1292734	0.3581007	0.5773503	0.7335191	0.8432492			
$\mu_{\ell 6}$	0.1292734	0.3800860	0.5776795	0.7335191	0.8432492	0.9330754		
$\mu_{\ell 7}$	0.1136154	0.3356467	0.5217463	0.7011734		0.9330754	0.9870071	
n=16								
w_ℓ	0.2222222	0.1944444	0.1666667	0.1388889	0.1111111	0.0833333	0.0555556	0.0277778
μ_ℓ	0.1111111	0.3203022	0.5016083	0.6550294	0.7805655	0.8782166	0.9479828	0.9898638
$\mu_{\ell 1}$	0.1004229							
$\mu_{\ell 2}$	0.1144522	0.2970343						
$\mu_{\ell 3}$	0.1144522	0.3381830	0.4643665					
$\mu_{\ell 4}$	0.1144522	0.3229862	0.5351610	0.6145064				
$\mu_{\ell 5}$	0.1144522	0.3229862	0.5027914	0.6692085	0.7805655			
$\mu_{\ell 6}$	0.1144522	0.3229862	0.5027914	0.7031370	0.7805655	0.8782166		
$\mu_{\ell 7}$	0.1144522	0.3381830	0.5351610	0.6692085	0.7805655	0.8782166	0.9479828	
$\mu_{\ell 8}$	0.1004229	0.2970343	0.4643665	0.6145064			0.9479828	0.9898638

The total outflow $TN_{h+\frac{1}{2}}$ and inflow $TN_{h-\frac{1}{2}}$ are defined by

$$TN_{h+\frac{1}{2}} = |\mu|AN_{i+\frac{1}{2}} + |\eta|BN_{j+\frac{1}{2}} + |\xi|CN_{k+\frac{1}{2}}, \quad (140)$$

$$TN_{h-\frac{1}{2}} = |\mu|AN_{i-\frac{1}{2}} + |\eta|BN_{j-\frac{1}{2}} + |\xi|CN_{k-\frac{1}{2}}, \quad (141)$$

with

$$T = |\mu|A + |\mu|B + |\xi|C. \quad (142)$$

Equations (140) and (141) refer to the case when all angular components are positive. The indices depend naturally on the signs of μ, η, and ξ, that is, on the general direction of numerical evaluation. Equation (131) can now be written

$$T(N_{h+\frac{1}{2}} - N_{h-\frac{1}{2}}) + \sigma VN = VS, \quad (143)$$

which resembles Eq. (1) with $|\mu|$ set to $T\Delta x/V$, and u, the apparent cell thickness, given by

$$u = \sigma V/T. \quad (144)$$

Equation (131) may be solved by assuming the difference relation

$$N_{h+\frac{1}{2}} - N_{h-\frac{1}{2}} = (1 + P)(N - N_{h-\frac{1}{2}}). \quad (145)$$

Substituting this in Eq. (143) and solving for N, one finds

$$N = \frac{(1 + P)N_{h-\frac{1}{2}} + u\ S/\sigma}{1 + P + u}, \quad (146)$$

and using this N in Eq. (145), one finds

$$N_{h+\frac{1}{2}} = \frac{(1 + P - Pu)\ N_{h-\frac{1}{2}} + (1 + P)\ u\ S/\sigma}{1 + P + u}, \quad (147)$$

where u S/σ is replaced by VS/T in both equations if $\sigma = 0$. In the normal, straight diamond case, with $1 + P = 2$, the above reduces to

$$N = \frac{2N_{h-\frac{1}{2}} + u\ S/\sigma}{2 + u}, \tag{148}$$

and

$$N_{h+\frac{1}{2}} = \frac{(2 - u)\ N_{h-\frac{1}{2}} + 2\ u\ S/\sigma}{2 + u}. \tag{149}$$

For discussions of various other schemes, see Refs. 9 and 10.

Assuming that the Reduced Source Limit scheme is followed (the third scheme discussed in Sec. II), the next step is to calculate u', the effective cell thickness, by using

$$u' = u(N' - S/\sigma)/N', \tag{150}$$

where N' is the value of N obtained from Eq. (148). If $u \leq 1$, or if $u > 1$ with $u' \leq 1$, the normal result from Eq. (148) is kept and the extrapolation is done using Eq. (149). If $u' > 1$, one takes $P = 1/u'$, recomputes N from Eq. (146) and goes to Eq. (147) for $N_{h+\frac{1}{2}}$.

