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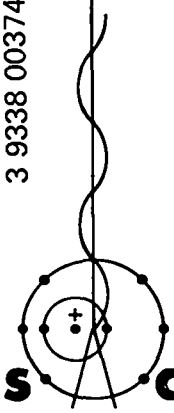

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A METHOD OF CHARACTERISTICS FOR THE TRANSPORT EQUATION SOLUTION

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Bengt G. Carlson

ABSTRACT

A method of characteristics is developed for the numerical solution of the multigroup discrete ordinates transport equation. A revised form of the diamond difference method is coordinated with the new approach and some alternate, possibly useful methods are developed. Also, several minor numerical difficulties that occasionally troubled calculations in the past have been resolved.

I. INTRODUCTION

This report discusses the numerical solution of the multigroup, discrete ordinates transport equation with special emphasis on neutron transport and diffusion, and develops an improved S_n-type method for such solution with several new features. Included among these is a method of characteristics that furnishes a different approach to the solution. For clarification, a transport method is a collection of methods, which typically includes discretizations, quadrature formulas, difference schemes, and iterative techniques, plus numerous special methods for special situations. Reference 1 should be regarded as a companion report to this one. To some extent, this report updates and rearranges material from Ref. 1.

The revised methods have many advantages over earlier methods, which will become apparent as the discussion progresses. The characteristic approach, for example, imparts more general and consistent properties to the final discretized equations. It facilitates the generation of physically realistic solutions even under very adverse conditions. Specifically, the positivity and smoothness of a solution can be enforced as the computations progress, which reduces or eliminates various types of oscillations, including, to some degree, so-called ray effects. This, in turn, has a beneficial effect on the convergence rate of iterative sequences. However, the revised method is not radically different from the S_n methods and codes now used, or from those explored or used in the past.

Solution by a discrete S_n (DSN) method typically involves piecing together a distribution function over a coordinate mesh in energy, direction, time, and position by means of straight-line segments, using continuous segments whenever this seems the most sensible thing to do. Based on various practical considerations, the discrete treatment has become the favored treatment for the energy variable. In other variables, including directional or angular, the normal treatment is by continuous segments, with occasional departures from that norm by means of so-called modified difference schemes. The finite element and spherical harmonic methods represent significant departures from the general approach of this report. The finite element method replaces simple difference schemes by more elaborate techniques, and the spherical harmonics method approximates the angular-dependent segment of the distribution by a continuous polynomial rather than by a net of connected straight-line segments.

The multigroup, discrete ordinates equation is a simplified form of the linear Boltzmann equation, an integro-differential equation. It governs the distribution N of particles, typically neutrons or

photons, as a function of particle class (g,m) location in space R, and time t, and consists of a system of G times M partial differential equations of the form

$$\frac{\partial}{\partial s} N_{g,m}(s) + \sigma_g(s)\, N_{g,m}(s) = S_g(s), \qquad (1.1)$$

where g = 1, 2, ..., G, and m = 1, 2, ..., M. The functions $N_{g,m}$ are the unknowns to be determined, given the other quantities. Here an index pair (g,m) refers to a beam or collection of neutrons, say, of velocity about v_g moving in the direction about Ω_m. The quantity s is measured along so-called characteristic lines, that is, in the direction Ω_m of streaming. Equation (1.1) assumes that time t and the components of R depend parametrically on s.

The multigroup transformation is largely a transformation of the physical data (mainly cross-section data for a variety of particle-nuclei interactions) from their more natural energy-dependent form to the multigroup or transfer matrix form. When done to any precision, this is a very complex and laborious transformation. The data include the total removal cross-section σ_g shown explicitly in Eq. (1.1) and similar, more detailed data used to form the source term S_g. This term is the principal coupling term in the above system of G times M equations.

For any given g, S_g generally depends on the $N_{g,m}$ for that g, as well as on $N_{g,m}$ for other or perhaps all g. Therefore, to arrive at a numerical solution in a simple way, a sequence of iterative cycles is performed. Initially, S_g is computed from given trial functions but at later stages it comes from previous iterates. Fortunately, in most practical situations, such sequences of iterates converge. Moreover, in cases of slow convergence, various means are available for the acceleration of convergence.

The solution for N in angle, space, and time is obtained by means of difference schemes. For angular components, quadrature methods are also involved. The solution is generated mesh cell by mesh cell in the (Ω,R,t) space, usually in a very particular sequence. Iteration is involved for each time step and each group g. Here, R may have up to three components, and $\Omega \equiv (\mu,\eta,\xi)$ with $\mu^2 + \eta^2 + \xi^2 = 1$, up to two independent components. Assuming regular mesh cells with d dimensions and two times d sides, the calculations first entail the determination of the midcell value of N and then d extrapolation across the cell. The latter, which may be based on the d input fluxes and the midcell flux, determine the cell output fluxes. Here by extrapolation scheme is meant the same as difference scheme. In the rectangular geometries (the Cartesian case), with R = (x,y,z) in the most general case, extrapolation in the angular variables is normally not necessary. In the simple curvilinear cases of spherical (r) and cylindrical geometry, only one extrapolation in angle is needed. Discontinuous extrapolation, used occasionally, is used chiefly to maintain positive output fluxes.

In the discrete S_n method, one normally chooses $M_o = n(n+2)/8$ directions per octant of the unit sphere, the general domain of Ω, where n is the order of angular approximation, n = 2, 4, ... The usual value of M is therefore $2^d M_o$, where d is the dimensionality of R. The calculations are greatly simplified if the total mesh in all the variables present is obtained as the logical product of the individual meshes. Although this restriction is convenient and generally reduces the calculation time per cell, it is not necessary, may not suit all applications, and may produce far too many cells.

The revised methods can be expected to save a great deal of computing time because, with smoother fluxes expected, the number of cells in one or several of the variables may be decreased markedly and the number of iterations needed for convergence may also be reduced. The basic procedure uses special schemes in a variety of situations. In general, such schemes are more elaborate than the regular ones. However, the special schemes are only used when actually needed and involve but a fraction of the cells, thus having little effect on the calculation time. The fraction depends on the locality in the configuration and on the cell sizes chosen, as well as on the particle speed and direction.

The main difficulty with the discrete ordinate, difference relation approach is the occasional development of flux distortions, often in the form of oscillations in the calculated fluxes with no basis in the physics of the problem. Oscillations in the forward direction (flux seesaw), oscillations at large angles to the main stream (flux skewing), and irregular, wave-like variations in the flux referred to as ray effects can be observed.

Oscillations generally develop as a consequence of rapid local variation in the flux with too large intervals and too stiff extrapolations to handle the situation. In this context, the importance of the optical dimensions that depend on cross-sections σ_g multiplied by cell dimensions is noted. Actually, as explained later, what counts is the effective optical dimensions. Oscillations can sometimes be controlled by inserting more intervals in the appropriate places. In such localities, however, they are better controlled by using modified difference schemes if a precise determination of the flux is not of prime concern.

Ray effects develop in certain situations as a result of the discrete ordinates approximation in the absence of sufficient natural smoothing, for example, by particle scattering. Ray effects can be mitigated readily by increasing the order n but, unfortunately, the mitigation tends to go slowly with increasing n. They can be effectively reduced or eliminated by introducing a fictitious source correction of total strength zero, which operates as a smoothing agent. In general, well-based, effective source corrections are very complex and are expensive in terms of computer time and storage. Also, they interfere seriously with the rate of iterative convergence. Other smoothing methods combined with a simplified fictitious source, as suggested in this report, may possibly be an answer to this occasional dilemma.

II. RECTANGULAR GEOMETRIES

For (x,y) rectangular geometry, the multigroup transport equation is given by

$$\mu \frac{\partial}{\partial x} N_g(x,y,\mu,\eta) + \eta \frac{\partial}{\partial y} N_g(x,y,\mu,\eta) + \sigma_g(x,y)\, N_g(x,y,\mu,\eta) = S_g(x,y). \qquad (2.1)$$

This is the analytical equation discretized in the energy variable. If the particles are neutrons, discrete energy is represented by a set of G discrete velocities v_g, g = 1, 2, ..., G. The simple form of Eq. (2.1) also reflects that isotropic scattering, isotropic sources, and a stationary situation have been assumed.

In the above, N_g means the number of particles of velocity about v_g streaming in the direction Ω, $\Omega \equiv (\mu,\eta,\xi)$ with $\mu^2 + \eta^2 + \xi^2 = 1$, per unit area normal to Ω at R, $R \equiv (x,y)$, per unit time. The quantity σ_g, called the total macroscopic cross section, denotes the probability per unit length of travel that a given particle experiences a collision (a change in Ω, a removal from the beam). The source term S_g denotes the number of particles of velocity about v_g being released (inserted into the beam) per unit volume at (x,y) per unit time. Therefore, $V\sigma_g N_g$ represents the interaction losses in a small volume V at (x,y), VS_g the interaction and other gains, and $V(S_g - \sigma_g N_g)$ the net change due to all local sources and sinks. In particular, the term S_g acts as a coupling term between the groups. It includes contributions from its own and other groups, from a selection of the groups if not from all. In the neutron case, it includes contributions from independent sources, scattering events, and fission reactions. The derivative terms in Eq. (2.1), however, have to do with the migration or propagation of particles in the (x,y) space.

Equation (2.1) illustrates the general rectangular case that may include as many as four derivative terms. Equation (2.1) is simplified to one less term if N_g depends on x only. It gains a term $\xi(\partial N_g/\partial z)$ if N_g depends on z as well as on x and y. Finally, it receives a term $\partial N_g/v_g\, \partial t$ if N_g is also a function of time t.

Equation (2.1) can be written more concisely in the characteristic form

$$\frac{\partial}{\partial s} N(s,\Omega) + \sigma(s)\, N(s,\Omega) = S(s,\Omega), \qquad (2.2)$$

where the variable s is measured along the path determined by Ω, with Ω assuming the role of a parameter. Here and following, the index g is suppressed. Equation (2.2) is the physically more meaningful equation that describes the attenuation and amplification of the intensity or flux of a unidirectional beam involving a single independent variable s. Given a change in s, the changes in the other variables can be calculated. Equation (2.1) can be derived from Eq. (2.2) by the operator relation

$$\frac{\partial}{\partial s} = \mu \frac{\partial}{\partial x} + \eta \frac{\partial}{\partial y}, \qquad (2.3)$$

where $\mu = dx/ds$ and $\eta = dy/ds$.

An important subcase in transport theory is diffusion theory, the result of taking the transport equation to the diffusion theory limit. This may be defined as the limit in which N can be approximated by a linear expression in the angular components

$$N(x,y,\mu,\eta) = \bar{N}(x,y) + 3\mu\, I(x,y) + 3\eta\, J(x,y), \tag{2.4}$$

where $\bar{N}$ is the scalar flux

$$N(x,y) = \frac{1}{2\pi}\int_0^{\pi}\int_{-1}^{1} d\eta\, d\theta\, N(x,y,\mu,\eta), \tag{2.5}$$

and I and J are the currents in the x and y directions, respectively.

$$I(x,y) = \frac{1}{2\pi}\int_0^{\pi}\int_{-1}^{1} \mu\, d\eta\, d\theta\, N(x,y,\mu,\eta), \tag{2.6}$$

and

$$J(x,y) = \frac{1}{2\pi}\int_0^{\pi}\int_{-1}^{1} \eta\, d\eta\, d\theta\, N(x,y,\mu,\eta). \tag{2.7}$$

Here, in the special case of $N \equiv 1$, $\bar{N} = 1$ and $I = J = 0$. The azimuthal variable θ is related to μ and η by

$$\mu = \sqrt{1 - \eta^2}\ \cos\theta\ . \tag{2.8}$$

The mixed moment Q, a second-order moment needed later, is defined by

$$Q(x,y) = \frac{1}{2\pi}\int_0^{\pi}\int_{-1}^{1} \mu\,\eta\, d\eta\, d\theta\, N(x,y,\mu,\eta). \tag{2.9}$$

If Eq. (2.1) is integrated over the Ω domain three separate times after multiplying the terms by 1, 3μ, and 3η, respectively, all times $1/2\pi$, one obtains the balance equation

$$\frac{\partial}{\partial x} I(x,y) + \frac{\partial}{\partial y} J(x,y) + \sigma(x,y)\, \bar{N}(x,y) = S(x,y), \tag{2.10}$$

the net flux equation in the x direction

$$\frac{\partial}{\partial x} \bar{N}(x,y) + 3\sigma(x,y)\, I(x,y) = 0, \tag{2.11}$$

and the net flux equation in the y direction

$$\frac{\partial}{\partial y} \bar{N}(x,y) + 3\sigma(x,y)\, J(x,y) = 0. \tag{2.12}$$

The last two assume that Eq. (2.4) is substituted in Eq. (2.1) before integration. The above three equations, which may be combined into a single second-order equation, define diffusion theory.

However, if Eq. (2.4) is not substituted in Eq. (2.1) before integration, the net flux equations are given by

$$\frac{\partial}{\partial x} \bar{N}(x,y) + 3\,\frac{\partial}{\partial y} Q(x,y) + 3\sigma(x,y)\, I(x,y) = 0 \tag{2.13}$$

and

$$3\,\frac{\partial}{\partial x} Q(x,y) + \frac{\partial}{\partial y} \bar{N}(x,y) + 3\sigma(x,y)\, J(x,y) = 0. \tag{2.14}$$

These two equations, plus Eq. (2.10), are consistent with the expansion

$$N(x,y,\mu,\eta) = \bar{N}(x,y) + 3\mu\, I(x,y) + 3\eta\, J(x,y) + 15\mu\eta\, Q(x,y). \tag{2.15}$$

The above procedure, coupled with the assumption that $Q(x,y) \equiv 0$, is an alternate, second route to diffusion theory.

Note that Eq. (2.15) is not a complete polynomial of second order in μ and η because the terms in μ^2 and η^2 are absent. Stated otherwise, Eq. (2.15) is a polynomial of first order with an excess term in Q. Therefore, if one desires not to propagate the excess term, done by writing Eq. (2.1) as

$$\mu\,\frac{\partial}{\partial x}\,(N - 15\mu\eta Q) + \eta\,\frac{\partial}{\partial y}\,(N - 15\mu\eta Q) + \sigma N = S, \tag{2.16}$$

Eqs. (2.10), (2.11), and (2.12) follow without assuming either Eq. (2.4) or (2.15). In this third approach, diffusion theory is obtained without assuming that $Q(x,y) \equiv 0$.

The next two steps represent successive discretizations of the angular variable $\Omega = (\mu,\eta,\xi)$ and the position variable $R = (x,y,z)$. The first step is the discrete ordinates transformation and the second step is the finite cell formulation. Following these steps with a third major step, difference schemes are introduced to effect the numerical solution.

The multigroup discrete ordinates equations are on the same physical basis as Eq. (2.1) and are given by

$$\mu_m \frac{\partial}{\partial x} N_m(x,y) + \eta_m \frac{\partial}{\partial y} N_m(x,y) + \sigma(x,y)\, N_m(x,y) = S(x,y), \tag{2.17}$$

where m refers to one of M discrete directions, $\Omega_m = (\mu_m, \eta_m, \xi_n)$, with

$$\mu_m^2 + \eta_m^2 + \xi_m^2 = 1 \tag{2.18}$$

assumed, m = 1, 2, ..., M. The direction cosine μ is normally attached to the x direction, η to the y direction, and ξ to the z direction. In (x,y) geometry, in which four octants of the unit sphere, or half of the Ω space, is normally involved, M is taken to be

$$M = n(n + 2)/2. \tag{2.19}$$

This implies n(n + 2)/8 directions per octant, where n is the order of angular approximation, n = 2, 4, ..., and also that

$$-1 \le \mu_m, \eta_m \le 1, \tag{2.20}$$

with $0 \le \xi_m \le 1$.

