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**FINITE DIFFERENCE METHODS FOR NONLINEAR
RADIATION TRANSPORT**

RELEASED FOR ANNOUNCEMENT
IN NUCLEAR SCIENCE ABSTRACTS

Livermore, California

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UCRL-12411
Physics, UC34,
TID-4500 (45th Ed.)

UNIVERSITY OF CALIFORNIA
Lawrence Radiation Laboratory
Livermore, California

AEC Contract No. W-7405-eng-48

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August 20, 1965

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Printed in USA. Price \$2.00. Available from the Clearinghouse for Federal
Scientific and Technical Information, National Bureau of Standards,
U. S. Department of Commerce, Springfield, Virginia.

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FINITE DIFFERENCE METHODS FOR NONLINEAR RADIATION TRANSPORT

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ABSTRACT

A formulation is given of the nonlinear, frequency-dependent transport problem in one dimension, assuming local thermodynamic equilibrium. Equivalent representations of the angular distribution are discussed, including the treatment of discontinuities. A method for the combination of transport and diffusion based on the equivalence of the angular representations is presented. The performance of this method is illustrated in a variety of sample calculations.

I. INTRODUCTION

In this report we shall consider numerical methods for the solution of the nonlinear frequency-dependent, radiation transport problem in one space dimension. In the nonlinear problem the temperature-dependent emitting and absorbing properties of the transport medium can be obtained only in terms of the past history of the radiation field, whereas in the linear problem the given characteristics of the transport medium remain unchanged.

The principal difficulty in frequency-dependent calculations is the enormous variation in cross section that can be encountered in a single problem. For example, since most of the energy in a blackbody radiation field at temperature T lies in the frequency range $[T/10, 10T]$, the resulting variation in a typical absorption cross section proportional to ν^{-3} is $[10^3 \sigma_0, 10^{-3} \sigma_0]$.

The first account of a nonlinear, frequency-dependent calculation is that of Barfield, von Holdt, and Zachariasen (1954). The accuracy of the method used by these authors is subject to the restriction that the distance a photon travels in a time step, $c\Delta t$, must be less than the absorption mean free path λ . This restriction, characteristic of many numerical methods for the transport equation, leads to prohibitively long running times for most frequency-dependent calculations.

It is therefore desirable that the accuracy of the transport method be as nearly independent of the cross section as possible. Two approaches have been successful in this respect: Monte Carlo methods¹ follow particles accurately through the transport medium whatever the cross section, and finite difference methods can be constructed so as to yield the correct diffusion properties in the limit of very large cross section.²

¹ Refer to Campbell and Nelson (1964).

² See for example Grant (1963).

In this report we propose a method for the combination of transport and diffusion which is based on the demonstrated equivalence between the Legendre polynomial, moment, and discrete ordinate representations of the angular distribution.

II. FORMULATION OF THE PROBLEM

In transport calculations (for which polarization effects³ are neglected) the state of the radiation field is given by the specific intensity, $I^\nu(\vec{r}, \vec{\Omega}, t)$.

For one-dimensional symmetry the monochromatic intensity of frequency ν , $I^\nu(r, \mu, t)$, is a function of the position coordinate, r , the direction cosine relative to the r axis, μ , and the time, t . In terms of the intensity we may obtain the radiation energy density,

$$E^\nu(r, t) = \frac{2\pi}{c} \int_{-1}^1 I^\nu(r, \mu, t) d\mu,$$

the r component of the radiation flux vector,

$$F^\nu(r, t) = 2\pi \int_{-1}^1 I^\nu(r, \mu, t) \mu d\mu,$$

and the $P_{r,r}$ component of the radiation pressure tensor,

$$P^\nu(r, t) = 2\pi \int_{-1}^1 I^\nu(r, \mu, t) \mu^2 d\mu.$$

The specific intensity obeys a continuity equation of the following form:

$$\frac{1}{c} \frac{\partial I^\nu}{\partial t} + \mu \frac{\partial I^\nu}{\partial r} + \frac{\alpha}{2} \frac{(1 - \mu^2)}{r} \frac{\partial I^\nu}{\partial \mu} + (\sigma_a^\nu + \sigma_s^\nu) I^\nu = S_e^\nu + S_s^\nu, \quad (1)$$

where $\alpha = 0$ for plane geometry and $\alpha = 2$ for spherical geometry. The forms for the absorption and scattering cross sections (σ_a and σ_s) and the emission and scattering sources (S_e and S_s) depend on the nature of the transport medium.