Section II showed that if $N_{h+\frac{1}{2}} < N$, then $N_{h+\frac{1}{2}}$ is limited from below by $\frac{1}{2}S/\sigma$, regardless of the size of u'. A test is necessary, however, for the upper limit if $N_{h+\frac{1}{2}} > N$. Here, if $N_{h+\frac{1}{2}} > \frac{3}{2}S/\sigma$, one sets

$$N_{h+\frac{1}{2}} = \frac{3}{2}S/\sigma, \tag{151}$$

and recomputes N from

$$N = N_{h-\frac{1}{2}}/u + (1 - 3/2u)S/\sigma. \tag{152}$$

Proceeding in conventional fashion, one now introduces the formulas for computing $N_{i+\frac{1}{2}}$, $N_{j+\frac{1}{2}}$, and $N_{k+\frac{1}{2}}$, the detailed output fluxes as follows.

$$N_{i+\frac{1}{2}} = (1 + P)N - PN_{i-\frac{1}{2}}, \tag{153}$$

$$N_{j+\frac{1}{2}} = (1 + P)N - PN_{j-\frac{1}{2}}, \tag{154}$$

and

$$N_{k+\frac{1}{2}} = (1 + P)N - PN_{k-\frac{1}{2}}, \tag{155}$$

which are consistent with Eq. (145). To obtain that equation one forms a linear combination of the above using, for example, the weight factors $|\mu|A/T$, $|\eta|B/T$, and $|\xi|C/T$.

After calculating the extrapolations, they are tested and corrected for skewing following the steps described in Sec. III. If, for example, $N_{i+\frac{1}{2}}$ is negative, set $N_{i+\frac{1}{2}} = 0$ after first computing a factor f,

$$f = -N_{i+\frac{1}{2}}/(N_{h+\frac{1}{2}} - N_{i+\frac{1}{2}}). \tag{156}$$

The set of extrapolations is then modified by

$$N_{s+\frac{1}{2}} + f(N_{h+\frac{1}{2}} - N_{s+\frac{1}{2}}) \rightarrow N_{s+\frac{1}{2}}, \tag{157}$$

where s = j and k. For s = i, Eq. (157) yields a zero result. The above test, and related corrections if such are required, are then repeated for $N_{j+\frac{1}{2}}$ and $N_{k+\frac{1}{2}}$.

Next, two methods for alleviating ray effects are described. Other methods were examined earlier (see Refs. 11 and 12). In the first method, smoothing is achieved by simplifying the extrapolations. The means is the "sloping step" method justified on the basis of solution along pseudocharacteristic lines. The lower differential accuracy of this method may be offset by going to a higher n and by some increase in the count of cells. In the second method ("input flaring"), one follows the general solution method described above after first smoothing out the input flux as detailed below.

To give some justification to the first method, note that the partial differential equation corresponding to Eq. (131), given by

$$\mu \frac{\partial}{\partial x} N(x, y, \mu_m, \eta_m) + \eta \frac{\partial}{\partial y} N(x, y, \mu_m, \eta_m)$$

$$+ \xi \frac{\partial}{\partial z} N(x, y, \mu_m, \eta_m)$$

$$+ \sigma N(x, y, \mu_m, \eta_m) = S(x,y), \tag{158}$$

is actually a transformation of a one-dimensional equation. The transformation is defined by

$$\frac{\partial}{\partial s} = \mu \frac{\partial}{\partial x} + \eta \frac{\partial}{\partial y} + \xi \frac{\partial}{\partial z}, \tag{159}$$

and the result is that Eq. (158) is equivalent to

$$\frac{\partial}{\partial s} N(s) + \sigma N(s) = S(s), \qquad (160)$$

where s is measured along the path determined by (μ_m, η_m, ξ_m) for each direction in the set. The solution of Eq. (143), the difference equation corresponding to Eq. (160), obtained above in terms of N and $N_{h+\frac{1}{2}}$, is clearly a one-dimensional result consistent with Eq. (160).