For discrete ordinates in the diffusion theory limit, one writes

$$N_m(x,y) = \bar{N}(x,y) + 3\mu_m I(x,y) + 3\eta_m J(x,y), \tag{2.21}$$

with

$$\bar{N}(x,y) = \Sigma_m w_m N_m(x,y), \tag{2.22}$$

$$I(x,y) = \Sigma_m w_m \mu_m N_m(x,y), \tag{2.23}$$

and

$$J(x,y) = \Sigma_m w_m \eta_m N_m(x,y). \tag{2.24}$$

For consistency with the analytical case, the following conditions must hold for the quadrature sets (w_m, μ_m, η_m).

$$\Sigma_m w_m = 1, \tag{2.25}$$

$$\Sigma_m w_m \mu_m = \Sigma w_m \eta_m = 0, \tag{2.26}$$

and

$$\Sigma_m w_m \mu_m^2 = \Sigma_m w_m \eta_m^2 = 1/3. \tag{2.27}$$

These are extended to include also the component ξ in the case of (x,y,z) geometry. The last of the conditions [Eq. (2.27)] is required to get consistent balance and net flux equations, which in this case are obtained by summations over m in Eq. (2.17) after multiplying by the factors 1, $3\mu_m$, and $3\eta_m$, respectively.

The finite cell formulation results from the discretization of position (x,y) in the discrete ordinates equations. Again, the physical principles of Eq. (2.1) are retained. The finite cell equation is written

$$\mu_m A_{i,j}\left(N_{m,i+\frac{1}{2},j} - N_{m,i-\frac{1}{2},j}\right) + \eta_m B_{i,j}\left(N_{m,i,j+\frac{1}{2}} - N_{m,i,j-\frac{1}{2}}\right) + \sigma_{i,j} V_{i,j} N_{m,i,j} = V_{i,j} S_{i,j}, \tag{2.28}$$

where the cell is defined by the coordinates $x_{i-\frac{1}{2}}$, $x_{i+\frac{1}{2}}$, $y_{j-\frac{1}{2}}$, and $y_{j+\frac{1}{2}}$, and the area and volume elements by

$$A_{i+\frac{1}{2},j} = A_{i-\frac{1}{2},j} = A_{i,j} = \Delta y_j, \tag{2.29}$$

$$B_{i,j+\frac{1}{2}} = B_{i,j-\frac{1}{2}} = B_{i,j} = \Delta x_i, \tag{2.30}$$

and

$$V_{i,j} = \Delta x_i \, \Delta y_j = \left(x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}\right)\left(y_{j+\frac{1}{2}} - y_{j-\frac{1}{2}}\right). \tag{2.31}$$

In general, area elements divided by volume elements (here A/V and B/V) have units of inverse length, that is, the units of σ. Note that here, for a regular rectangular mesh, $A_{i,j}$ depends only on the y index j and $B_{i,j}$ only on the x index i. In conventional, simplified notation, omitting all central subscripts, Eq. (2.28) becomes

$$\mu A(N_{i+\frac{1}{2}} - N_{i-\frac{1}{2}}) + \eta B(N_{j+\frac{1}{2}} - N_{j-\frac{1}{2}}) + \sigma V N = V S. \tag{2.32}$$

If the variable z is present, a flux difference with

the factor ξ C is added. In this case A = $\Delta y\ \Delta z$, B = $\Delta x\ \Delta z$, C = $\Delta x\ \Delta y$, and V = $\Delta x\ \Delta y\ \Delta z$. If the time variable is present, a flux difference with a factor $V/v\Delta t$ is added.

Equation (2.28) is to be solved numerically for the central flux $N_{g,m,i,j}$ and the extrapolations to the cell boundaries which, in the case of μ_m and η_m positive, are $N_{g,m,i+\frac{1}{2},j}$ and $N_{g,m,i,j+\frac{1}{2}}$. With three unknowns involved, Eq. (2.28) must be supplemented by two auxiliary equations, that is, by difference schemes. The source terms depend on the $N_{g,m,i,j}$ functions but usually not strongly, therefore iterative means of solution can be used effectively. In other words, in any iterative step, the term $V_{i,j}$ $S_{i,j}$ in Eq. (2.28) is assumed to be known.

Equation (2.28) is taken to be exact in the sense that $\sigma_{i,j}$, $\sigma_{i,j}\ N_{m,i,j}$, and $S_{i,j}$ represent appropriate volume averages of σ, σN, and S, and the remaining N's similarly represent appropriate surface averages. Equations (2.28) and (2.32) clearly reveal the conservation nature of the transport equation. The term $|\mu|AN_{i+\frac{1}{2}}$ signifies, for example, the number of particles leaving (entering if $\mu < 0$) the cell over the face defined by the index pair $(i+\frac{1}{2},j)$; $|\eta|BN_{j-\frac{1}{2}}$ the number entering (leaving if $\eta > 0$) the cell over the face $(i,j-\frac{1}{2})$; and $V(S-\sigma N)$ the net change of particles in the cell from emissions and removals. Here the source term VS includes in-scattering from its own and other groups, the collision term $V\sigma N$ losses in the form of out-scattering to its own or other groups.

The finite cell equation for the characteristic formulation may be written

$$T\left(N_{h+\frac{1}{2}} - N_{h-\frac{1}{2}}\right) + VN = VS, \tag{2.33}$$

where the effective input or output area, or target area, is defined by

$$T = |\mu|A + |\eta|B, \tag{2.34}$$

and where $TN_{h+\frac{1}{2}}$ and $TN_{h-\frac{1}{2}}$ are given by

$$TN_{h+\frac{1}{2}} = |\mu|AN_{i+\frac{1}{2}} + |\eta|BN_{j+\frac{1}{2}} \tag{2.35}$$

and

$$TN_{h-\frac{1}{2}} = |\mu|AN_{i-\frac{1}{2}} + |\eta|BN_{j-\frac{1}{2}}. \tag{2.36}$$

These two formulas are valid for the principal octant. In the following text, most formulas will only be developed for that octant. The sign and index rules by octant are given in Table II-1.

Equation (2.33), the one-dimensionalized form of Eq. (2.32), is readily solved by the methods described in the next section for infinite plane (x) geometry. The solution is generated in a prescribed sequence, mesh cell by mesh cell, for each discrete direction and for each velocity group. To control round-off errors in the calculations, the direction of evaluation through the mesh must be consistent with Ω_m. Therefore, if μ_m is negative and η_m positive, the evaluation progresses in the negative x-direction and the positive y-direction. The process assumes an estimate for the source term, as it begins, the updating of the source whenever practical, as it continues, and the recalculation of the source, as it terminates, thereby setting up an iterative loop. In many problems, the calculations entail two or more iterative loops, usually nested, in which the number of cycles is limited by prescribed convergence criteria. The process also assumes known inputs from adjoining cells, previous in the calculating sequence, or, in exceptional cases, from boundary conditions. As a result, Eq. (2.33) is an equation in two unknowns, N and $N_{h+\frac{1}{2}}$. But, as stated above, solution is made possible by introducing a difference scheme.

As indicated, the solution of Eq. (2.33) appears as a pair of positive numbers, one for the midcell flux N and the other for the extrapolated flux $N_{h+\frac{1}{2}}$. A weight P is associated with the pair, where P = 1 in the normal, small cell case, and a P subject to $0 \le P < 1$ is determined in the large cell case. The solution, as explained further in Sec. III, depends on the difference relation

TABLE II-1

SIGN AND INDEX RULES FOR (x,y) GEOMETRY

Octant Number	Sign of μ	Sign of η	Indices in the Terms of $TN_{h+\frac{1}{2}}$
1	+	+	$i+\frac{1}{2}$, $j+\frac{1}{2}$
2	-	+	$i-\frac{1}{2}$, $j+\frac{1}{2}$
3	+	-	$i+\frac{1}{2}$, $j-\frac{1}{2}$
4	-	-	$i-\frac{1}{2}$, $j-\frac{1}{2}$

$$N_{h+\frac{1}{2}} - N_{h-\frac{1}{2}} = (1 + P)(N - N_{h-\frac{1}{2}}), \tag{2.37}$$

and is found to be

$$N = \frac{(1 + P)\ T\ N_{h-\frac{1}{2}} + V\ S}{(1 + P)\ T + \sigma\ V}, \tag{2.38}$$

together with

$$N_{h+\frac{1}{2}} = \frac{[(1 + P)T - P\ V\sigma]N_{h-\frac{1}{2}} + (1 + P)\ V\ S}{(1 + P)T + \sigma\ V}. \tag{2.39}$$

The difference scheme [Eq. (2.37)] implies an S_n-type approximation to the flux for $P = 1$, that is, an approximation by means of connected straight-line segments. In the exceptional case, $0 \leq P < 1$, the line segments are allowed to be discontinuous. The $P = 0$ case is referred to as the step scheme and the $0 < P < 1$ case is referred to as the sloping step scheme. Equation (2.37) with $P = 1$ implies the diamond difference scheme, accurate to second-order terms in Δs.

It remains to determine the individual extrapolations, or average outputs, knowing the combined average output $N_{h+\frac{1}{2}}$. If the direction lies in the principal octant, these outputs are $N_{i+\frac{1}{2}}$ and $N_{j+\frac{1}{2}}$. Several methods will be discussed.

In the diamond difference scheme, $N_{i+\frac{1}{2}}$ and $N_{j+\frac{1}{2}}$ are obtained from the following detailed schemes.

$$N_{i+\frac{1}{2}} = (1 + P)N - PN_{i-\frac{1}{2}} \tag{2.40}$$

and

$$N_{j+\frac{1}{2}} = (1 + P)N - PN_{j-\frac{1}{2}}, \tag{2.41}$$

which are consistent with Eq. (2.37). This is readily seen by combining the two equations with the weights $|\mu|A$ and $|\eta|B$, respectively, which yields

$$TN_{h+\frac{1}{2}} = T(1 + P)N - TPN_{h-\frac{1}{2}}. \tag{2.42}$$

In some situations, Eqs. (2.40) and (2.41) may produce one negative extrapolation. This is referred to as flux skewing, and positivity of the errant extrapolation may be restored by a skewing correction as follows. The correction is formulated so that $N_{h+\frac{1}{2}}$ is left unchanged. The set of extrapolations is revised each time a particular one is found to be negative. The following simple skewing correction, satisfying the condition, may be used. If $N_{i+\frac{1}{2}}$ is tested and found to be negative, $N_{i+\frac{1}{2}}$ is set to zero after first computing a factor f.

$$f = -N_{i+\frac{1}{2}}/(N_{h+\frac{1}{2}} - N_{i+\frac{1}{2}}). \tag{2.43}$$

The set of extrapolations is then modified by

$$N_{\ell+\frac{1}{2}} + f(N_{h+\frac{1}{2}} - N_{\ell+\frac{1}{2}}) \rightarrow N_{\ell+\frac{1}{2}}, \tag{2.44}$$

where ℓ denotes the sequence of indices, here i and j. The calculation for $\ell = i$ can of course be omitted because in this case the revised $N_{i+\frac{1}{2}}$ equals zero by construction. If $N_{i+\frac{1}{2}}$ is not negative, one goes on to test $N_{j+\frac{1}{2}}$, etc. In the (x,y) case, if $N_{i+\frac{1}{2}} < 0$, $N_{j+\frac{1}{2}}$ need not be tested because at least one of the outputs must be positive.

The extrapolations may be based on the idea that one is dealing with a single stream and that therefore the coordinate directions are auxiliary, less important directions. This is the characteristic approach in which Eq. (2.33), not Eq. (2.32), is the basic equation. The simplest extrapolation of this type is based on

$$N_{i+\frac{1}{2}} = N_{j+\frac{1}{2}} = N_{h+\frac{1}{2}}. \tag{2.45}$$

This rather crude scheme implies a sloping step scheme in the coordinate directions and it requires no skewing corrections. A more refined method is based on interpolation using N and $N_{h+\frac{1}{2}}$ and the projections of the output points on the line through the N and $N_{h+\frac{1}{2}}$ points. This leads to

$$N_{i+\frac{1}{2}} = N + D|\mu|\Delta x\ (N_{h+\frac{1}{2}} - N) \tag{2.46}$$

and

$$N_{j+\frac{1}{2}} = N + D|\eta|\Delta y\ (N_{h+\frac{1}{2}} - N), \tag{2.47}$$

with D to be determined so that the correct combined output $TN_{h+\frac{1}{2}}$ is obtained. One finds

$$D = T/(\mu^2 + \eta^2)V. \tag{2.48}$$

Finally, the most refined characteristic scheme is

in this geometry equivalent to the diamond scheme. In this and the previous case, it becomes necessary to test for skewing corrections.

The extrapolation methods based on Eq. (2.45) or Eqs. (2.46) and (2.47) exercise considerable restraint on the variation of the angular flux N. They may therefore be regarded as methods for smoothing the flux and may, together with the diamond scheme, be combined with a smoothing of the inputs by one of the methods described in Ref. 1, Sec. V. In general, smoothing methods can bring about considerable mitigation of ray effects. However, from all indications, the effect of smoothing extends over rather few intervals. Therefore, smoothing is not likely to be a complete remedy for ray effects.

The discrete S_n method, based on solving Eq. (2.32) or Eq. (2.33) by means of the diamond scheme, performs rather well over a wide range of applications. Actually, in some instances it performs too well -- too much in accordance with the assumptions made, particularly to the discrete ordinates approximation. In that basic, rather crude approximation, isotropic sources are replaced by spoke-like sources with fairly sparse spokes. In many problems this does not matter because scattering and other natural smoothing processes are present. In some problems, however, the natural smoothing is not sufficient in magnitude or uniform distribution over the system. In such cases, wavelike distortions in the flux may become evident. This is referred to as ray effects. It is a form of extraneous behavior, an imprint on N of the discrete representation for Ω. Ray effects become possible when two or more time and position variables are present.

Several methods have been proposed for major reduction or elimination of ray effects. A few, rather elaborate procedures have proved to be effective. However, these have also proved to be costly in computer time and storage and to slow down the convergence of iterative sequences. The most direct means of alleviating ray effects is of course to increase the order n of approximation. Unfortunately, this is an ineffective method because a very large n is required.

A simplified method, which probably has some adverse effect on convergence but demands little in terms of added computer time and storage, is based on a modified form of the transport equation, like Eq. (2.16). Here, for n = 2, a single excess term, $15\mu\eta Q$, is excluded from the derivative terms. In the general case, fluxes are obtained for $n(n+2)/2$ directions which can be used to determine a polynomial in μ and η, complete to degree $n-1$, plus a few terms of degree n. The complete part requires $n(n+1)/2$ fluxes, leaving $\frac{1}{2}n$ terms to determine as many excess terms. In the simplified method, as an approximation, one sets the excess terms equal to $15\, c_n\, \mu\eta Q$ where $c_2 = 1.0$, and c_n, $n > 2$, is determined by solving some basic problem for a few n's, say n = 4, 6, 8, and 12. The quantities c_n would be selected to give as smooth a solution as possible. A suitable problem might be a centrally located source in a vacuous and square (x,y) configuration. Assuming that such c_n can be determined, the regular difference procedure with P = 1 leads to a source correction ΔS of the form

$$\Delta S = 30 c_n\, \mu\eta(|\mu|A + |\eta|B)Q. \tag{2.49}$$

More explicitly, the VS source terms in Eqs. (2.32) and (2.33) are replaced by $V(S + \Delta S)$.

The mitigation of ray effects has two main results, one highly desirable, the other undesirable but usually acceptable. The desirable result is that the scalar flux $\overline{N}$ becomes smoother and more realistic. The undesirable result is that the angular flux generally becomes less smooth.

III. SOLUTION IN THE ONE-DIMENSIONAL PLANE CASE

In infinite plane (x,μ) geometry the differential equation for particle transport is given by

$$\mu \frac{\partial}{\partial x} N(x,\mu) + \sigma(x)\, N(x,\mu) = S(x). \tag{3.1}$$

This assumes isotropic emissions and interactions, so that S and σ are independent of μ, and a single component μ of Ω, $-1 \le \mu \le 1$, representing direction relative to the space coordinate x.