Throughout this report we shall assume that local thermodynamic equilibrium is valid,⁴ in which case the emission function is given by Kirchhoff's law:

$$S_e = \sigma_a^\nu B^\nu(T),$$

where $B^\nu(T)$ is the Planck function,

$$B^\nu(T) = \frac{2}{(hc)^2} \frac{(h\nu)^3}{e^{h\nu/kT} - 1}. \quad (2)$$

³ The most general radiation field encountered in nature can be specified by four quantities, the Stokes parameters, each with the dimensions of an intensity. For example see Chandrasekhar (1950), p. 24.

⁴ The hypothesis of local thermodynamic equilibrium is discussed by Woolley and Stibbs (1953), p. 57, and Goody (1964), p. 29.

For the purposes of this report we need to consider only conservative scattering, for which

$$S_s^\nu(r, \mu, t) = \sigma_s \int_0^{2\pi} \int_{-1}^1 K(\mu; \mu', \phi') I^\nu(r, \mu', t) d\mu' d\phi'.$$

If the scattering kernel in the center-of-mass system is expressed in terms of Legendre polynomials

$$K(\cos \theta) = \sum_{\ell=0}^{\infty} K_\ell P_\ell(\cos \theta),$$

the scattering integral becomes

$$S_s^\nu(r, \mu, t) = \sigma_s \int_{-1}^1 K(\mu, \mu') I^\nu(r, \mu', t) d\mu', \quad (3a)$$

where

$$K(\mu, \mu') = 2\pi \sum_{\ell=0}^{\infty} K_\ell P_\ell(\mu) P_\ell(\mu'), \quad (3b)$$

by virtue of the addition theorem for the Legendre functions:

$$P_\ell(\cos \theta) = P_\ell(\mu) P_\ell(\mu') + 2 \sum_{k=1}^{\ell} P_\ell^k(\mu) P_\ell^k(\mu') \frac{(\ell-k)!}{(\ell+k)!} \cos k\phi.$$

For isotropic scattering, for example, we have

$$K_0 = \frac{1}{4\pi}; K_\ell = 0, \ell = 1, 2, \dots,$$

and for Thompson scattering by free electrons at rest

$$K_0 = \frac{1}{4\pi}; K_2 = \frac{1}{2\pi}; K_\ell = 0, \ell = 1, 3, 4, \dots$$

A. The Basic Equations

Under the restrictions of local thermodynamic equilibrium and conservative scattering, the transport equation in one dimension becomes

$$\begin{aligned} \frac{1}{c} \frac{\partial I^\nu}{\partial t} + \mu \frac{\partial I^\nu}{\partial r} + \frac{\alpha}{2} \frac{(1-\mu^2)}{r} \frac{\partial I^\nu}{\partial \mu} + (\sigma_a^\nu + \sigma_s) I^\nu \\ = \sigma_a^\nu B^\nu(T) + \sigma_s \int_{-1}^1 K(\mu, \mu') I^\nu(\mu') d\mu'. \end{aligned} \quad (4)$$

In order to evaluate the source function, $\sigma_a^\nu B^\nu(T)$, we must keep and account of the energy exchange between the radiation field and the material. When we integrate Eq. (4) over all μ and ν , the (conservative) scattering terms drop out with the result:

$$\frac{\partial E}{\partial t} + \frac{1}{r^\alpha} \frac{\partial}{\partial r} (r^\alpha F) = \int_0^\infty c \sigma_a^\nu \left[\frac{4\pi}{c} B^\nu(T) - E^\nu \right] d\nu. \quad (5a)$$

The right-hand side of Eq. (5a) is the difference between the rates of emission and absorption of energy in a unit volume. Thus if $E_m(T)$ is the material energy density, the net exchange of energy is given by Eqs. (5a) and (5b).

$$\frac{\partial E_m(T)}{\partial t} = \int_0^\infty c \sigma_a^\nu \left[E^\nu - \frac{4\pi}{c} B^\nu(T) \right] d\nu. \quad (5b)$$

Finally the material energy density must be expressed in terms of the temperature T by an equation of state. In this report we shall use the ideal-gas equation of state

$$E_m = \rho c_v T, \quad (6)$$

where ρ is the mass density and c_v the specific heat.

The transport equation (4) and the appropriate boundary conditions together with the energy balance equations (5) and the equation of state (6) constitute the complete set of basic relations which define the problem to be considered in this study.