The change of variables from Eq. (160) to Eq. (158), replacing one variable by three, is a convenient but otherwise rather arbitrary transformation which does not add any physics to the problem. One may therefore argue that the presence of several inputs to a cell is simply the manifestation of a system of mesh cells not lined up with the directions of flow and that, therefore, the calculated average output flux $N_{h+\frac{1}{2}}$ should represent all the extrapolations. According to this, one sets

$$N_{i+\frac{1}{2}} = N_{j+\frac{1}{2}} = N_{k+\frac{1}{2}} = N_{h+\frac{1}{2}}, \qquad (161)$$

which is a Sloping Step scheme applied to all the coordinate directions. It differs from the ordinary step scheme in that $N_{h+\frac{1}{2}} \neq N$. Using the relations above [Eq. (161)] eliminates the skewing problem and also exercises a strong smoothing action on the fluxes since several, usually unequal, inputs are made to produce equal outputs. This method, which is essentially a step function method as far as variation of flux normal to the discrete directions is concerned, probably benefits from having more than the normal count of mesh cells. In practice, the larger count is generally supplied because it is normally required for an adequate description of the problem. It is needed for placing sources and internal boundaries, for getting detail in the output, etc.

The second method for smoothing out ray effects is more elaborate than the first; it is based on making exchanges of particles between the detailed input beams entering a cell; and it is done before the regular calculation described at the beginning of this section. It represents a means for making a distribution of parallel beams simulate a distribution of conical beams. The method requires that certain data input be furnished specifying the conical spread for each discrete ray, that is, a spread for each direction (μ_m, η_m, ξ_m).

The input flaring method, as it may be called, is based on the observation that the inflow on one side of the cell [say, $\mu\Delta y N_{i-\frac{1}{2}}$ on the left side of an (x,y) cell], which on the assumption that

$$R \equiv |\mu|\Delta y \,/\, |\eta|\Delta x \leq 1, \qquad (162)$$

is directed toward the adjoining side, perhaps also should, to some extent because of flaring, be directed toward the opposite side. Here the extent would depend on the flare in the rays entering the cell and on how close R is to unity. Likewise some fraction of $\eta\Delta x N_{j-\frac{1}{2}}$, the input at the bottom of the cell, should perhaps be diverted to exit at the top rather than on the right.

The partial exchanges between the cell surfaces must conserve the number of particles. For (x,y) geometry, for example, write

$$\mu\Delta y\ N_{i-\frac{1}{2}}(1 - F) + \eta\Delta x\ N_{j-\frac{1}{2}}\overline{F} \rightarrow \mu\Delta y\ N_{i-\frac{1}{2}}, \qquad (163)$$

and

$$\mu\Delta y\ N_{i-\frac{1}{2}}F + \eta\Delta x\ N_{j-\frac{1}{2}}(1 - \overline{F}) \rightarrow \eta\Delta x\ N_{j-\frac{1}{2}}. \qquad (164)$$

The sum of these exchange equations produces an identity. Here F represents the fraction of particles transferred to the $(i,j-\frac{1}{2})$ side.

Another condition on the exchange is that it should have no effect if $N_{i-\frac{1}{2}} = N_{j-\frac{1}{2}}$. Therefore,

$$\mu\Delta y(1 - F) + \eta\Delta x\overline{F} = \mu\Delta y, \qquad (165)$$

which gives

$$\mu\Delta yF = \eta\Delta x\overline{F}. \qquad (166)$$

It remains, therefore, to produce a formula for F. In (x,y) geometry there is only one exchange; in (x,y,z) geometry this count goes to three, and for four variables the count goes to six. Each exchange is like the one outlined above and is defined by equations similar to Eqs. (163) through (166).

A few formulas are derived below for F = F(R) in the simple case of n = 2 and (x,y) geometry. For

flow in the principal octant in the single direction, $\mu_1 = \eta_1 = \sqrt{3}/3$. In this instance the spread of the beam represented by $(\sqrt{3}/3, \sqrt{3}/3, \sqrt{3}/3)$ is over an entire octant of solid angle.