In the discrete ordinates formulation of the above, with ordinates N_m defined by

$$N_m(x) = N(x,\mu_m), \tag{3.2}$$

Eq. (3.1) is replaced by a system of equations.

$$\mu_m \frac{\partial}{\partial x} N_m(x) + \sigma(x)\, N_m(x) = S(x). \tag{3.3}$$

Here a μ-interval of length $\Delta\mu_m = \mu_{m+\frac{1}{2}} - \mu_{m-\frac{1}{2}}$, or weight $w_m = \frac{1}{2}\Delta\mu_m$, is assigned to each distinct μ_m, $m = 1, 2, \ldots, n$, where n is the order of angular approximation, $n = 2, 4, \ldots$. In general, a quadrature set (w_m, μ_m) for Eq. (3.3) must satisfy the following conditions.

$$\Sigma_m w_m = 1, \tag{3.4}$$

$$\Sigma_m w_m \mu_m = 0, \tag{3.5}$$

and

$$\Sigma_m w_m \mu_m^2 = 1/3. \tag{3.6}$$

The abscissas μ_m and related μ neighborhoods are normally placed symmetrically with respect to $\mu = 0$ on the interval $(-1, 1)$, an arrangement that implies Eq. (3.5). The subject of quadrature is discussed in more detail in Sec. VI.

The finite difference equation corresponding to Eq. (3.3) is written

$$\mu_m(A_{i+\frac{1}{2}} N_{m,i+\frac{1}{2}} - A_{i-\frac{1}{2}} N_{m,i-\frac{1}{2}}) + \sigma_i V_i N_{m,i} = V_i S_i, \tag{3.7}$$

where, in plane geometry,

$$A_{i+\frac{1}{2}} = A_{i-\frac{1}{2}} = A_i = 1 \tag{3.8}$$

and

$$V_i = \Delta x_i = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}, \tag{3.9}$$

with A_i defined by

$$A_i = \tfrac{1}{2}(A_{i+\frac{1}{2}} + A_{i-\frac{1}{2}}). \tag{3.10}$$

In Eq. (3.7), S_i, $N_{m,i}$, and $\sigma_i N_{m,i}$ represent volume averages of $S(x)$, $N_m(x)$, and $\sigma(x)N_m(x)$ over $(x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}})$. In many situations σ is constant within intervals so that $\sigma(x) = \sigma_i$. Physically, $V_i S_i$ and $\sigma_i V_i N_{m,i}$ represent total releases and removals of particles, respectively.

Using the above formulas for area and volume elements, and the convention of omitting central subscripts, Eq. (3.7) becomes

$$\mu(N_{i+\frac{1}{2}} - N_{i-\frac{1}{2}}) + \sigma\Delta x N = \Delta x S. \tag{3.11}$$

In the general context of the method of characteristics, Eq. (3.11) is written

$$(N_{h+\frac{1}{2}} - N_{h-\frac{1}{2}}) + uN = uS/\sigma, \tag{3.12}$$

where $u = \sigma V/T$ and, for the present geometry,

$$u = \sigma V/T = \sigma_h \Delta x_h / |\mu_m|. \tag{3.13}$$

Here h is defined so that $x_{h-\frac{1}{2}}$ is the boundary of inflow and $x_{h+\frac{1}{2}}$ is the boundary of outflow. Therefore

$$N_{h+\frac{1}{2}} - N_{h-\frac{1}{2}} = \begin{cases} N_{m,i+\frac{1}{2}} - N_{m,i-\frac{1}{2}}, & \mu_m \text{ positive}, \\ N_{m,i-\frac{1}{2}} - N_{m,i+\frac{1}{2}}, & \mu_m \text{ negative}. \end{cases} \tag{3.14}$$

The thickness of a given mesh cell V/T is obtained by dividing the volume element V by the effective target area A. $(V/T)S$ replaces uS/σ in Eq. (3.12) if $\sigma = u = 0$.

Because σ often varies a great deal, and irregularly, with particle velocity and material composition (hence with position in space), it is frequently impossible to construct a mesh so that u is sufficiently small everywhere for all velocity groups and all beam directions. Therefore, in finding numerical solutions, one must be prepared for large as well as small u dimensions.

The source uS/σ and sink uN terms in Eq. (3.12) can clearly be decreased (or increased) by the same amount with no real change to the equation, which points to an ambiguity in the transport equation. The magnitude of this depends in general on x and μ, may vary irregularly, and may be difficult to define in any precise manner. However, when present, the ambiguity can be used to advantage to decrease u, by decreasing uN, to obtain an <u>effective</u> optical thickness u'. If one permits a negative u' but not a negative modified source, uN can be decreased by as much as uS/σ. Performing the maximum subtraction, one obtains

$$N_{h+\frac{1}{2}} - N_{h-\frac{1}{2}} + u\,\frac{N - S/\sigma}{N}\,N = 0 \tag{3.15}$$

as a replacement for Eq. (3.12). On this basis, and with some means for estimating N, u' may be defined by

$$u' = u \frac{N - S/\sigma}{N} . \tag{3.16}$$

Further, u' may be written

$$u' = \sigma' V/T, \tag{3.17}$$

thus defining σ', the effective removal probability.

Two derived functions, the scalar flux $\overline{N}$ and the current or net flux I, are of particular importance in transport theory. They are defined by

$$\overline{N}(x) = \tfrac{1}{2} \int_{-1}^{1} N(x,\mu) d\mu \tag{3.18}$$

and

$$I(x) = \tfrac{1}{2} \int_{-1}^{1} N(x,\mu) \mu d\mu. \tag{3.19}$$

Associated with these functionals are two derived equations, the balance equation and the net flux equation, given by

$$\frac{\partial}{\partial x} I(x) + \sigma(x) \overline{N}(x) = S(x) \tag{3.20}$$

and

$$\frac{\partial}{\partial x} \overline{N}(x) + 3\sigma(x) I(x) = 0. \tag{3.21}$$

The derivation is by integration of Eq. (3.1) over μ from -1 to 1 after multiplying the terms by $\tfrac{1}{2}d\mu$ and $\frac{3}{2}\mu d\mu$, respectively, and by using, in the second integration, the diffusion approximation to $N(x,\mu)$.

$$N(x,\mu) = \overline{N}(x) + 3\mu I(x). \tag{3.22}$$

In the finite difference case, the corresponding functionals and equations, consistent with the analytical formulas in the limit of small Δx and $\Delta\mu$, are

$$\overline{N}_i = \Sigma_m w_m N_{m,i}, \tag{3.23}$$

$$I_i = \Sigma_m w_m \mu_m N_{m,i}, \tag{3.24}$$

$$I_{i+\frac{1}{2}} - I_{i-\frac{1}{2}} + \sigma_i \Delta x_i \overline{N}_i = \Delta x_i S_i, \tag{3.25}$$

and

$$\overline{N}_{i+\frac{1}{2}} - \overline{N}_{i-\frac{1}{2}} + 3\sigma_i \Delta x_i I_i = 0 \tag{3.26}$$

with the approximation

$$N_{m,i} = \overline{N}_i + 3\mu_m I_i \tag{3.27}$$

used with Eq. (3.26).

Physically, the flux functions N_m, $\overline{N}$, and I should be continuous in x, also in μ with some exceptions. In the numerical work, N_m is sometimes made discontinuous at a cell boundary just after the particles it represents have crossed the boundary. Nevertheless, continuity of $\overline{N}$ and I can be maintained if, in forming $\overline{N}$ and I at a boundary, values of N_m just before (or at) the boundary are used. The consistency of the above finite difference equations with their analytical counterparts depends, in the first place, on making sure that $\overline{N}$ and I are continuous and, in the second place, on the quadrature conditions [Eqs. (3.4) through (3.6)].

The consistency of the analytical and finite difference formulations is important for the proper convergence of the solutions with n, the order of directional approximation, and for obtaining high accuracy for relatively low n, say for n = 4, 6, and 8. The second consideration is important because convergence as n is increased tends to be slow. As seen above, consistency for plane geometry is readily established. For spherical and cylindrical geometry, however, consistency is somewhat more difficult to achieve and has a definite effect on the method of numerical solution.

Equation (3.12) is solved numerically by using the weighted diamond scheme, a simple difference scheme, given by

$$N_{h+\frac{1}{2}} = (1 + P)N - PN_{h-\frac{1}{2}}, \tag{3.28}$$

which may also be written

$$N_{h+\frac{1}{2}} - N_{h-\frac{1}{2}} = (1 + P)(N - N_{h-\frac{1}{2}}), \tag{3.29}$$

where P is a parameter, $0 \le P \le 1$. The auxiliary relation [Eq. (3.28)], together with the main equation [Eq. (3.12)], gives two equations for obtaining the two unknowns: the midcell flux N and the extrapolated flux $N_{h+\frac{1}{2}}$. In the modified diamond scheme (MDS), P is set to unity for small intervals and

computed from a given formula for large intervals. The use of P = 1 (the DS scheme) assumes that N is linear in x in the interval $(x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}})$. Physically, P = 1 means that the situation may be regarded as elliptic, or mildly or moderately hyperbolic and P < 1 means that the situation is decisively hyperbolic.

The weighted diamond scheme, also called the sloping step scheme, may be given the interpretation illustrated in Fig. 3.1. One finds $N'_{h-\frac{1}{2}}$, the past-crossing value of $N_{h-\frac{1}{2}}$, to be

$$N'_{h-\frac{1}{2}} = 2N_h - N_{h+\frac{1}{2}} = (1 - P)N_h + PN_{h-\frac{1}{2}}, \qquad (3.30)$$

and, for the discontinuity $N_{h-\frac{1}{2}} - N'_{h-\frac{1}{2}}$ at $x_{h-\frac{1}{2}}$,

$$N'_{h-\frac{1}{2}} - N_{h-\frac{1}{2}} = (1 - P)(N_h - N_{h-\frac{1}{2}}). \qquad (3.31)$$

Note that continuity of N requires that P be unity.

Substituting Eq. (3.28) with P = 1 in the difference equation [Eq. (3.12)], and solving for N, one obtains

$$N = \frac{2N_{h-\frac{1}{2}} + uS/\sigma}{2 + u}, \qquad (3.32)$$

and, from this, the extrapolation

$$N_{h+\frac{1}{2}} = 2N - N_{h-\frac{1}{2}} = \frac{(2 - u)N_{h-\frac{1}{2}} + 2uS/\sigma}{2 + u}. \qquad (3.33)$$

For the general case of arbitrary P, one finds

$$N = \frac{(1 + P)N_{h-\frac{1}{2}} + uS/\sigma}{1 + P + u} \qquad (3.34)$$

and

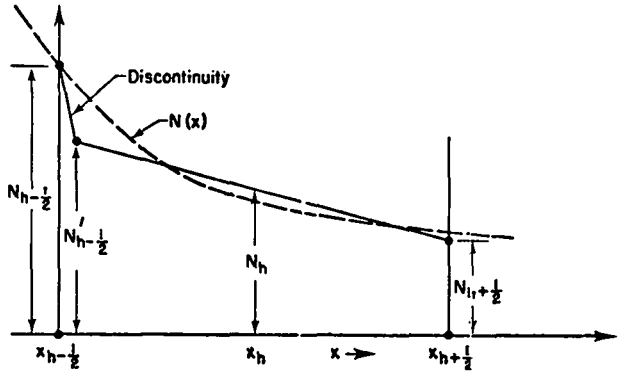

Fig. 3.1. Interpretation of difference scheme.

$$N_{h+\frac{1}{2}} = (1 + P)N - PN_{h-\frac{1}{2}}$$
$$= \frac{(1 + P - uP)N_{h-\frac{1}{2}} + (1 + P)uS/\sigma}{1 + P + u}. \qquad (3.35)$$

Here, one notes first that Eqs. (3.32) through (3.35) represent weighted averages of $N_{h-\frac{1}{2}}$ and S/σ with weights that sum to unity. Second, one notes that the coefficient of $N_{h-\frac{1}{2}}$ in Eq. (3.35), which analytically should equal the penetration probability e^{-u}, is an approximation to e^{-u}. Expanding for small u one obtains

$$\frac{1 + P - uP}{1 + P + u} = 1 - \frac{u}{1 + \frac{u}{1+P}}$$
$$= 1 - u + \frac{u^2}{1+P} - \frac{u^3}{(1+P)^2} + \ldots . \qquad (3.36)$$

This is accurate to second-order terms for all P and to third-order terms for P = 1. The ratio is clearly not a good approximation to e^{-u} if u is so large that it becomes negative, that is, if $u > (1 + P)/P$ or $P > 1/(u - 1)$.

Further, from the numerical solutions, one observes that the sequence of fluxes, $N_{h-\frac{1}{2}}$, N_h, $N_{h+\frac{1}{2}}$, is monotonely increasing if $S/\sigma > N_{h-\frac{1}{2}}$ (the growth case), and nonincreasing if $S/\sigma \leq N_{h-\frac{1}{2}}$ (the decay case). Also, by using Eq. (3.34), Eq. (3.31) for the discontinuity can be written

$$N'_{h-\frac{1}{2}} - N_{h-\frac{1}{2}} = \frac{u(1 - P)(S/\sigma - N_{h-\frac{1}{2}})}{1 + P + u}, \qquad (3.37)$$

which shows (if P < 1) that the discontinuity at $x = x_{h-\frac{1}{2}}$ is positive in the growth case and negative or zero in the decay case. Using the diamond solution (DS) for N, one deduces a second form for u'.

$$u' = u\,\frac{N - S/\sigma}{N} = \frac{N_{h-\frac{1}{2}} - N}{\frac{1}{2}N}, \qquad (3.38)$$

and, from these equalities,

$$(u - u')N = uS/\sigma \qquad (3.39)$$

and

$$N_{h-\frac{1}{2}} = (1 + \tfrac{1}{2}u')N. \qquad (3.40)$$

Hence, in terms of $N_{h-\frac{1}{2}}$ and u',

$$N = \frac{N_{h-\frac{1}{2}}}{1 + \frac{1}{2}u'}, \tag{3.41}$$

and

$$N_{h+\frac{1}{2}} = \frac{(1 - \frac{1}{2}u')N_{h-\frac{1}{2}}}{1 + \frac{1}{2}u'} = (1 - \frac{1}{2}u')N. \tag{3.42}$$

The weighted diamond scheme has two primary virtues. First, it is arithmetically simple, especially for P = 1, and is therefore economical with computer time. Second, it is invariant with respect to the source/sink ambiguity in the transport equation. This makes it very accurate, basically to second-order terms in u' rather than in u as one would first expect. The invariance of the scheme is established in Theorem 3.1 below. Note that u' is often substantially smaller than u and may, in high-scattering situations, be smaller by one or more orders of magnitude.

The modified diamond scheme (MDS) can now be more precisely defined. One first computes values for N and $N_{h+\frac{1}{2}}$ from Eqs. (3.32) and (3.33) based on P = 1 and then u' from Eq. (3.38). These values constitute the final solution for the interval unless u' is greater than u'_o, where u'_o is a given parameter, $u'_o \sim 1$. If $u' > u'_o$, which presumably would be infrequent, N and $N_{h+\frac{1}{2}}$ are recalculated using Eqs. (3.34) and (3.35) and a given formula for P, P = P(u'). Continuity of P(u') at $u' = u'_o$ is assumed so that $P(u'_o) = 1$. A simplified version of the MDS method, the limit version, will be defined and discussed later.

Theorem 3.1. The solution of Eq. (3.12) by the weighted diamond scheme, using a constant P, is independent of the source/sink ambiguity in the equation, that is, of any equal reduction in the source and sink terms.

Here, assuming a reduction of the source term by quS/σ and an invariant solution, one wants to show that the sink term is also reduced by quS/σ. From Eq. (3.34), without reduction, one has

$$(1 + P + u)(N - N_{h-\frac{1}{2}}) = u(S/\sigma - N_{h-\frac{1}{2}}). \tag{3.43}$$

With the source reduced and u replaced by u', assuming the same solution for N, one has

$$(1 + P + u')(N - N_{h-\frac{1}{2}}) = u'[(1-q)S/\sigma' - N_{h-\frac{1}{2}}]. \tag{3.44}$$

Subtraction of Eq. (3.44) from Eq. (3.43), noting that $u/\sigma = u'/\sigma'$, gives

$$(u - u')(N - N_{h-\frac{1}{2}}) = quS/\sigma - (u - u')N_{h-\frac{1}{2}}. \tag{3.45}$$

Consequently,

$$u'N = u(N - qS/\sigma), \tag{3.46}$$

which shows that uN is also reduced by quS/σ.

Theorem 3.1 provides a reasonable basis for using Eqs. (3.16) and (3.38) to estimate the effective optical thickness u'. The estimate appears to be on the low side. It does not seem worthwhile, however, to iterate on N.