III. EQUIVALENT REPRESENTATIONS OF THE ANGULAR DISTRIBUTION

In transport problems a number of different representations of the angular distribution have been used, resulting in a variety of calculational procedures. Most of these procedures are formally equivalent,⁵ a fact of considerable assistance in the task of assimilating the transport literature.

A. Orthogonal Polynomial Representation

The angular distribution is represented in terms of a series expansion in orthogonal polynomials, $P_\ell(\mu)$:

$$I(r, \mu, t) = \frac{1}{4\pi} \sum_{\ell=0}^{\infty} (2\ell + 1) \psi_\ell(r, t) P_\ell(\mu). \quad (7)$$

The polynomials orthogonal on the interval $[-1, 1]$ are the Legendre polynomials, which may be written

$$P_\ell(\mu) = \sum_{k=0}^{\ell} C_k^\ell \mu^k.$$

By means of the orthogonality relation for the $P_\ell(\mu)$ we obtain the inversion

$$\psi_\ell(r, t) = 2\pi \int_{-1}^1 I(r, \mu, t) P_\ell(\mu) d\mu,$$

which may be expressed directly in terms of the moments of the angular distribution, M_k :

$$\psi_\ell(r, t) = 2\pi \sum_{k=0}^{\ell} C_k^\ell \int_{-1}^1 I(r, \mu, t) \mu^k d\mu = \sum_{k=0}^{\ell} C_k^\ell M_k(r, t). \quad (8)$$

⁵ Relations between the different methods have been variously discussed by Chandrasekhar (1950), p. 366, Krook (1955), Richtmyer (1957), p. 139, and Goldstein (1957).

In order to derive an equation for the expansion coefficients $\psi_\ell(r, t)$ we make use of the following recurrence relations,

$$(2\ell + 1)\mu P_\ell(\mu) = (\ell + 1)P_{\ell+1}(\mu) + \ell P_{\ell-1}(\mu),$$

$$(1 - \mu^2) \frac{dP_\ell(\mu)}{d\mu} = \frac{\ell(\ell + 1)}{2\ell + 1} [-P_{\ell+1}(\mu) + P_{\ell-1}(\mu)],$$

to obtain, after rearrangement of terms,

$$\frac{1}{c} \frac{\partial I}{\partial t} = \frac{1}{4\pi} \sum_{\ell=0}^{\infty} (2\ell + 1) \frac{1}{c} \frac{\partial \psi_\ell}{\partial t} P_\ell(\mu),$$

$$\mu \frac{\partial I}{\partial r} = \frac{1}{4\pi} \sum_{\ell=0}^{\infty} \left\{ \ell P_{\ell-1} + (\ell + 1) P_{\ell+1} \right\} \frac{\partial \psi_\ell}{\partial r} = \frac{1}{4\pi} \sum_{\ell=0}^{\infty} \left\{ \ell \frac{\partial \psi_{\ell-1}}{\partial r} + (\ell + 1) \frac{\partial \psi_{\ell+1}}{\partial r} \right\} P_\ell(\mu),$$

$$\begin{aligned} (1 - \mu^2) \frac{\partial I}{\partial \mu} &= \frac{1}{4\pi} \sum_{\ell=0}^{\infty} \frac{\ell(\ell + 1)}{(2\ell + 1)} \left\{ P_{\ell-1} - P_{\ell+1} \right\} \psi_\ell \\ &= \frac{1}{4\pi} \sum_{\ell=0}^{\infty} \left\{ (\ell + 1)(\ell + 2) \psi_{\ell+1} - \ell(\ell - 1) \psi_{\ell-1} \right\} P_\ell(\mu). \end{aligned}$$

The scattering integral (3) is given by

$$S(r, \mu, t) = \int_{-1}^1 2\pi \sum_{\ell=0}^{\infty} K_\ell P_\ell(\mu) P_\ell(\mu') \frac{1}{4\pi} \sum_{j=0}^{\infty} (2j + 1) \psi_j P_j(\mu') d\mu' = \sum_{\ell=0}^{\infty} K_\ell \psi_\ell(r, t) P_\ell(\mu).$$