Assuming that the flux on the left face of the cell is uniformly equal to $N_{i-\frac{1}{2}}$ and that $R \leq 1$, the fraction F(R) of particles reaching for the opposite side is given by

$$F(R) = (2/\pi)\int_0^1 \arctan(Rr)dr = (2/\pi)[\arctan(R) - (1/2R)\,\ell n(1 + R^2)] \tag{167}$$

from which one can calculate F(1) = 0.279, F(0.8) = 0.233, F(2/3) = 0.199, and F(1/2) = 0.153. Asymptotically, for R going to zero,

$$F(R) \sim R/\pi \tag{168}$$

holds. Using a crude but useful approximation to the subtended angle, the area of some part of the output surface divided by the total area, one obtains

$$F(R) \approx \int_0^1 Rrdr/(1 + Rr) = 1 - (1/R)\,\ell n(1 + R), \tag{169}$$

which yields F(1) = 0.307, F(0.8) = 0.265, F(2/3) = 0.234, and F(1/2) = 0.189. F(R) from Eq. (167) is, however, very well approximated by

$$F(R) \approx R/\pi = 0.3183R. \tag{170}$$

On the basis of the above and a few other investigations, the following preliminary estimate for F in the general case is proposed.

$$F = (R - \gamma)/\pi, \tag{171}$$

where F is set to zero if negative, and where $\gamma = 0$ for the example above and otherwise equal to unity minus the given spread, $0 \leq \gamma \leq 1$. In the ES_n quadrature with the triangular arrangement of points and level weights

$$w_\ell = 8(\tfrac{1}{2}n - \ell + 1)/n(n + 2), \tag{172}$$

one can let γ be given by

$$\gamma = 1 - 1/(\tfrac{1}{2} - \ell + 1). \tag{173}$$

After computating F, one finds $\overline{F}$ from $\overline{F} = RF$. If $R > 1$, replace R as follows.

$$1/R \rightarrow R, \tag{174}$$

and, by using the new R, compute

$$\overline{F} = (R - \gamma)/\pi, \tag{175}$$

setting it to zero if negative, and finally find F from $F = R\overline{F}$. In all of this, one can assume that the coefficient of $1/\pi$ in the formulas for F and $\overline{F}$, as well as the γ quantities, can be manipulated to a limited extent if this is a way to enhance the smoothing.

As shown, the above can be extended to (x,y,z) and other geometries. On the (x,y,z) case one has three exchanges with separate R's, $R_1 = \mu\Delta y/\eta\Delta x$, $R_2 = \mu\Delta z/\xi\Delta x$, and $R_3 = \eta\Delta z/\xi\Delta y$. Also, on the basis of the ES_n quadrature, one can let γ be given by

$$\gamma = 1/2n \tag{176}$$

for all points. In (x,y,z) one probably has to do something special if a beam interacts with three cell faces simultaneously.

Splitting mesh cells in rectangular geometries is regarded as a method for handling complicated geometrical arrangements of materials. The present discussion will be confined to (x,y) geometry and to splitting by a single straight diagonal line. However, ideas also apply to (x,y,z) geometry. It is assumed that up to two inputs may be divided and that up to two split outputs may be produced by the calculation. It is also assumed, of course, that the two parts of the cell can have different materials and that two values of N are generated, one for each part. Finally, it is assumed that, in general, relatively few cells are split, say from 5 to 15% of the total.

The diagonals may be defined by two numbers, f_1 and f_2. The splits may be divided into eight cases depending on the sign and magnitude of these parameters. A negative f_1 defines a point on the $(i - \frac{1}{2}, j)$ side, a positive f_1 defines a point on the $(i, j-\frac{1}{2})$ side, a negative f_2 defines a point on the $(i + \frac{1}{2}, j)$ side, and a positive f_2 defines a point on the $(i, j+\frac{1}{2})$ side. Here, to illustrate, the case of positive f_1 and f_2 will be discussed with incident particles from below and from the left. The situation is shown in Fig. 1.

The important area elements in the illustration are given by the following.