Theorem 3.2. If P = P(u') is chosen so that P = 1 for $u' \le 2$ and $P \le 1/(u' - 1)$ for $u' > 2$, then, on the normal assumption that u, $N_{h-\frac{1}{2}}$, and uS/σ are nonnegative, $N_{h+\frac{1}{2}}$ is also nonnegative.

This theorem is verified by first writing Eq. (3.35) as follows and by adding and subtracting equal terms.

$$N_{h+\frac{1}{2}} = \frac{(1+P-u'P)N_{h-\frac{1}{2}} - (u-u')PN_{h-\frac{1}{2}} + (1+P)uS/\sigma}{1 + P + u}. \tag{3.47}$$

By application of Eqs. (3.39) and (3.40), this is simplified to

$$N_{h+\frac{1}{2}} = \frac{(1+P-u'P)N_{h-\frac{1}{2}} + (1-\frac{1}{2}u'P)uS/\sigma}{1 + P + u} \tag{3.48}$$

Clearly, if P = 1 and $u' \le 2$, $N_{h+\frac{1}{2}}$ is nonnegative. Also, if $P \le 1/(u' - 1)$, the coefficient of $N_{h-\frac{1}{2}}$ is nonnegative. With this restriction on P, and with $u' > 2$, one can write

$$1 - \tfrac{1}{2}u'P \ge \tfrac{1}{2}\frac{u' - 2}{u' - 1} > 0. \tag{3.49}$$

Therefore, the coefficient of S/σ is also nonnegative, which completes the proof. Note that if P approaches 1/u' for very large u', $N_{h+\frac{1}{2}}$ approaches $\frac{1}{2}S/\sigma$.

Theorem 3.3. If P satisfies $P \le 1/u' < 1/(u' - 1)$, then, in the decay case, $N_{h+\frac{1}{2}}$ is limited from below by $\frac{1}{2}S/\sigma$.

To prove this, one observes first, by using Eq. (3.40), that

$$N_{h-\frac{1}{2}} = (1 + \tfrac{1}{2}u')N \ge (1 + \tfrac{1}{2}u')S/\sigma. \tag{3.50}$$

After using this in Eq. (3.48) to put $N_{h-\frac{1}{2}}$ in terms of S/σ and decrease the numerator, it remains to demonstrate that

$$(1 + P - u'P)(1 + \tfrac{1}{2}u')$$

$$+ (1 - \tfrac{1}{2}u'P)u \ge \tfrac{1}{2}(1 + P + u). \tag{3.51}$$

Solving this inequality for P, one obtains

$$P \le \frac{u + u' + 1}{u'(u + u' + 1) - 1}, \tag{3.52}$$

which is satisfied by $P \le 1/u'$.

It seems reasonable, in view of the above, to complete the MDS scheme by taking $u'_o = 1$ and using $P(u') = 1/u'$ if $u' > u'_o$. An acceptable generalization of this is to use

$$P(u') = \frac{u' + (1 - 2u'_o)}{(u')^2 + (1 - 2u'_o)u' + (u'_o - 1)^2}, \tag{3.53}$$

valid for $0 \le u'_o \le 1$ where $P(u'_o) = 1$ and

$$P'(u')_{u'=u'_o} = 0, \tag{3.54}$$

$u'_o < 1$. This reduces to $P = 1/u'$ for $u'_o = 1$ and to

$$P(u') = u'/[(u')^2 + 1/4] \tag{3.55}$$

for $u'_o = 1/2$. Table III-1 gives some comparisons for P.

Many other possibilities exist for choosing $P(u')$ for $u' > u'_o$. For example,

$$P(u') = \frac{u' + 2(1 - u'_o)}{(u')^2 + (1 - 2u'_o)u' + (u'_o - 1)^2 + 1}, \tag{3.56}$$

$0 \le u'_o \le 2$, with $P(u'_o) = 1$ and Eq. (3.54) is satisfied for $u'_o < 2$. For $u'_o = 2, 1, \frac{1}{2}$, Eq. (3.56) gives

$$P(u') = 1(/(u' - 1), \tag{3.57}$$

$$P(u') = u'/[(u')^2 - u' + 1], \tag{3.58}$$

and

$$P(u') = (u' + 1)/[(u')^2 + 1.25], \tag{3.59}$$

respectively. It is not clear here if, for some sufficiently small u_o, the relation $N_{h+\frac{1}{2}} \ge \frac{1}{2}S/\sigma$ holds.

Assuming a constant source S over the interval $(x_{h-\frac{1}{2}}, x_{h+\frac{1}{2}})$, one can derive an analytical expression

TABLE III-1

VALUES OF P FROM FORMULAS AS GIVEN

u	1/(u-1)	$u/(u^2+1/4)$	1/u	Eq. (3.63)
0.5		1.0000		0.8467
1.0		0.8000	1.0000	0.7183
1.5		0.6000	0.6667	0.6115
2.0	1.0000	0.4706	0.5000	0.5232
2.5	0.6667	0.3846	0.4000	0.4505
3.0	0.5000	0.3243	0.3333	0.3907
4.0	0.3333	0.2462	0.2500	0.3010
5.0	0.2500	0.1980	0.2000	0.2395

for $N_{h+\frac{1}{2}}$ by integration, obtaining the total penetration

$$N_{h+\frac{1}{2}} = N_{h-\frac{1}{2}} e^{-u} + (1 - e^{-u})S/\sigma, \tag{3.60}$$

where $u = \sigma V/T$. Substituting this in Eq. (3.12), an analytical expression for N is found.

$$N = N_{h-\frac{1}{2}} (1 - e^{-u}/u) + [1 - (1 - e^{-u}/u)] S/\sigma. \tag{3.61}$$

Here, as in the case of Eqs. (3.34) and (3.35), one observes that N and $N_{h+\frac{1}{2}}$ are weighted averages of $N_{h-\frac{1}{2}}$ and S/σ. One also notes that N and $N_{h+\frac{1}{2}}$ are limited by S/σ as u becomes very large. In the growth case, S/σ is an upper limit and in the decay case, it is a lower limit. By solving the equation

$$\frac{1 + P - uP}{1 + P + u} = e^{-u}, \tag{3.62}$$

one finds the following formula for P.

$$P = \frac{1 - (1 + u)e^{-u}}{u - 1 + e^{-u}}, \tag{3.63}$$

with

$$P \approx 1 - u/3 \tag{3.64}$$

for small u and

$$P \approx 1/(u - 1) \tag{3.65}$$

for large u. Also, P can be shown to be monotonely decreasing.

For several reasons, the exponential method is not a good method to use. Constant S in each interval is a rather crude approximation. Also, it is time consuming to compute e^{-u} and then P from Eq. (3.63), especially since this has to be done for every interval. Finally, the error in the method is controlled by u rather than u' which is not good because often $u' \ll u$ in much of the mesh. To some degree, the same disadvantages apply to P based on high-order approximations to e^{-u}, Padé-type or other types. Note that in all these cases P varies with u so that Theorem 3.1 does not apply.

The limit version of the modified diamond scheme is defined as follows. N and $N_{h+\frac{1}{2}}$ are computed from Eqs. (3.32) and (3.33) with $P = 1$. In most cases these are final values for the interval. But if $N_{h+\frac{1}{2}} > (2 - \beta)S/\sigma$ occurs in the decay case, $N_{h+\frac{1}{2}}$ is set by $L_{h+\frac{1}{2}}$, the limit used in the test.

$$N_{h+\frac{1}{2}} = L_{h+\frac{1}{2}}, \tag{3.66}$$

and N is computed from

$$N = S/\sigma + (N_{h-\frac{1}{2}} - L_{h+\frac{1}{2}})/u, \tag{3.67}$$

whereupon P, if needed, can be computed from

$$P = (N - N_{h+\frac{1}{2}})/(N_{h-\frac{1}{2}} - N) = \frac{(N_{h-\frac{1}{2}} - L) + u(S/\sigma - L)}{(u - 1)(N_{h-\frac{1}{2}} - L) - u(S/\sigma - L)} = \frac{N_{h-\frac{1}{2}} + u\, S/\sigma - (u + 1)L}{(u - 1)N_{h-\frac{1}{2}} - u\, S/\sigma + L}. \tag{3.68}$$

The most restrictive limits are those based on Eqs. (3.60) and (3.61), that is, on setting $\beta = 1$. It was shown earlier that β can be relaxed to $\beta = \frac{1}{2}$ in the decay case. This is the motivation for introducing the coefficient β, and for using $2 - \beta$ in the growth case. In the zero fix-up scheme, a limit scheme used a great deal in the past, β is set to zero. This scheme, however, is in clear violation of the physics, which probably explains why it sometimes failed to control adequately oscillatory tendencies in the numerical solutions.

A way to compare the MDS method with other methods is to examine how well exponential decay is approximated when $S/\sigma = 0$ ($u' = u$). A few approximations are listed in Table III-2.

In some situations it may be useful to accept negative S/σ and, as a result, also negative $N_{h-\frac{1}{2}}$. In most cases, this would occur for a few intervals, directions, and groups. This is not in any way upsetting in the MDS methods. If both $N_{h-\frac{1}{2}}$ and S/σ are negative in an interval, the procedure is not changed, the same formula for u' is used, etc. If one of these quantities is negative and the other positive, the only change is that u' may be larger than u, which is quite acceptable. If N from the

TABLE III-2

APPROXIMATION TO e^{-u} IN VARIOUS METHODS

Scheme	P	e^{-u} Approximation	Good in u Range	Positive in u Range
Diamond	1	$\frac{1 - \frac{1}{2}u}{1 + \frac{1}{2}u}$	(0,1)	(0,2)
Step Scheme	0	$\frac{1}{1 + u}$	(0,½)	(0,∞)
MDS	$\begin{cases} 1, u \le 1 & \frac{1-\frac{1}{2}u}{1+\frac{1}{2}u} \\ 1/u, u > 1 & \frac{1}{1+u+u^2} \end{cases}$		(0,2)	(0,∞)

DS calculation is equal to zero, one sets P = 0. Growth and decay of flux are interpreted as increase or decrease in magnitude.

In conclusion, therefore, the modified diamond scheme (MDS) seems to take care of the difficulties of the past, those encountered with the straight diamond scheme (DS) or with improperly defined MDS schemes. It does not increase the requirements for computer storage and, although the computing time per cell is increased slightly, the total time is likely to be less because of the decreased interference with the inner iteration convergence resulting from the smoother MDS solutions.

IV. SOLUTION IN SPHERICAL GEOMETRY

The solution of the transport equation in curvilinear geometries, compared to solution in rectangular cases, is more involved. Here, starting with spherical geometry, the partial differential equation is given by

$$\mu \frac{\partial}{\partial r} A(r)\, N(r,\mu) + A'(r) \frac{\partial}{\partial \mu} \frac{1}{2}(1 - \mu^2)\, N(r,\mu) + \sigma(r)\, A(r)\, N(r,\mu) = A(r)\, S(r), \qquad (4.1)$$

where

$$A(r) = 4\pi r^2 \qquad (4.2)$$

and

$$A'(r) = \frac{\partial}{\partial r} A(r) = 8\pi r. \qquad (4.3)$$

This represents the conservation form of the equation because the coefficients μ and A', respectively, of $\frac{\partial}{\partial r}$ and $\frac{\partial}{\partial \mu}$ are independent of the variables of differentiation. Transformed to the regular form, with terms in $\frac{\partial}{\partial r} N$ and $\frac{\partial}{\partial \mu} N$, Eq. (4.1) becomes

$$\mu \frac{\partial}{\partial r} N(r,\mu) + \frac{1}{r}(1 - \mu^2) \frac{\partial}{\partial \mu} N(r,\mu) + \sigma(r)\, N(r,\mu) = S(r), \qquad (4.4)$$

where the 1/r coefficient comes from

$$\frac{1}{2} A'(r)/A(r) = 1/r. \qquad (4.5)$$

In the discrete ordinates formulation, Eq. (4.1) is written

$$\mu_m \frac{\partial}{\partial r} A(r)\, N_m(r) + \frac{A'(r)}{w_m} [\alpha_{m+\frac{1}{2}} N_{m+\frac{1}{2}}(r) - \alpha_{m-\frac{1}{2}} N_{m-\frac{1}{2}}(r)] + \sigma(r)\, A(r)\, N_m(r) = A(r)\, S(r), \qquad (4.6)$$

where $w_m = \frac{1}{2}\Delta\mu_m$ and $\alpha_{m-\frac{1}{2}}$, m = 1, 2, ..., n + 1, are coefficients to be determined.

$$\alpha_{m-\frac{1}{2}} \approx \frac{1}{4}(1 - \mu_{m-\frac{1}{2}}^2), \qquad (4.7)$$

with equality specified for m = 1, for which $\mu_{m-\frac{1}{2}} = -1$, and hence

$$\alpha_{\frac{1}{2}} = \frac{1}{4}(1 - \mu_{\frac{1}{2}}^2) = 0. \qquad (4.8)$$

The terms in $\alpha_{m+\frac{1}{2}}$ and $\alpha_{m-\frac{1}{2}}$ have the meaning of losses and gains, respectively, to the m^{th} discrete ray, or bundle of particles, in the course of streaming. As a consequence of streaming, such changes can occur in a system described by curvilinear coordinates. In such streaming, the value of μ associated with the moving particle depends on r and is monotonely increasing.

The differential operator in Eq. (4.6), as in Eq. (4.1), must clearly vanish in any situation with constant N. This condition on the derivative terms yields the following recursion for α.

$$\alpha_{m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}} = - w_m \mu_m. \qquad (4.9)$$

Therefore, $\alpha_{3/2} = - w_1 \mu_1$, where μ_1 is the discrete

μ that is closest to $\mu = -1$, and $\alpha_{m+\frac{1}{2}} \geq 0$ for all m. Summing both sides of Eq. (4.9) over m, one derives

$$\alpha_{n+\frac{1}{2}} - \alpha_{\frac{1}{2}} = -\Sigma_m w_m \mu_m = 0 \tag{4.10}$$

where the second equality comes from Eq. (3.5) and the last α, $\alpha_{n+\frac{1}{2}}$, equals zero. The midpoint α_m is defined by

$$\alpha_m = \frac{1}{2}(\alpha_{m+\frac{1}{2}} + \alpha_{m-\frac{1}{2}}). \tag{4.11}$$

Note that if the quadrature is symmetric in the sense discussed in Sec. III, the coefficients are also symmetric, $\alpha_{n+\frac{1}{2}} = \alpha_{\frac{1}{2}} = 0$, $\alpha_n = \alpha_1$, $\alpha_{n-\frac{1}{2}} = \alpha_{3/2}$, $\alpha_{n-1} = \alpha_2$, etc., with

$$\alpha_{\frac{1}{2}(n+1)} = \tfrac{1}{2} \Sigma_m w_m |\mu_m| \approx \frac{1}{4}. \tag{4.12}$$

In solving Eq. (4.6) numerically, the progression is clearly from smaller μ_m toward larger μ_m, and is, as in the infinite plane case for x, in the r direction indicated by the sign of μ, that is, inward for negative μ and outward for positive μ. The first ray equation (m = 1) possesses no streaming source, since $\alpha_{\frac{1}{2}} = 0$, and the last ray equation (m = n) no streaming sink, since $\alpha_{n+\frac{1}{2}} = 0$. However, because $N_{m+\frac{1}{2}}$ is obtained by extrapolation from N_m and $N_{m+\frac{1}{2}}$, values for $N_{\frac{1}{2}}$ for an initializing ray are needed. The equation for $N_{\frac{1}{2}}$, obtained from Eq. (4.4) by setting $\mu = -1$, is

$$-\frac{\partial}{\partial r} N_{\frac{1}{2}}(r) + \sigma(r)\, N_{\frac{1}{2}}(r) = S(r). \tag{4.13}$$

Next, by a process of adding and subtracting terms (shown in detail later), and by setting

$$N_m(r) = \frac{1}{2}[N_{m-\frac{1}{2}}(r) + N_{m+\frac{1}{2}}(r)], \tag{4.14}$$

Eq. (4.6) can be put in a regular form, as follows.

$$\mu_m \frac{\partial}{\partial r} N_m(r) + \frac{2\,\alpha_m}{r\, w_m} [N_{m+\frac{1}{2}}(r) - N_{m-\frac{1}{2}}(r)] + \sigma(r)\, N_m(r) = S(r). \tag{4.15}$$

The balance and net flux equations for continuous and discrete μ, respectively, are obtained on the basis of the definitions

$$\bar{N}(r) = \frac{1}{2} \int_{-1}^{1} N(r,\mu)\,d\mu = \Sigma_m w_m N_m(r) \tag{4.16}$$

and

$$I(r) = \frac{1}{2} \int_{-1}^{1} N(r,\mu)\mu\,d\mu = \Sigma_m w_m \mu_m N_m(r), \tag{4.17}$$

and the quadrature operators

$$\frac{1}{2} \int_{-1}^{1} d\mu(\ ) = \Sigma_m w_m (\ ) \tag{4.18}$$

and

$$\frac{3}{2} \int_{-1}^{1} \mu\,d\mu(\ ) = 3 \Sigma_m w_m \mu_m (\ ). \tag{4.19}$$

The operators in Eq. (4.18) are applied to Eqs. (4.1) and (4.6), respectively, and the operators in Eq. (4.19) to Eqs. (4.4) and (4.15). In applying Eq. (4.19) to the continuous and discrete cases, respectively, the diffusion approximations

$$N(r,\mu) = \bar{N}(r) + 3\mu I(r) \tag{4.20}$$

and

$$N_m(r) = \bar{N}(r) + 3\mu_m I(r) \tag{4.21}$$

are also used.