When the above expressions are substituted into the transport equation (4) and the coefficients of the $P_\ell(\mu)$ are set equal to zero, one obtains the required equations for the expansion coefficients:

$$\begin{aligned} (2\ell + 1) \frac{1}{c} \frac{\partial \psi_\ell}{\partial t} + \frac{\partial \psi_{\ell-1}}{\partial r} + (\ell + 1) \frac{\partial \psi_{\ell+1}}{\partial r} + \frac{\alpha}{2r} \left[(\ell + 1)(\ell + 2) \psi_{\ell+1} - \ell(\ell - 1) \psi_{\ell-1} \right] \\ + (2\ell + 1) \sigma_T \psi_\ell = 4\pi \delta_\ell \sigma_a B(T) + 4\pi \sigma_s K_\ell \psi_\ell, \quad \ell = 0, 1, 2, \dots, \quad (9) \end{aligned}$$

where $\delta_\ell = 1$ for $\ell = 0$ and $\delta_\ell = 0$ for $\ell = 1, 2, \dots$.

In any $n - 1$ equations there are n unknowns. In order to obtain a useful procedure for computation, we truncate the series by

$$\psi_n = 0,$$

where n is sufficiently large.

Since the expansion coefficients $\psi_\ell(r, t)$ can be expressed directly in terms of the $M_k(r, t)$, it is clear that the angular distribution can be represented equally well in terms of the moments. Indeed the correct moment equations result when the relations (8) are inserted into the equations (9) for the Legendre coefficients ψ_ℓ .

B. Moment Representation

The moments of the angular distribution are defined by the relation

$$M_k(r, t) = 2\pi \int_{-1}^1 I(r, \mu, t) \mu^k d\mu, \quad k = 0, 1, 2, \dots$$

When the transport equation (4) is multiplied by $2\pi\mu^k d\mu$ and integrated over the interval $[-1, 1]$, the following sequence of moment equations is obtained:

$$\frac{1}{c} \frac{\partial M_k}{\partial t} + \frac{\partial M_{k+1}}{\partial r} + \frac{\alpha}{2r} [(k+2)M_{k+1} - kM_{k-1}] + \sigma_T M_k = 2\pi \frac{[1 + (-1)^k]}{(k+1)} \sigma_a B(T) + 2\pi \sigma_s G, \quad (10)$$

$$k = 0, 1, 2, \dots,$$

where

$$G(k) = \int_{-1}^1 S(\mu) \mu^k d\mu = \sum_{\ell=0}^{\infty} K_{\ell} \sum_{j=0}^{\ell} C_j^{\ell} M_j \int_{-1}^1 P_{\ell}(\mu) \mu^k d\mu.$$

In any $n-1$ equations there are n unknowns. The series is therefore terminated by the expression

$$\sum_{k=0}^n C_k^n M_k = 0, \quad (11)$$

which, according to (8), is also the terminal relation for the Legendre polynomial representation.

C. Discrete Ordinate Representation

The μ interval $[-1, 1]$ is divided by n points $(\mu_{\ell}; \ell=1, \dots, n)$ into $n-1$ subintervals, $\Delta\mu_{\ell}$. The points of division can be considered as the zeros of a factorable polynomial,

$$P_n(\mu) = \prod_{\ell=1}^n (\mu - \mu_{\ell}).$$

The basis of the discrete ordinate representation is an interpolating function for the intensity:

$$I(r, \mu, t) \approx \sum_{\ell=1}^n L_{\ell}^{(n)}(\mu) I_{\ell}(r, t),$$

where the Lagrangian coefficients⁶ are given by

$$L_{\ell}^{(n)}(\mu) = \frac{P_n(\mu)}{(\mu - \mu_{\ell})} \left[\frac{dP_n(\mu)}{d\mu} \right]_{\mu_{\ell}}^{-1} = \frac{(\mu - \mu_1) \dots (\mu - \mu_{\ell-1})(\mu - \mu_{\ell+1}) \dots (\mu - \mu_n)}{(\mu_{\ell} - \mu_1) \dots (\mu_{\ell} - \mu_{\ell-1})(\mu_{\ell} - \mu_{\ell+1}) \dots (\mu_{\ell} - \mu_n)}.$$

The derivative of the intensity with respect to μ at any of the points of division is approximated by

$$\left(\frac{\partial I}{\partial \mu} \right)_{\mu_k} \approx \sum_{\ell=1}^n I_{\ell} \left[\frac{dL_{\ell}^{(n)}(\mu)}{d\mu} \right]_{\mu_k} = \sum_{\ell=1}^n D_{\ell, k} I_{\ell},$$

⁶ See Milne (1949), p. 83.