$$(A,C) = (B,D) = \Delta x, \tag{177}$$

$$(A,B) = (C,D) = \Delta y, \tag{178}$$

$$(A,E) = f_1 \Delta x, \tag{179}$$

$$(B,F) = f_2 \Delta x, \tag{180}$$

and the volume of parts I and II are given by

$$V_I = \tfrac{1}{2}(f_1 + f_2)V, \tag{181}$$

and

$$V_{II} = V - V_I. \tag{182}$$

The figure indicates a flow from left to right across the diagonal (E,F). The total effective input area, hence also the output area, is given by

$$A_I = \mu \Delta y + F_1 \eta \Delta x, \tag{183}$$

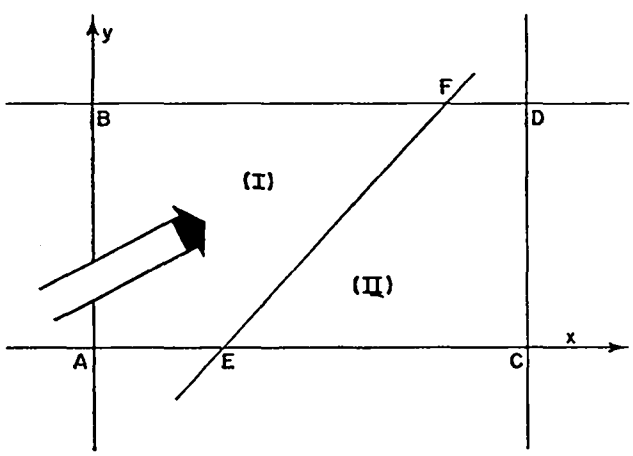


Fig. 1. Schematic diagram of split (x,y) mesh cell.

where the terms give the two partial areas. Looking at A_I as the sum of effective output areas, one writes

$$A_I = f_2 \eta \Delta x + (A_I - f_2 \eta \Delta x). \tag{184}$$

Therefore, if $A_I - f_2 \eta \Delta x$ is positive, the flow is from left to right, otherwise it is the reverse. The calculations must first be done for the part which transmits particles to the other part.

Because of splitting a single cell into two, one can expect the accuracy of the calculation to increase. This may be offset to some degree because cell splitting implies a material discontinuity.

Turning to the calculation, it is easy to determine N and $N_{h+\frac{1}{2}}$ for the two parts of the cell given the inputs, but somewhat cumbersome to determine the extrapolations by the detailed (x,y) method, including smoothing the inputs to control ray effects, and correcting for skewing by Eqs. (156) and (157).

The easiest method for the split cell is, of course, to determine N and $N_{h+\frac{1}{2}}$ in the normal manner, but to use the sloping step scheme for the extrapolations, a scheme which also serves to mitigate ray effects and to eliminate skewing problems.

REFERENCES

1. Bengt G. Carlson, in Methods in Computational Physics, B. Alder, S. Fernbach, and M. Rotenburg, Eds. (Academic Press, New York and London, 1963), Vol. 1.

2. B. G. Carlson and K. D. Lathrop, Computing Methods in Reactor Physics, H. Greenspan, C. N. Kelber, and D. Okrent, Eds. (Gordon and Breach, Science Publishers, Inc., New York, 1968).

3. K. D. Lathrop, "Discrete-Ordinates Methods for Numerical Solution of the Transport Equation," Reactor Technol. 15, No. 2 (1972).

4. William H. Reed, "New Difference Schemes for the Neutron Transport Equation," Nucl. Sci. Eng. 46, No. 2, 309 (1971).

5. I. P. Grant, "Numerical Analysis of Discrete Ordinates Methods," J. Comput. Phys. 2, No. 4 (1968).

6. Wm. H. Reed and K. D. Lathrop, "Truncation Error Analysis of Finite Difference Approximations to the Transport Equation," Nucl. Sci. Eng. 41, No. 2, 237 (1970).

7. B. G. Carlson, "Tables of Symmetric Equal Weight Quadrature EQ_n Over the Unit Sphere," Los Alamos Scientific Laboratory report LA-4734 (1971).

8. B. G. Carlson, "Transport Theory: Discrete Ordinates Quadrature Over the Unit Sphere," Los Alamos Scientific Laboratory report LA-4554 (1970).

9. K. Lathrop and B. Carlson, "Numerical Solution of the Boltzmann Equation," J. Comput. Phys. 2, 173 (1966).

10. K. D. Lathrop, "Spatial Differencing of the Transport Equation: Positivity vs Accuracy," J. Comput. Phys. 4, No. 4, 475 (1969).

11. K. D. Lathrop, "Remedies for Ray Effects," Nucl. Sci. Eng. 45, No. 3, 255 (1971).

12. K. D. Lathrop and B. G. Carlson, "Properties of New Numerical Approximations to the Transport Equation," J. Quant. Spectrosc. Radiat. Transfer 11, 921 (1971).