In applying Eq. (4.18) to Eq. (4.6), the terms in α vanish since

$$A'(r)\, \Sigma_m(\alpha_{m+\frac{1}{2}} N_{m-\frac{1}{2}} - \alpha_{m-\frac{1}{2}} N_{m-\frac{1}{2}}) = 0 \tag{4.22}$$

because of cross cancellation and $\alpha_{n+\frac{1}{2}} = \alpha_{\frac{1}{2}} = 0$. Also, after applying Eq. (4.19) to Eq. (4.15), the terms in α in that equation vanish since

$$(6/r)\, \Sigma_m \mu_m \alpha_m (N_{m+\frac{1}{2}} - N_{m-\frac{1}{2}}) = 0, \tag{4.23}$$

first because, by using Eq. (4.21), the difference of the N's is replaced by $6w_m I$ and second because α_m, like w_m, is an even function in μ. As a result of the above, the balance and net flux equations are given by

$$\frac{\partial}{\partial r} A(r)\, I(r) + \sigma(r)\, A(r)\, \bar{N}(r) = A(r)\, S(r) \tag{4.24}$$

and

$$\frac{\partial}{\partial r}\bar{N}(r) + 3\sigma(r)\, I(r) = 0 \qquad (4.25)$$

for the discrete ordinates as well as the analytical case. Note that the construction of unsymmetric quadrature sets is not simple since μ_m selections must satisfy the condition

$$\Sigma_m\, w_m\, \mu_m\, \alpha_m = 0, \qquad (4.26)$$

with α_m depending on μ_s, $s \le m$, through Eqs. (4.9) and (4.11).

The finite cell formulation of the transport equation for sphere, derived independently of Eq. (4.6), is given by

$$\mu_m(A_{i+\frac{1}{2}}\, N_{m,i+\frac{1}{2}} - A_{i-\frac{1}{2}}\, N_{m,i-\frac{1}{2}}) + (C_i/w_m)(\alpha_{m+\frac{1}{2}}\, N_{m+\frac{1}{2},i} - \alpha_{m-\frac{1}{2}}\, N_{m-\frac{1}{2},i}) + \sigma_i\, V_i\, N_{m,i} = V_i\, S_i, \qquad (4.27)$$

where

$$A_{i+\frac{1}{2}} = 4\pi r_{i+\frac{1}{2}}^2, \qquad (4.28)$$

$$A_i = \tfrac{1}{2}(A_{i+\frac{1}{2}} + A_{i-\frac{1}{2}}) = 4\pi(\bar{r}_i^{\,2} + \tfrac{1}{4}\Delta r_i^{\,2}), \qquad (4.29)$$

$$C_i = A_{i+\frac{1}{2}} - A_{i-\frac{1}{2}} = 8\pi\bar{r}_i\Delta r_i, \qquad (4.30)$$

and

$$V_i = (4\pi/3)(r_{i+\frac{1}{2}}^3 - r_{i-\frac{1}{2}}^3) = 4\pi(\bar{r}_i^{\,2} + \tfrac{1}{12}\Delta r_i^{\,2})\Delta r_i, \qquad (4.31)$$

with

$$\Delta r_i = r_{i+\frac{1}{2}} - r_{i-\frac{1}{2}} \qquad (4.32)$$

and

$$\bar{r}_i = \tfrac{1}{2}(r_{i-\frac{1}{2}} + r_{i+\frac{1}{2}}). \qquad (4.33)$$

In simplified notation, Eq. (4.27) is written

$$\mu(A_{i+\frac{1}{2}}\, N_{i+\frac{1}{2}} - A_{i-\frac{1}{2}}\, N_{i-\frac{1}{2}}) + (C/w)(\alpha_{m+\frac{1}{2}}\, N_{m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}}\, N_{m-\frac{1}{2}}) + \sigma V N = V\, S. \qquad (4.34)$$

In the finite cell equation, S_i, $N_{m,i}$, $\sigma_i N_{m,i}$, and $C_i N_{m,i}$ represent volume average of $S(r)$, $N_m(r)$, $\sigma(r)N_m(r)$, and $(2/r)N_m(r)$, respectively, over intervals $(r_{i-\frac{1}{2}}, r_{i+\frac{1}{2}})$.

To arrive at the correct net flux equation, Eq. (4.27) is also needed in the regular form. By adding and subtracting terms in Eq. (4.34), that equation becomes

$$\mu(V/\Delta r)(N_{i+\frac{1}{2}} - N_{i-\frac{1}{2}}) + (C\alpha/w)(N_{m+\frac{1}{2}} - N_{m-\frac{1}{2}}) + \mu(A_{i+\frac{1}{2}} - V/\Delta r)N_{i+\frac{1}{2}} + \mu(V/\Delta r - A_{i-\frac{1}{2}})N_{i-\frac{1}{2}} - \tfrac{1}{2}C\mu(N_{m+\frac{1}{2}} + N_{m-\frac{1}{2}}) + \sigma V N = VS. \qquad (4.35)$$

Here the relations

$$\alpha_{m+\frac{1}{2}}/w_m = \alpha_m/w_m - \tfrac{1}{2}\mu_m \qquad (4.36)$$

and

$$\alpha_{m-\frac{1}{2}}/w_m = \alpha_m/w_m + \tfrac{1}{2}\mu_m \qquad (4.37)$$

were used. For further simplification, the following formulas are useful.

$$A_{i+\frac{1}{2}} - V/\Delta r = \tfrac{1}{2}C + (A - V/\Delta r) \qquad (4.38)$$

and

$$V/\Delta r - A_{i-\frac{1}{2}} = \tfrac{1}{2}C - (A - V/\Delta r). \qquad (4.39)$$

To obtain the desired consistency between Eqs. (4.15) and (4.35), the terms in the second line of Eq. (4.35) plus the term in $-\frac{1}{2}C\mu$, must vanish. This leads to the following difference relation.

$$\tfrac{1}{2}(N_{m+\frac{1}{2}} + N_{m-\frac{1}{2}}) = (\tfrac{1}{2} + \Delta r/12\bar{r})N_{i+\frac{1}{2}} + (\tfrac{1}{2} - \Delta r/12\bar{r})N_{i-\frac{1}{2}}, \quad (4.40)$$

where the coefficient $\Delta r/6\bar{r}$ comes from

$$(A - V/\Delta r)/C = \Delta r/12\bar{r}, \quad (4.41)$$

which has its maximum value of 1/6 for the first r interval $(0,\Delta r)$. With this difference relation, Eq. (4.35) simplifies to

$$\mu(N_{i+\frac{1}{2}} - N_{i-\frac{1}{2}}) + (C\alpha\Delta r/Vw)(N_{m+\frac{1}{2}} - N_{m-\frac{1}{2}}) + \sigma\Delta rN = \Delta rS \quad (4.42)$$

as the finite cell equivalent to Eqs. (4.4) and (4.15). If one multiplies the terms by w and takes Δrw as the volume element, Eq. (4.42) may be regarded as the rectangularized version of Eq. (4.27). For the special straight-in direction, $\mu = -1$, with $\alpha = 0$ erasing the α term in the equation, the result is a planar-type equation.

$$-(N_{i+\frac{1}{2}} - N_{i-\frac{1}{2}}) + \sigma\Delta rN = \Delta rS, \quad (4.43)$$

corresponding to Eq. (4.13). The same equation is obtained from Eq. (4.34) by setting $N_{m+\frac{1}{2}} = N_{m-\frac{1}{2}}$, $\alpha_{m+\frac{1}{2}}/w = 1$ (the correct limit for a small μ interval near $\mu = -1$), and $\alpha_{m-\frac{1}{2}} = 0$, and then eliminating $N_{m+\frac{1}{2}}$ by means of Eq. (4.40).

The above analysis shows that there are special restraints on the difference relations in curved geometries. In the spherical case, one can select one difference relation in the usual manner, joining this with Eq. (4.40), the principal relation. Subsequently, upon substitution of these relations, Eq. (4.42) can be solved for its three unknowns, N, $N_{m+\frac{1}{2}}$, and $N_{h+\frac{1}{2}}$, where $N_{h+\frac{1}{2}} = N_{i+\frac{1}{2}}$ for $\mu > 0$, and $N_{h+\frac{1}{2}} = N_{i-\frac{1}{2}}$ for $\mu < 0$. Truncation error analysis (as made in Refs. 2 and 3) suggest the following scheme as a supplement to Eq. (4.40).

$$N = (\tfrac{1}{2} + \Delta r/12\bar{r})N_{i+\frac{1}{2}} + (\tfrac{1}{2} - \Delta r/12\bar{r})N_{i-\frac{1}{2}}, \quad (4.44)$$

a weighted scheme, which in combination with Eq. (4.40) gives

$$N = \tfrac{1}{2}(N_{m+\frac{1}{2}} + N_{m-\frac{1}{2}}) = (\tfrac{1}{2} + \Delta r/12\bar{r})N_{i+\frac{1}{2}} + (\tfrac{1}{2} - \Delta r/12\bar{r})N_{i-\frac{1}{2}}, \quad (4.45)$$

where, moreover, the first equality is consistent with Eq. (4.14). This total scheme may be completed for $P < 1$ by replacing N in the above by

$$\tfrac{1}{2}(1 + P)N + \tfrac{1}{2}(1 - P)N_{m-\frac{1}{2}}. \quad (4.46)$$

The scheme defined by Eq. (4.44), involving unequal weights, does not seem proper, however, for the straight-in case, Eq. (4.43). It seems that the total scheme should be replaced, in some way, by

$$N = \tfrac{1}{2}(N_{i+\frac{1}{2}} + N_{i-\frac{1}{2}}) + \tfrac{1}{2}(N_{m+\frac{1}{2}} + N_{m-\frac{1}{2}}). \quad (4.47)$$

By a slightly different procedure, partly empirical but in other respects like that used to establish Eq. (4.40), one can indeed (as shown in Ref. 1) terminate by Eq. (4.47). This involves the replacements

$$\sigma A\Delta r/V \to \sigma \quad (4.48)$$

and

$$S/\sigma + (A\Delta r/V - 1)\bar{N} \to S/\sigma. \quad (4.49)$$

This method, which manipulates the source and sink terms so that the number of particles is preserved, is not perfect as applied to Eq. (4.43), but it is probably better than the method based on Eq. (4.45). Some of the earlier methods for coping with the diffusion condition should be mentioned. These methods, which were unsatisfactory for other reasons, involved the manipulation of area and volume elements, computing, for example, $A_{i+\frac{1}{2}}$ from the exact V_i using the recursion

$$A_{i+\frac{1}{2}} = 2V/\Delta r - A_{i-\frac{1}{2}} \quad (4.50)$$

so that $A\Delta r = V$, or computing V from the exact A's by

$$V = A\Delta r. \quad (4.51)$$

The method of characteristics resolves the above problem very nicely, at least analytically. Final judgment on this approach must be reserved until a

number of numerical tests have been made. In characteristic from, Eq. (4.34) is written

$$(N_{h+\frac{1}{2}} - N_{h-\frac{1}{2}}) + uN = u\,S/\sigma, \tag{4.52}$$

where

$$u = \sigma V/T. \tag{4.53}$$

Here T has the meaning of total effective outflow area (equal to inflow area) of the cell, being the sum of the individual areas (in this case $|\mu|A_{i+\frac{1}{2}}$ and $C\alpha_{m+\frac{1}{2}}/w$) and is given by

$$\begin{aligned} T &= |\mu|A_{i+\frac{1}{2}} + C\alpha_{m+\frac{1}{2}}/w \\ &= |\mu|A_{i-\frac{1}{2}} + C\alpha_{m-\frac{1}{2}}/w \\ &= |\mu|A + C\alpha/w. \end{aligned} \tag{4.54}$$

These expressions, and those below, are for positive μ; for negative μ, $i+\frac{1}{2}$ is replaced by $i-\frac{1}{2}$ and $i-\frac{1}{2}$ by $i+\frac{1}{2}$. Also, if Eq. (4.52) is to be equivalent to Eq. (4.34), $N_{h+\frac{1}{2}}$ and $N_{h-\frac{1}{2}}$, the average outflow and inflow for the cell must be defined by

$$TN_{h+\frac{1}{2}} = |\mu|A_{i+\frac{1}{2}}\,N_{i+\frac{1}{2}} + (C\alpha_{m+\frac{1}{2}}/w)N_{m+\frac{1}{2}} \tag{4.55}$$

and

$$TN_{h-\frac{1}{2}} = |\mu|A_{i-\frac{1}{2}}\,N_{i-\frac{1}{2}} + (C\alpha_{m-\frac{1}{2}}/w)N_{m-\frac{1}{2}}, \tag{4.56}$$

respectively. To solve Eq. (4.52), one introduces the difference relation

$$N_{h+\frac{1}{2}} = (1 + P)N - PN_{h-\frac{1}{2}} \tag{4.57}$$

and proceeds as in Sec. III to obtain P, N, and $N_{h+\frac{1}{2}}$. Then to detail the output, given $N_{h+\frac{1}{2}}$, one uses the definition of $N_{h+\frac{1}{2}}$ in terms of $N_{i+\frac{1}{2}}$ and $N_{m+\frac{1}{2}}$ or $N_{i-\frac{1}{2}}$ and $N_{m+\frac{1}{2}}$, as the case may be, plus the difference relation Eq. (4.40). The straight-in case is handled somewhat differently because Eq. (4.40) implies Eq. (4.43). Therefore, in this case

$$u = \sigma\Delta r/T, \tag{4.58}$$

with T = 1, $N_{h+\frac{1}{2}} = N_{i-\frac{1}{2}}$, and $N_{h-\frac{1}{2}} = N_{i+\frac{1}{2}}$.