and the integral of the intensity is given by a corresponding quadrature formula,

$$\int_{-1}^1 I d\mu \approx \sum_{\ell=1}^n I_{\ell} \int_{-1}^1 L_{\ell}(\mu) d\mu = \sum_{\ell=1}^n A_{\ell} I_{\ell}.$$

The discrete ordinates, I_{ℓ} , obey the equation

$$\frac{1}{c} \frac{\partial I_{\ell}}{\partial t} + \mu_{\ell} \frac{\partial I_{\ell}}{\partial r} + \frac{\alpha}{2} \frac{(1 - \mu_{\ell}^2)}{r} \sum_{\ell'} D_{\ell', \ell} I_{\ell'} + \sigma_T I_{\ell} = \sigma_a B(T) + \sigma_s S(\mu_{\ell}), \quad (12)$$

where

$$S(\mu_{\ell}) = \sum_{\ell'} I_{\ell'} \int_{-1}^1 K(\mu_{\ell}, \mu') L_{\ell'}(\mu') d\mu'.$$

It is easy to show that the discrete ordinate representation is equivalent to the Legendre polynomial representation and hence equivalent to the moment representation also. According to (7) the n discrete ordinates are given in terms of the $n+1$ Legendre coefficients by

$$I_{\ell} = I(\mu_{\ell}) = \frac{1}{4\pi} \sum_{k=0}^n (2k+1) \psi_k P_k(\mu_{\ell}), \quad \ell = 1, 2, \dots, n. \quad (13)$$

If we choose the μ_{ℓ} to be the zeros of $P_n(\mu)$, ψ_n is arbitrary since $P_n(\mu_{\ell}) \equiv 0$. When the relations (13) are inverted for the ψ_k and substituted into the equations for the Legendre coefficients (9), the discrete ordinate equations (12) are obtained.

In the discrete ordinate representation the moments are given by

$$M_k = 2\pi \sum_{\ell=1}^n I_{\ell} \int_{-1}^1 L_{\ell}(\mu) \mu^k d\mu, \quad k = 0, 1, \dots, n. \quad (14)$$

When the μ_{ℓ} are the zeros of the Legendre function $P_n(\mu)$, the expression for the moments reduces to the surprisingly simple result⁷

$$M_k = 2\pi \sum_{\ell=1}^n A_{\ell} I_{\ell} \mu_{\ell}^k, \quad k = 0, 1, \dots, n, \quad (15)$$

where

$$A_{\ell} = \int_{-1}^1 L_{\ell}(\mu) d\mu.$$

⁷ For example:

$$\frac{1}{P'(\mu_{\ell})} \int_{-1}^1 \frac{P_n(\mu)}{\mu - \mu_{\ell}} \mu^k d\mu = \frac{1}{P'(\mu_{\ell})} \int_{-1}^1 P_n(\mu) \mu^{k-1} d\mu + \frac{1}{P'(\mu_{\ell})} \int_{-1}^1 \frac{P_n(\mu)}{\mu - \mu_{\ell}} \mu^{\ell} \mu^{k-1} d\mu$$

$$= \dots = \mu_{\ell}^k A_{\ell}.$$

It should be emphasized that only for Gaussian quadrature does the relation (15) hold. If Newton-Cotes quadrature is used, for example, the moments must be calculated by (14).

The expression (15) may be inverted to obtain the M_k in terms of the A_{ℓ}^I if the rank of the $(n+1) \times (n)$ coefficient matrix $[\mu_{\ell}^k]$ is equal to the rank of the $(n+1) \times (n+1)$ augmented matrix $[M_k, \mu_{\ell}^k]$.⁸ This will be the case if

$$\begin{vmatrix} M_0 & 1 & 1 & \cdots & 1 \\ M_1 & \mu_1 & \mu_2 & \cdots & \mu_n \\ \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & & \cdot \\ M_n & \mu_1^n & \mu_2^n & \cdots & \mu_n^n \end{vmatrix} = 0,$$

which is actually (11), since $P_n(\mu)$ may be expressed in the form of a determinant:

$$\begin{vmatrix} 1 & 1 & 1 & \cdots & 1 \\ \mu & \mu_1 & \mu_2 & \cdots & \mu_n \\ \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & & \cdot \\ \mu^n & \mu_1^n & \mu_2^n & \cdots & \mu_n^n \end{vmatrix} = P_n(\mu).$$

D. Discontinuities in the Angular Distribution

Most radiation transport problems involve a boundary between the transport medium and free space. The boundary conditions are such that the angular distribution at an interface contains a finite discontinuity at $\mu = 0$.