Detailing of outputs is done as follows. For the straight-in direction it remains to calculate $N_{\frac{1}{2},i}$, the initial function for extrapolation in μ.

$$N_{\frac{1}{2}} = (\tfrac{1}{2} + \Delta r/6\bar{r})N_{h-\frac{1}{2}} + (\tfrac{1}{2} - \Delta r/6\bar{r})N_{h+\frac{1}{2}}. \tag{4.59}$$

For the case of negative μ,

$$TN_{h+\frac{1}{2}} = -\mu A_{i-\frac{1}{2}}\,N_{i-\frac{1}{2}} + (C\alpha_{m+\frac{1}{2}}/w)N_{m+\frac{1}{2}}, \tag{4.60}$$

combined with Eq. (4.40) to eliminate $N_{m+\frac{1}{2}}$, gives

$$N_{i-\frac{1}{2}} = \frac{N_{h+\frac{1}{2}} + (C\alpha_{m+\frac{1}{2}}/Tw)[N_{m-\frac{1}{2}} - (1 + \Delta r/6\bar{r})N_{i+\frac{1}{2}}]}{1 - (C\alpha_{m+\frac{1}{2}}/Tw)(\Delta r/6\bar{r})}. \tag{4.61}$$

Since for i = 1, the factors in the denominator equal 1 and 1/3, respectively, the equation simplifies in this case to

$$N_{m,\frac{1}{2}} = \frac{3}{2}(N_{h+\frac{1}{2}} + N_{m-\frac{1}{2}}) - 2N_{i+\frac{1}{2}}. \tag{4.62}$$

For the positive μ directions,

$$TN_{h+\frac{1}{2}} = \mu A_{i+\frac{1}{2}}\,N_{i+\frac{1}{2}} + (C\alpha_{m+\frac{1}{2}}/w)N_{m+\frac{1}{2}}, \tag{4.63}$$

combined with Eq. (4.40) to eliminate $N_{m+\frac{1}{2}}$, gives

$$N_{i+\frac{1}{2}} = \frac{N_{h+\frac{1}{2}} + (C\alpha_{m+\frac{1}{2}}/Tw)[N_{m-\frac{1}{2}} - (1 - \Delta r/6\bar{r})N_{i-\frac{1}{2}}]}{1 + (C\alpha_{m+\frac{1}{2}}/Tw)(\Delta r/6\bar{r})}. \tag{4.64}$$

For m = n, in which case $\alpha_{m+\frac{1}{2}} = 0$, this reduces to $N_{i+\frac{1}{2}} = N_{h+\frac{1}{2}}$. After the extrapolation in the r-direction has been done, $N_{m+\frac{1}{2}}$ is calculated from

$$N_{m+\frac{1}{2}} = (1 + \Delta r/6\bar{r})N_{i+\frac{1}{2}} + (1 - \Delta r/6\bar{r})N_{i-\frac{1}{2}} - N_{m-\frac{1}{2}}. \tag{4.65}$$

The final step in the calculation is the correction for skewing as described in Sec. II.

V. SOLUTION IN CYLINDRICAL GEOMETRY

In infinite cylindrical (r) geometry with two variables for direction, the radial and axial components μ and ξ, the transport equation is given by

$$\begin{aligned} &\mu\frac{\partial}{\partial r}A(r)\,N(r,\mu,\xi) - A'(r)\frac{\partial}{\partial\phi}\eta\,N(r,\mu,\xi) \\ &\quad + \sigma(r)\,A(r)\,N(r,\mu,\xi) = A(r)\,S(r), \end{aligned} \tag{5.1}$$

where A is the area element

$$A(r) = 2\pi r, \tag{5.2}$$

with $A'(r) = 2\pi$, and where ϕ and η are related to μ and ξ by

$$\mu = \sqrt{1 - \xi^2} \cos \phi \tag{5.3}$$

and

$$\eta = \sqrt{1 - \xi^2} \sin\phi, \tag{5.4}$$

with $\pi \geq \phi \geq 0$ and $0 \leq \xi \leq 1$. It follows from this that $-1 \leq \mu \leq 1$ and $0 \leq \eta \leq 1$, and that the domain of Ω is comprised of two octants of the unit sphere. Note that if $N(r,\mu,\xi)$ is constant, the differential operator in Eq. (5.1) vanishes because

$$\mu \frac{\partial}{\partial r} A(r) - A'(r) \frac{\partial}{\partial \phi} \eta = 0. \tag{5.5}$$

As in the spherical case, the discretization of Eq. (5.1) is accomplished by means of quadrature methods and difference schemes. Numerical quadrature combines with finite intervals in μ and ξ, and difference methods combine with finite intervals in r. The construction is such that in the limit of small intervals the discrete and analytical equations are consistent. An intermediate step in the construction is the discrete ordinates formulation where the treatment is discrete in μ and ξ and continuous in r.

A number of equations are involved in the consistency arguments: first the conservation equation [Eq. (5.1) and its alternate, regular form, Eq. (5.6) below], second the basic derived equations, the balance and net flux equations [Eqs. (5.7) and (5.8) below], and third the associated diffusion approximation [Eq. (5.9)] used in the derivation of Eq. (5.8). These equations are given by

$$\mu \frac{\partial}{\partial r} N(r,\mu,\xi) - (\eta/r) \frac{\partial}{\partial \phi} N(r,\mu,\xi) + \sigma(r)\, N(r,\mu,\xi) = S(r), \tag{5.6}$$

$$\frac{\partial}{\partial r} A(r)\, I(r) + \sigma(r)\, A(r)\, \bar{N}(r) = A(r)\, S(r), \tag{5.7}$$

$$(1/3) \frac{\partial}{\partial r} \bar{N}(r) + \sigma(r)\, I(r) = 0. \tag{5.8}$$

and

$$N(r,\mu,\xi) \approx \bar{N}(r) + 3\mu\, I(r). \tag{5.9}$$

In the above, the scalar flux $\bar{N}(r)$ and current $I(r)$, two functionals of $N(r,\mu,\xi)$ may be defined as the result of two operators.

$$F_0 = \frac{1}{\pi} \int_0^1 d\xi \int_0^\pi d\phi \tag{5.10}$$

and

$$F_1 = \frac{1}{\pi} \int_0^1 d\xi \int_0^\pi \mu d\phi \tag{5.11}$$

applied to $N(r,\mu,\xi)$.

Equation (5.6) is found by continued differentiation in Eq. (5.1); Eq. (5.7) by applying the first operator [Eq. (5.10)], term by term to Eq. (5.1); and Eq. (5.8) by applying the second operator after substitution of Eq. (5.9). However, Eq. (5.8) is more readily obtained if the second operator [Eq. (5.11)] is applied to Eq. (5.6) rather than to Eq. (5.1).

In constructing the discrete ordinates formulation, one starts with

$$\mu_{\ell,m} \frac{\partial}{\partial r} A(r)\, N_{\ell,m}(r) + \frac{A'(r)}{w_{\ell,m}} \left[\alpha_{\ell,m+\frac{1}{2}}\, N_{\ell,m+\frac{1}{2}}(r) - \alpha_{\ell,m-\frac{1}{2}}\, N_{\ell,m-\frac{1}{2}}(r)\right] + \sigma(r)\, A(r)\, N_{\ell,m}(r) = A(r)\, S(r), \tag{5.12}$$

where ℓ is the level index (the index associated with ξ) and m the μ (or ϕ) index, where the quantities $\mu_{\ell,m}$ are discrete values of μ depending on ξ as well as ϕ, and where the second term approximates the term in Eq. (5.1) with the ϕ derivative. The meaning of $N_{\ell,m}(r)$ is

$$N_{\ell,m}(r) = N(r,\, \mu_{\ell,m},\, \xi_{\ell,m}) \tag{5.13}$$

and weights $w_{\ell,m}$, together with the points or nodes, $(\mu_{\ell,m},\, \eta_{\ell,m},\, \xi_{\ell,m})$ constitute the quadrature set.

By requiring that the differential operator in Eq. (5.12) vanish in the case of constant N, as for the analytical equation, the following recursion formula for α is obtained.

$$\alpha_{\ell,m+\frac{1}{2}} - \alpha_{\ell,m-\frac{1}{2}} = - w_{\ell,m}\, \mu_{\ell,m}, \tag{5.14}$$

which can be used to compute α because $\alpha_{\ell,\frac{1}{2}}$ can be set to zero as seen later.

In the following, the point weights $w_{\ell,m}$ are assumed to be equal.

$$w_{\ell,m} \equiv w = 4/n(n+2) \tag{5.15}$$

for any given order n of approximation, n = 2, 4, ... The associated nodes ($\mu_{\ell,m}$, $\eta_{\ell,m}$, $\xi_{\ell,m}$) are assumed to be arranged in a triangular fashion on $\frac{1}{2}n$ levels with n = 2ℓ + 2 nodes on level ℓ, m = 1, 2, ..., n - 2ℓ + 2, ℓ = 1, 2, ..., $\frac{1}{2}n$. This yields a total of n(n + 2)/4 nodes, with n(n + 2)/8 per octant. From this, with the level weights W_ℓ defined by

$$W_\ell = \Sigma_m w_{\ell,m} = (n - 2\ell + 2)w, \tag{5.16}$$

the normalization is

$$\Sigma_{\ell,m} w_{\ell,m} = \Sigma_\ell W_\ell = 1. \tag{5.17}$$

It is further assumed that the nodes are chosen so that

$$\mu_{\ell,m}^2 + \eta_{\ell,m}^2 + \xi_{\ell,m}^2 = 1 \tag{5.18}$$

and

$$\Sigma_{\ell,m} w_{\ell,m} \mu_{\ell,m}^2 = \Sigma_{\ell,m} w_{\ell,m} \xi_m^2 = 1/3, \tag{5.19}$$

m = 1, 2, ..., n - 2ℓ + 2, ℓ = 1, 2, ..., $\frac{1}{2}n$, from which it follows that

$$\Sigma_{\ell,m} w_{\ell,m} \eta_{\ell,m}^2 = 1/3. \tag{5.20}$$

Defining the level cosines $\bar{\xi}_\ell$ by

$$\bar{\xi}_\ell = \sqrt{(\Sigma_m w_{\ell,m} \xi_{\ell,m}^2)/W_\ell}\,, \tag{5.21}$$

it also follows that

$$\Sigma_\ell W_\ell \bar{\xi}_\ell^2 = 1/3. \tag{5.22}$$

Finally, it is assumed that if ($\mu_{\ell,m}$ $\eta_{\ell,m}$ $\xi_{\ell,m}$) is a node in the set, so is (- $\mu_{\ell,m}$, $\eta_{\ell,m}$, $\xi_{\ell,m}$). With this sign reversal symmetry and equal weights, it follows that

$$\Sigma_{\ell,m} w_{\ell,m} \mu_{\ell,m} = 0 \tag{5.23}$$

and also that $\alpha_{\ell,m}$ is an even function of $\mu_{\ell,m}$ for each ℓ. As a consequence,

$$\Sigma_{\ell,m} w_{\ell,m} \mu_{\ell,m} \alpha_{\ell,m} = 0. \tag{5.24}$$

As in the spherical case, the basic quadrature set is augmented by special zero-weight points, one for each ξ level, say for m = 1. This changes the m sequence to m = 1, 2, ..., n = 2ℓ + 3 and the totality of points to n(n + 4)/4. For the special points one has $w_{\ell,1} = 0$, $\eta_{\ell,1} < 0$, $\xi_{\ell,1} = \sqrt{1 - \mu_{\ell,1}^2}$, and $\alpha_{3/2} = \alpha_1 = \alpha_{1/2} = 0$. The indices for the nodes with negative μ are m = 2, 3, ..., $\frac{1}{2}n$ - ℓ + 2.

Returning to the discrete ordinates formulation, one observes that $w_{\ell,m}$ can be related to $\Delta\phi$ by

$$w_{\ell,m} = - (W_\ell/\pi)\, \Delta\phi. \tag{5.25}$$

Therefore, if Eq. (5.12) is to be consistent with Eq. (5.1), the α coefficients as computed from Eq. (5.14) must satisfy

$$\alpha_{\ell,m-\frac{1}{2}} \approx (W_\ell/\pi)\, \eta_{\ell,m-\frac{1}{2}} \tag{5.26}$$

as well as

$$\alpha_{\ell,m} = \tfrac{1}{2}(\alpha_{\ell mn+\frac{1}{2}} + \alpha_{\ell,m-\frac{1}{2}}) \approx (W_\ell/\pi)\, \eta_{\ell,m}, \tag{5.27}$$

and do this with increasing accuracy as n increases. In the one-dimensional case for spheres, the corresponding relations are

$$\alpha_{m-\frac{1}{2}} \approx \tfrac{1}{4}(1 - \mu_{m-\frac{1}{2}}^2) \tag{5.28}$$

and

$$\alpha_m \approx \tfrac{1}{4}(1 - \mu_m^2). \tag{5.29}$$

Note that for the special points in which case $\eta_{\ell,\frac{1}{2}} = 0$, Eq. (5.26) justifies that $\alpha_{\ell,\frac{1}{2}}$ be set to zero.

The accuracy of the relations of Eqs. (5.26) and (5.28) are tested in the next section in the case of ES_n quadrature, an easily constructed quadrature defined and tabulated in that section.

To put Eq. (5.12) in the regular form, the first term is differentiated with the result

$$A(r)\, \mu_{\ell,m} \frac{\partial}{\partial r} N_{\ell,m}(r) + \mu_{\ell,m} A'(r)\, N_{\ell,m}(r) \tag{5.30}$$

where the first term is the desired term. Second, the terms in α can be written

$$\frac{A'(r)}{w_{\ell,m}} \alpha_{\ell,m} \left[N_{\ell,m+\frac{1}{2}}(r) - N_{\ell,m-\frac{1}{2}}(r)\right] + (\alpha_{\ell,m+\frac{1}{2}} - \alpha_{\ell,m-\frac{1}{2}}) \frac{A'(r)}{2w_{\ell,m}} \left[N_{\ell,m+\frac{1}{2}}(r) + N_{\ell,m-\frac{1}{2}}(r)\right]. \quad (5.31)$$

Here the first term with the factor $\alpha_{\ell,m}$ is the desired term. Noting that $(\alpha_{\ell,m+\frac{1}{2}} - \alpha_{\ell,m-\frac{1}{2}})$ in the second term can be replaced by $- w_{\ell,m} \mu_{\ell,m}$, that term can be made to cancel the second term in Eq. (5.30) by assuming the difference relation

$$N_{\ell,m}(r) = \frac{1}{2}[N_{\ell,m+\frac{1}{2}}(r) + N_{\ell,m-\frac{1}{2}}(r)]. \quad (5.32)$$

In this way, Eq. (5.12) is put in the regular form

$$\mu_{\ell,m} \frac{\partial}{\partial r} N_{\ell,m}(r) + \frac{\alpha_{\ell,m}}{r\, w_{\ell,m}} [N_{\ell,m+\frac{1}{2}}(r) - N_{\ell,m-\frac{1}{2}}(r)] + \sigma(r)\, N_{\ell,m}(r) = S(r), \quad (5.33)$$

consistent with Eq. (5.6).

Next, defining the discrete operators corresponding to Eqs. (5.10) and (5.11) by

$$F_0 = \Sigma_{\ell,m}\, w_{\ell,m} \quad (5.34)$$

and

$$F_1 = \Sigma_{\ell,m}\, w_{\ell,m}, \mu_{\ell,m} \quad (5.35)$$

$\bar{N}(r)$ and $I(r)$ may be defined as the result of these operators operating on $N_{\ell,m}(r)$. Furthermore, on the basis of the properties assigned to the quadrature set, the operators Eqs. (5.34) and (5.35) applied to Eqs. (5.12) and (5.6), respectively, yield exactly Eqs. (5.7) and (5.8). In arriving at Eq. (5.8), Eq. (5.24) and the following discrete version of Eq. (5.9) are used.

$$N_{\ell,m}(r) \approx \bar{N}(r) + 3\, \mu_{\ell,m}\, I(r). \quad (5.36)$$

For the final step in the discretization, Eq. (5.12) is first written as a finite cell conservation law.

$$\mu_{\ell,m} A_{i+\frac{1}{2}} N_{\ell,m,i+\frac{1}{2}} - \mu_{\ell,m} A_{i-\frac{1}{2}} N_{\ell,m,i-\frac{1}{2}} + (C_i/w_{\ell,m})(\alpha_{\ell,m+\frac{1}{2}} N_{\ell,m+\frac{1}{2},i} - \alpha_{\ell,m-\frac{1}{2}} N_{\ell,m-\frac{1}{2},i}) + \sigma_i V_i N_{\ell,m,i} = V_i S_i, \quad (5.37)$$

where

$$A_{i+\frac{1}{2}} = 2\pi r_{i+\frac{1}{2}}, \quad (5.38)$$

$$A_i = \frac{1}{2}(A_{i+\frac{1}{2}} + A_{i-\frac{1}{2}}) = 2\pi \bar{r}_i, \quad (5.39)$$

$$C_i = A_{i+\frac{1}{2}} - A_{i-\frac{1}{2}} = 2\pi \Delta r_i, \quad (5.40)$$

and

$$V_i = \pi(r_{i+\frac{1}{2}}^2 - r_{i-\frac{1}{2}}^2) = 2\pi \bar{r}_i \Delta r_i = A_i \Delta r_i. \quad (5.41)$$

The correct balance equation,

$$A_{i+\frac{1}{2}} I_{i+\frac{1}{2}} - A_{i-\frac{1}{2}} I_{i-\frac{1}{2}} + \sigma_i V_i \bar{N}_i = V_i S_i, \quad (5.42)$$

is obtained by applying the operators Eqs. (5.34) and (5.35) to Eq. (5.37). In this case $\bar{N}_i$ and I_i are defined by

$$N_i = \Sigma_{\ell,m}\, w_{\ell,m}\, N_{\ell,m,i} \quad (5.43)$$

and

$$I_i = \Sigma_{\ell,m}\, w_{\ell,m}\, \mu_{\ell,m}\, N_{\ell,mi}, \quad (5.44)$$

respectively. To obtain the correct net flux equation,

$$(1/3)(\bar{N}_{i+\frac{1}{2}} - \bar{N}_{i-\frac{1}{2}}) + \sigma_i \Delta r_i I_i = 0, \quad (5.45)$$

one uses Eq. (5.37) put in a regular form together with the diffusion approximation

$$N_{\ell,m,i} = \bar{N}_i + 3\,\mu_{\ell,m}\,I_i. \tag{5.46}$$

The regular form of Eq. (5.37) is found by adding and subtracting equal terms in that equation, obtaining

$$\mu_{\ell,m}\,A_i(N_{\ell,m,i+\frac{1}{2}} - N_{\ell,m,i-\frac{1}{2}}) + \frac{1}{2}\,\mu_{\ell,m}\,(A_{i+\frac{1}{2}} - A_{i-\frac{1}{2}})(N_{\ell,m,i+\frac{1}{2}} + N_{\ell,m,i-\frac{1}{2}})$$

$$+ (C_i\,\alpha_{\ell,m}/w_{\ell,m})(N_{\ell,m+\frac{1}{2},i} - N_{\ell,m-\frac{1}{2},i}) - \frac{1}{2}\,\mu_{\ell,m}\,C_i(N_{\ell,m+\frac{1}{2},i} + N_{\ell,m-\frac{1}{2},i}) + \sigma_i\,V_i\,N_{\ell,m,i} = V_i\,S_i. \tag{5.47}$$

Here the first and second terms equal the first two terms in Eq. (5.37) and the two terms in C_i equal the term in C_i in Eq. (5.37). If the following difference is introduced,

$$\frac{1}{2}(N_{\ell,m+\frac{1}{2},i} + N_{\ell,m-\frac{1}{2},i})$$

$$= \frac{1}{2}(N_{\ell,m,i+\frac{1}{2}} + N_{\ell,m,i-\frac{1}{2}}), \tag{5.48}$$

the two terms in $\frac{1}{2}\mu_{\ell,m}$ in Eq. (5.47) cancel because $C_i = A_{i+\frac{1}{2}} - A_{i-\frac{1}{2}}$, and the proper regular difference equation, consistent with Eqs. (5.6) and (5.33), is obtained.

$$\mu_{\ell,m}(N_{\ell,m,i+\frac{1}{2}} - N_{\ell,m,i-\frac{1}{2}}) + \frac{\Delta r_i\,\alpha_{\ell,m}}{\bar{r}_i\,w_{\ell,m}}(N_{\ell,m+\frac{1}{2},i} - N_{\ell,m-\frac{1}{2},i}) + \sigma_i\,\Delta\,r_i\,N_{\ell,m,i} = \Delta\,r_i\,S_i, \tag{5.49}$$

after dividing through by A_i noting that $C_i/A_i = \Delta\,r_i/\bar{r}_i$ and $V_i/A_i = \Delta\,r_i$. Equation (5.49) corresponds to Eq. (4.40) in the spherical case. Note that the relation is simpler in cylindrical geometry because $V_i = A_i\,\Delta\,r_i$. The remaining steps in finding solutions in the cylindrical case by the method of characteristics parallel and are almost identical to the steps in spherical geometry. These are described in Sec. IV beginning with the paragraph of Eq. (4.52). The difference in the equations is that the terms in $\Delta\,r/6\bar{r}$ in the spherical case are not present in the cylindrical case.

For the choice of special directions, more than one method is available. In a first method, $\mu_{\ell,1}$ is computed from

$$\mu_{\ell,1} = -\sqrt{1 - \bar{\xi}_\ell^{\,2}}\,, \tag{5.50}$$

in a second, from

$$\mu_{\ell,1} = -\sum_{m=1}^{\frac{1}{2}n-\ell+1} w_m, \tag{5.51}$$

and in a third method only one special direction is used, $\mu_{1,1} = -1.0$. In this case, for $\ell > 1$, one sets

$$N_{\ell,1}(r) = N_{\ell-1,5/2}(r). \tag{5.52}$$

VI. ES_n MECHANICAL QUADRATURE

The requirements on numerical quadrature as used in transport calculations have been discussed in previous sections as well as in several earlier reports.[4,5] In this section a simple quadrature method labeled ES_n is described based on equal point weights and on approximating rather than precisely satisfying a set of moment conditions. The simplicity comes from the fact that no solution of a system of nonlinear (or linear) equations is involved. Here n controls the accuracy of the quadrature, n = 2, 4, ... The basic ES_n quadrature sets are defined on the interval (0,1) in the one-dimensional case and on the principal octant in the two-dimensional case. In the first instance, $\frac{1}{2}n$ nodes μ_m are placed on the μ-interval (0,1), m = 1, 2, ..., M = $\frac{1}{2}n$, with weights w_m which are sums of $(\frac{1}{2}n - m + 1)$ point weights, and in the second instance M(n) nodes $\Omega_m \equiv (\mu_m,\eta_m,\xi_m)$ on the principal octant (where the components of Ω are positive), m = 1, 2, ..., M = n(n+2)/8, with equal weights w_m,

$$w_m = w = 8/n(n + 2). \tag{6.1}$$

Here Ω_m may also be written $(\mu_{\ell,m},\eta_{\ell,m},\xi_{\ell,m})$ in terms of a μ-index m, m = 1, 2, ..., $\frac{1}{2}n - \ell + 1$, and

a ξ or level index ℓ, $\ell = 1, 2, \ldots, \frac{1}{2}n$. The components are assumed to satisfy

$$\mu_{\ell,m}^2 + \eta_{\ell,m}^2 + \xi_{\ell,m}^2 = 1. \tag{6.2}$$

In the two-dimensional case, as indicated above, the octant is covered by a triangular pattern of equal areas $\frac{1}{2}\pi w_{\ell,m} = \frac{1}{2}\pi w$, $n(n+2)/8$ in number, so that

$$\Sigma_{\ell,m}\, w_{\ell,m} = 1. \tag{6.3}$$

The one-dimensional weights w_m may be regarded as level weights, that is, sums of point weights by level

$$w_m = \Sigma_\ell w_{\ell,m} = (\tfrac{1}{2}n - m + 1)w. \tag{6.4}$$

Here $\frac{1}{2}\pi w_m$ correspond to areas of latitudinal bands on the octant. The weights given by Eq. (6.4) do not differ greatly from the ordinary Gauss quadrature weights.

The quadrature nodes (or points) are also placed in a triangular fashion on the octant with one node per point weight and $\frac{1}{2}n - \ell + 1$ nodes per level. They are placed in a symmetric pattern with respect to the three axes so as to form a closed set with respect to permutation of the components. Therefore, if (μ,η,ξ) is a node in the set so are (μ,ξ,η), (η,ξ,μ), (η,μ,ξ), (ξ,μ,η), and (ξ,η,μ). Such groupings may consist of less than six points, three points if two of the components are equal, and one point $(\sqrt{3}/3, \sqrt{3}/3, \sqrt{3}/3)$ if all three are equal. Altogether one can count $[(n^2 + 8n + 28)/48]$ groupings and $[n(n + 2)/24]$ independent components.

In EQ_n quadrature, based on certain assumptions discussed in Ref. 5, one is able to reduce the number of independent components to $[n(n + 12)/48]$. By correlating these with the same number of independent even moments $M_{k,j}$, $k + j \le n$, one can set up a system of nonlinear equations for determining the EQ_n set for any n.

Because of the triangular symmetry, Ω_m can be written $(\mu_{\ell,m}, \mu_{\ell,k}, \mu_{m,\ell})$ where $k = \frac{1}{2}n - \ell - m + 2$. The permutation invariance combined with Eq. (6.2) implies that the $M_{2,0}$ moment condition is satisfied.

$$M_{2,0} = \Sigma_{\ell,m}\, w_{\ell,m}\, \mu_{\ell,m}^{\,2} = 1/3. \tag{6.5}$$

Extension of the basic quadrature from (0,1) to (-1,1) or from one to two, four, or eight octants, as a given problem may require, is defined in terms of symmetry about coordinate planes with the appropriate sign changes in direction cosines. Because M changes from $\frac{1}{2}n$ to n or from $n(n + 2)/8$ to $n(n + 2)/4$, $n(n + 2)/2$, or $n(n + 2)$, respectively, the weights are renormalized so that their sum remains at unity.

The one-dimensional ES_n sets may be generated independently of the two-dimensional ones. This gives us simple means for describing the steps in the construction and examining some of the more immediate consequences. In the first step the weights are selected, here

$$w_m = (\tfrac{1}{2}n - m + 1)\ [8/n(n + 2)]. \tag{6.6}$$

In the second, certain μ coordinates are computed, the lower μ-interval boundaries $\mu_{m-\frac{1}{2}}$,

$$\mu_{m-\frac{1}{2}} = 1 - \frac{1}{2}(\tfrac{1}{2}n - m + 2)w_m, \tag{6.7}$$

and the interval midpoint values $\bar{\mu}_m$,

$$\bar{\mu}_m = \mu_{m-\frac{1}{2}} + \tfrac{1}{2}w_m = 1 - \frac{1}{2}(\tfrac{1}{2}n - m + 1)w_m. \tag{6.8}$$

Here $\mu_{\frac{1}{2}} = 0$, $\mu_{3/2} = w_1$, $\mu_{5/2} = w_1 + w_2$, etc., and $\mu_1 = \frac{1}{2}w_1$, $\mu_2 = w_1 + \frac{1}{2}w_2$, etc.

In the third step, a scaling process is applied to $\bar{\mu}_m$. In method I μ_m is written

$$\mu_m = R\,\bar{\mu}_m, \tag{6.9}$$

with R determined so that

$$\Sigma_m\, w_m\, \mu_m^{\,2} = 1/3. \tag{6.10}$$

For transport work, a slightly different method (II) is considerably better. Here μ_m is written

$$\mu_m = R\,\mu_{m-\frac{1}{2}} + \bar{\mu}_m, \tag{6.11}$$

with R determined so that Eq. (6.10) is satisfied. This is the method selected here and the one examined below. Table VI-1 gives values of R, $R = R(n)$, for a sequence of n. For large n, R appears to behave as $1/n^2$. The one-dimensional ES_n sets, based

TABLE VI-1

VALUES OF THE SCALE FACTOR R VS n

n	R	n	R
4	0.0728757	24	0.0017172
6	0.0287804	28	0.0012627
8	0.0157065	32	0.0009675
10	0.0099458	40	0.0006200
12	0.0068776	48	0.0004310
14	0.0050444	56	0.0003169
16	0.0038600	64	0.0002428
20	0.0024709		

on method II, n = 2, 4, ..., 16, are included in Table VI-8.

In a first test of the quadrature, the linear extrapolation length z_o is obtained as a function of n. The accuracy of this quantity is important to the accuracy of the results to a number of benchmark problems in transport theory. The exact value of z_o is known to be 0.71044609. For finite n, z_o may be obtained as the sum of the poles minus the sum of the zeroes of the following equation.

$$\Sigma_m \frac{w_m}{1 - \mu_m^2/\mu^2} - 1 = 0. \qquad (6.12)$$

The poles are clearly located at the quadrature nodes. There are $\frac{1}{2}n - 1$ zeroes. For n = 4 one finds $\mu = \sqrt{3}\,\mu_1\mu_2$ to be the single zero, hence for n = 4

$$z_o = \mu_1 + \mu_2 - \sqrt{3}\,\mu_1\mu_2. \qquad (6.13)$$

Values of z_o for several sequences of n are given in Table VI-2. The errors in the ES_n-based values behave approximately as $-0.09/n^2$. Here ES_n by scaling II represents a significant improvement over Gauss quadrature which, for n = 4, 8, and 16, gives z_o = 0.694025, 0.706918, and 0.709609, respectively. ES_n by scaling I gives similar values.

Incidentally, Gauss quadrature can be very closely simulated by the ES_n technique with scaling I using in the first step either the exact Gauss weights or approximate values from $w_m = \mu_{m+\frac{1}{2}} - \mu_{m-\frac{1}{2}}$ where

$$\mu_{m-\frac{1}{2}} = \sin\frac{\pi}{2}\frac{2(m-1)}{n+\frac{1}{2}} \Big/ \sin\frac{\pi}{2}\frac{n}{n+\frac{1}{2}}. \qquad (6.14)$$

TABLE VI-2

THE EXTRAPOLATION LENGTH z_o FOR c = 1 AND ES_n QUADRATURE

n	z_o	n	z_o
4	0.706075	6	0.708304
8	0.709205	12	0.709874
16	0.710116	24	0.710295
32	0.710359	48	0.710407
64	0.710424		
		14	0.710020
10	0.709636	28	0.710334
20	0.710231	56	0.710417
40	0.710390		
		Exact	0.710446

In a second test, the moments M_k are computed from the ES_n data and compared to the exact values, $M_k = 1/(k+1)$, for a sequence of k for several values of n. For k = 0 and 2 the ES_n data give correct values by construction. Table VI-3 gives values of M_k for k = 4, 6, 8, 12, and 16, and n = 4, 6, 8, 12, 16, 32, and 64. The errors for large n behave as A_k/n^2 where $A_4 \approx 1.35$, $A_6 \approx 1.94$, $A_8 \approx 2.26$, and $A_{16} \approx 2.80$. The coefficients A_k appear to be bounded with respect to k. In this test, Gauss quadrature is clearly superior giving exact values by definition for M_k for even k to $k = 2n - 2$ inclusive. However, in S_n-type transport calculations, as far as has been observed, exactness for k > 2 appears to have no clear advantages over 1/n or faster convergence.

In a third test, values of the coefficients $2\alpha_{m-\frac{1}{2}}$, of special importance in spherical geometry, are computed using

$$2\alpha_{m-\frac{1}{2}} = 2\sum_{\ell=m}^{\frac{1}{2}n} w_\ell\,\mu_\ell, \qquad (6.15)$$

and compared to the exact values from

$$2\alpha_{m-\frac{1}{2}} = 1 - \bar{\mu}_{m-\frac{1}{2}}^2. \qquad (6.16)$$

As can be seen from the data in Table VI-4 and also confirmed analytically, there is rapid convergence of $2\alpha_{m-\frac{1}{2}}$ as obtained from Eq. (6.15) as n increases.

TABLE VI-3

ACCURACY OF MOMENTS FOR ES_n QUADRATURE

(zeroeth and second moments exact)

Moment	4	6	8	12	16
n					
4	0.209877	0.157750			
6	0.204154	0.148843	0.117595		
8	0.202293	0.146140	0.114841	0.080968	
12	0.200998	0.144286	0.112766	0.078794	0.060774
16	0.200554	0.143651	0.112035	0.077979	0.059940
32	0.200135	0.143051	0.111337	0.077184	0.059102
64	0.200033	0.142905	0.111167	0.076987	0.058892
Exact	0.200000	0.142857	0.111111	0.076923	0.058824

TABLE VI-4

VALUES OF $2\alpha_{m-\frac{1}{2}}$ FOR SELECTED n

n = 4	Approx	Exact	n = 16	Approx	Exact
$\alpha_{\frac{1}{2}}$	1.0324	1.0000	$\alpha_{\frac{1}{2}}$	1.0033	1.0000
$\alpha_{3/2}$	0.5879	0.5556	$\alpha_{3/2}$	0.9539	0.9506
n = 8			$\alpha_{5/2}$	0.8293	0.8264
$\alpha_{\frac{1}{2}}$	1.0110	1.0000	$\alpha_{7/2}$	0.6621	0.6597
$\alpha_{3/2}$	0.8510	0.8400	$\alpha_{9/2}$	0.4802	0.4784
$\alpha_{5/2}$	0.5172	0.5100	$\alpha_{11/2}$	0.3067	0.3056
$\alpha_{7/2}$	0.1928	0.1900	$\alpha_{13/2}$	0.1603	0.1597
			$\alpha_{15/2}$	0.0550	0.0548

The two-dimensional ES_n quadrature sets are also obtained by a three-step method as follows.

1. The principal octant is divided into $n(n + 2)/8$ mesh cells of equal area located in a triangular and symmetric manner as discussed earlier. The associated mesh points, also invariant with respect to permutation of components, can be determined from certain trigonometric equations. The mesh division is illustrated in Fig. 6.1 for n = 16. Note the successive $[(n+2)/6]$ annular regions containing $3(\frac{1}{2}n - 1)$, $3(\frac{1}{2}n - 4)$, ..., equal areas.

2. The midpoint coordinates $\bar{\mu}_m$, $\bar{\eta}_m$, and $\bar{\xi}_m$ are computed for each mesh cell. These coordinates, which may also be written $\bar{\mu}_{\ell,m}$, $\bar{\mu}_{\ell,k}$, and $\bar{\mu}_{m,\ell}$ $(k = \frac{1}{2}n - \ell - m + 2)$, can also be found from analytical formulas.

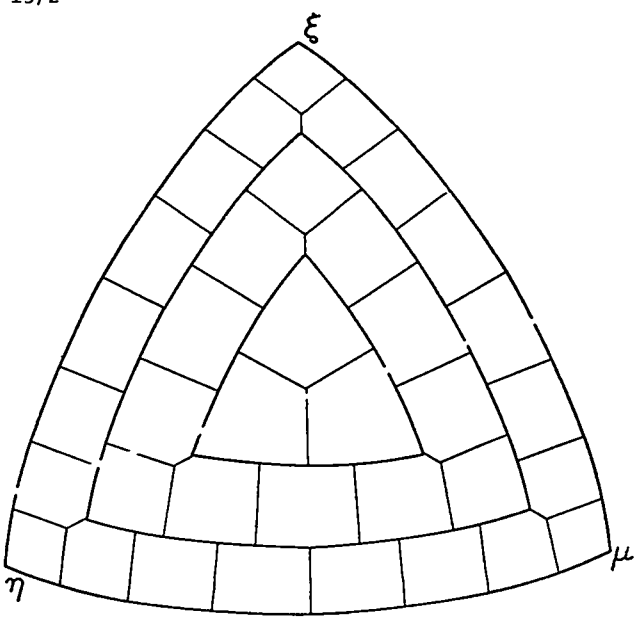

Fig. 6.1. Mesh division for n = 16.

3. The midpoint coordinates are scaled using

$$\mu_{\ell,m} = R\,\mu_{m-\frac{1}{2}} + \bar{\mu}_{\ell,m} \tag{6.17}$$

with $\mu_{m-\frac{1}{2}}$ from Eq. (6.7) and R determined for each grouping of points so that

$$(R\,\mu_{m-\frac{1}{2}} + \bar{\mu}_{\ell,m})^2 + (R\,\mu_{k-\frac{1}{2}} + \bar{\mu}_{\ell,k})^2 + (R\,\mu_{\ell-\frac{1}{2}} + \bar{\mu}_{m,\ell})^2 = 1. \tag{6.18}$$

The formulas and procedure in ES_n quadrature will be discussed in more detail in a future report.

As a first test of two-dimensional quadrature, a selection of moments $M_{k,o}$ is calculated and presented in Table VI-5 to be compared to data in Table VI-3. As shown, the agreement with exact values is better in the two-dimensional case.

In a second test, comparison of three variations of ES_n with EQ_n are made. Table VI-6 gives $\mu_{\ell,m}$ for n = 4, 8, and 16 for a previous version of ES_n (A) and the present version (B) with scaling I as well as for (B) with scaling II. In all cases the agreement is very close which may be taken as a confirmation of the reasonableness of all these quadratures, EQ_n included.

Method A is based on a simple half-symmetric division of the octant, splitting bands defined by $(\xi_{\ell-\frac{1}{2}}, \xi_{\ell+\frac{1}{2}})$, $\ell = 1, 2, \ldots, \frac{1}{2}n$, into $\frac{1}{2}n - \ell + 1$ equal sectors for a total of $n(n+2)/8$ sectors (mesh cells) where the ξ's are taken from Eq. (6.7). After computing the midpoint coordinates $\bar{\mu}_{\ell,m}$, $\bar{\eta}_{\ell,m}$, $\bar{\xi}_{\ell,m}$ for each cell, the following symmetrizing operation is performed before scaling

$$\frac{1}{3}(\bar{\mu}_{\ell,m} + \bar{\mu}_{k,m} + \bar{\xi}_m) \to \bar{\mu}_{\ell,m}. \tag{6.19}$$

As a third test, the values of $\eta_{\ell,\frac{1}{2}}$ are determined, of special significance in cylindrical geometry, where

TABLE VI-6

VALUES OF $\mu_{\ell,m}$ FOR VARIOUS METHODS

	ℓ	m	EQ_n (LA-4734)	ES_n Method A Scaling I	ES_n Method B Scaling I	ES_n Method B Scaling II
n = 4	1	1	0.3500212	0.3505622	0.3496826	0.3344052
	1	2	0.8688903	0.8684540	0.8691629	0.8811052
n = 8	4	1	0.1971380	0.1944296	0.1957928	0.1932356
	3	1	0.2133981	0.2137991	0.2103019	0.2075330
	3	2	0.5512958	0.5473098	0.5503087	0.5497634
	2	2	0.5773503	0.5773503	0.5773503	0.5773503
	2	3	0.8065570	0.8091612	0.8080430	0.8091294
	1	4	0.9603506	0.9614543	0.9609008	0.9619356
n = 16	8	1	0.1050159	0.1029811	0.1040726	0.1036946
	7	1	0.1152880	0.1130805	0.1137610	0.1133421
	6	1	0.1152880	0.1160605	0.1145198	0.1140958
	5	1	0.1152880	0.1172276	0.1145198	0.1140958
	7	2	0.3016701	0.3009446	0.3005210	0.3002897
	6	2	0.3284315	0.3238364	0.3266520	0.3263778
	5	2	0.3332906	0.3329597	0.3315867	0.3313218
	4	2	0.3332906	0.3355448	0.3325955	0.3323335
	6	3	0.4743525	0.4774090	0.4750315	0.4749405
	5	3	0.5107319	0.5085062	0.5121306	0.5120317
	4	3	0.5215431	0.5210090	0.5205894	0.5205236
	5	4	0.6327389	0.6329970	0.6321897	0.6321909
	4	4	0.6666774	0.6661117	0.6668509	0.6669162
	3	4	0.6752671	0.6760911	0.6767373	0.6768386
	4	5	0.7657351	0.7652271	0.7653038	0.7663660
	3	5	0.7925089	0.7940776	0.7923210	0.7924957
	3	6	0.8727534	0.8709825	0.8724851	0.8725902
	2	6	0.8855877	0.8889657	0.8869030	0.8871049
	2	7	0.9464163	0.9469135	0.9469665	0.9470901
	1	8	0.9889102	0.9893381	0.9891096	0.9891890

TABLE VI-5

ACCURACY OF MOMENTS $M_{k,0}$ for ES_n TWO-DIMENSIONAL CASE

k / n	4	6	8	12	16
4	0.209241	0.156904			
6	0.203230	0.147185	0.115398		
8	0.201376	0.144602	0.112958	0.078808	
12	0.200632	0.143655	0.111954	0.077764	0.059632
16	0.200325	0.143266	0.111552	0.077390	0.059295
32	0.200077	0.142954	0.111217	0.077038	0.058943
64	0.200019	0.142881	0.111137	0.076952	0.058854
Exact	0.200000	0.142857	0.111111	0.076923	0.058824

$$\eta_{\ell,\frac{1}{2}} = (\pi/2w_\ell)\alpha_{\ell,\frac{1}{2}}, \tag{6.20}$$

given exactly by

$$\eta_{\ell,\frac{1}{2}} = \sqrt{1 - \xi_\ell^2} = \sqrt{1 - \mu_\ell^2} \tag{6.21}$$

with μ_ℓ^2 obtained from

$$\mu_m^2 = (\Sigma_\ell\, w_{\ell,m}\, \mu_{\ell,m}^2)/w_m, \tag{6.22}$$

and given approximately by

$$\eta_{\ell,\frac{1}{2}} = (\pi w/2w_\ell)\Sigma_m\, \mu_{\ell,m}. \tag{6.23}$$

The differences between approximate and exact values for $\eta_{\ell,\frac{1}{2}}$ are given in Table VI-7 for n = 4, 6, ..., 16, and ℓ = 1, 2, ..., $\frac{1}{2}$n. Also, in the first column, the average absolute error is given, a weighted average with w_ℓ as weights. Similar tables have been constructed for $\eta_{\ell,3/2}$, $\eta_{\ell,5/2}$, etc., giving similar results.

Table VI-7 is only mildly reassuring in regard to convergence with n. However, this is not as much a test of the quadrature as a test of the numerical procedure for handling direction-to-direction transfer by streaming in cylindrical geometry. The procedure is built on the assumption of within-level transfer only, the basis for Eq. (6.23). Further tests are indicated here.

Table VI-8 gives one-dimensional and two-dimensional ES_n quadrature sets for n = 4, 6, ..., 16. In the one-dimensional case w_m and two sets of nodes μ_m are given, the first based on Eq. (6.11) and the second on Eq. (6.22).

REFERENCES

1. Bengt G. Carlson, "Modified Difference Schemes for the Transport Equation Solution," Los Alamos Scientific Laboratory report, LA-5760 (1974).
2. I. P. Grant, "Numerical Analysis of Discrete Ordinates Methods," J. Comput. Phys. 2, No. 4 (1968).
3. 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).
4. B. G. Carlson, "Transport Theory: Discrete Ordinates Quadrature Over the Unit Sphere," Los Alamos Scientific Laboratory report, LA-4554 (1970).
5. B. G. Carlson, "Tables of Symmetric Equal Weight Quadrature EQ_n Over the Unit Sphere," Los Alamos Scientific Laboratory report, LA-4734 (1971).

TABLE VI-7

ERROR IN $\eta_{\ell,\frac{1}{2}}$ FOR ES_n AND SELECTED n

n	Average Error	ℓ=1	ℓ=2	ℓ=3	ℓ=4	ℓ=5	ℓ=6	ℓ=7	ℓ=8
4	0.0256	0.0122	0.0524						
6	0.0143	0.0089	0.0104	0.0384					
8	0.0091	0.0076	0.0055	0.0071	0.0303				
10	0.0062	0.0066	0.0045	0.0021	0.0057	0.0249			
12	0.0046	0.0059	0.0048	0.0009	0.0006	0.0049	0.0212		
14	0.0038	0.0054	0.0053	0.0011	-0.0012	-0.0001	0.0043	0.0184	
16	0.0036	0.0049	0.0057	0.0016	-0.0013	-0.0021	-0.0003	0.0039	0.00162

TABLE VI-8

ES_n QUADRATURE SETS

m	1	2	3	4	5
n=4					
w_m	0.6666667	0.3333333			
μ_m	0.3344052	0.8819171			
μ_m	0.3333333	0.8819171			
$\mu_{2,m}$	0.3344052				
$\mu_{1,m}$	0.3344052	0.8811052			
n=6					
w_m	0.5000000	0.3333333	0.1666667		
μ_m	0.2500000	0.6810569	0.9406503		
μ_m	0.2508939	0.6825427	0.9377780		
$\mu_{3,m}$	0.2455325				
$\mu_{2,m}$	0.2612869	0.6825427			
$\mu_{1,m}$	0.2455325	0.6825427	0.9377780		
n=8					
w_m	0.4000000	0.3000000	0.2000000	0.1000000	
μ_m	0.2000000	0.5562826	0.8109946	0.9641359	
μ_m	0.2005118	0.5591103	0.8091294	0.9619356	
$\mu_{4,m}$	0.1932356				
$\mu_{3,m}$	0.2075330	0.5497634			
$\mu_{2,m}$	0.2075330	0.5773503	0.8091294		
$\mu_{1,m}$	0.1932356	0.5497634	0.8091294	0.9619356	
n=10					
w_m	0.3333333	0.2666667	0.2000000	0.1333333	0.0666667
μ_m	0.1666667	0.4699819	0.7059675	0.8746233	0.9759494
μ_m	0.1671001	0.4717345	0.7064294	0.8728505	0.9743667
$\mu_{5,m}$	0.1590747				
$\mu_{4,m}$	0.1717616	0.4567603			
$\mu_{3,m}$	0.1732011	0.4862478	0.6964199		
$\mu_{2,m}$	0.1717616	0.4862478	0.7260345	0.8728505	
$\mu_{1,m}$	0.1590747	0.4567603	0.6964199	0.8728505	0.9743667

TABLE VI-8 (cont)

m	1	2	3	4	5	6	7	8
n=12								
w_m	0.2857143	0.2380952	0.1904762	0.1428571	0.0952381	0.0476190		
μ_m	0.1428571	0.4067269	0.6226502	0.7906269	0.9106570	0.9827406		
μ_m	0.1432328	0.4082299	0.6231948	0.7902040	0.9092277	0.9815823		
$\mu_{6,m}$	0.1350855							
$\mu_{5,m}$	0.1465973	0.3896334						
$\mu_{4,m}$	0.1476756	0.4185322	0.6053009					
$\mu_{3,m}$	0.1476756	0.4234281	0.6405890	0.7821782				
$\mu_{2,m}$	0.1465973	0.4185322	0.6405890	0.8060158	0.9092277			
$\mu_{1,m}$	0.1350855	0.3896334	0.6053009	0.7821782	0.9092277	0.9815823		
n=14								
w_m	0.2500000	0.2142857	0.1785714	0.1428571	0.1071429	0.0714286	0.0357143	
μ_m	0.1250000	0.3584040	0.5559135	0.7175286	0.8432492	0.9330754	0.9870071	
μ_m	0.1253259	0.3596677	0.5573845	0.7167122	0.8425374	0.9319493	0.9861350	
$\mu_{7,m}$	0.1173407							
$\mu_{6,m}$	0.1278521	0.3392997						
$\mu_{5,m}$	0.1287323	0.3669064	0.5329202					
$\mu_{4,m}$	0.1287323	0.3719382	0.5709843	0.7012232				
$\mu_{3,m}$	0.1287323	0.3719382	0.5773503	0.7318735	0.8363158			
$\mu_{2,m}$	0.1278521	0.3669064	0.5709843	0.7318735	0.8548447	0.9319493		
$\mu_{1,m}$	0.1173407	0.3392997	0.5329202	0.7012232	0.8363158	0.9319493	0.9861350	
n=16								
w_m	0.2222222	0.1944444	0.1666667	0.1388889	0.1111111	0.0833333	0.0555556	0.0277778
μ_m	0.1111111	0.3203022	0.5016083	0.6550294	0.7805655	0.8782166	0.9479828	0.9898639
μ_m	0.1113942	0.3214668	0.5028882	0.6552855	0.7795403	0.8774551	0.9470901	0.8981890
$\mu_{8,m}$	0.1036946							
$\mu_{7,m}$	0.1133421	0.3002897						
$\mu_{6,m}$	0.1140958	0.3263778	0.4749405					
$\mu_{5,m}$	0.1140958	0.3313218	0.5120317	0.6321909				
$\mu_{4,m}$	0.1140958	0.3323335	0.5205236	0.6669162	0.7663660			
$\mu_{3,m}$	0.1140958	0.3313218	0.5205236	0.6768386	0.7924957	0.8725902		
$\mu_{2,m}$	0.1133421	0.3263778	0.5120317	0.6669162	0.7924957	0.8871049	0.9470901	
$\mu_{1,m}$	0.1036946	0.3002897	0.4749405	0.6321909	0.7663660	0.8725902	0.9470901	0.9891890

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