In order to correctly deal with such a discontinuity, the angular distribution must be approximated separately on each of the intervals $[-1, 0]$ and $[0, 1]$.⁹ The procedure is based on two sets of polynomials orthogonal on the half-intervals:

$$Q_{\ell}(\mu) = P_{\ell}(2\mu - 1), \quad 0 \leq \mu \leq 1,$$

$$R_{\ell}(\mu) = P_{\ell}(2\mu + 1), \quad -1 \leq \mu \leq 0,$$

where $P_{\ell}(\mu)$ is the Legendre function orthogonal on $[-1, 1]$.

Owing to its special utility as a calculational procedure, the half-range moment formulation is developed in detail in the appendix.

⁸ Refer to Hahn (1958), Chapter V.

⁹ This procedure is mentioned by Kourganoff (1952), p. 101, more fully treated by Sykes (1951), and later emphasized by Krook (1955).

IV. THE LIMITS OF STRONG AND WEAK INTERACTION

In a typical frequency-dependent transport problem, different components of the radiation field interact in varying degrees with the transport medium over rather wide limits. It is of value therefore to investigate the dynamics of radiation flow in the limits of strong and weak interaction with the material. We note that the equations of the moment representation are appropriate to this purpose. For convenience we transcribe them here in terms of energy density, flux, and radiation pressure:

$$\frac{\partial E}{\partial t} + \frac{1}{r^\alpha} \frac{\partial}{\partial r} (r^\alpha F) + c \sigma_a E = 4\pi \sigma_a B(T), \quad (16a)$$

$$\frac{1}{c} \frac{\partial F}{\partial t} + c \frac{\partial P}{\partial r} + \frac{\alpha}{2r} (3P - E) + \sigma_T F = 0, \quad (16b)$$

etc.

For radiation of moderately weak interaction, $\frac{1}{c} \frac{\partial F}{\partial t} \gg \sigma_T F$ and we know that far from the source $P \approx E$, the relation for a plane wave. We then have the equations

$$\begin{aligned} \frac{\partial E}{\partial t} + \frac{1}{r^\alpha} \frac{\partial}{\partial r} (r^\alpha F) + c \sigma_a E &= 4\pi \sigma_a B(T), \\ \frac{1}{c} \frac{\partial F}{\partial t} + \frac{c}{r^\alpha} \frac{\partial}{\partial r} (r^\alpha E) &\approx 0, \end{aligned} \quad (17)$$

$$\frac{\partial E_m}{\partial t} = \int_0^\infty c \sigma_a^\nu \left[E^\nu - \frac{4\pi}{c} B^\nu(T) \right] d\nu,$$

which for vanishingly small interaction reduce to the equations of wave propagation in free space.

For radiation of moderately strong interaction, $\sigma_T F \gg \frac{1}{c} \frac{\partial F}{\partial t}$; and we know that in this case the radiation field will be very nearly isotropic, $P \approx E/3$. In this situation Eq. (16b) reduces to the relation for the flux in a diffusing medium. Transport is then described by the nonequilibrium diffusion formulation:

$$\begin{aligned} \frac{\partial E}{\partial t} + \frac{1}{r^\alpha} \frac{\partial}{\partial r} (r^\alpha F) + c \sigma_a E &= 4\pi \sigma_a B(T), \\ F &\approx -\frac{c}{3} \frac{1}{\sigma_T} \frac{\partial E}{\partial r}, \end{aligned} \quad (18)$$

$$\frac{\partial E_m}{\partial t} = \int_0^\infty c \sigma_a^\nu \left[E^\nu - \frac{4\pi}{c} B^\nu(T) \right] d\nu.$$

When the cross section is exceedingly large for all frequencies, the temperature distribution rapidly adjusts itself so that everywhere $E^\nu \approx \frac{4\pi}{c} B^\nu(T)$. In this case the frequency spectrum is determined, thereby permitting the use of frequency-integrated equations in the equilibrium diffusion formulation:

$$\begin{aligned} E &= aT^4, \quad F \approx \frac{c}{3} \bar{\lambda}_R \frac{\partial E}{\partial r}, \\ \frac{\partial E_m}{\partial t} + \frac{\partial E}{\partial t} + \frac{1}{r^\alpha} \frac{\partial}{\partial r} (r^\alpha F) &= 0, \end{aligned} \quad (19)$$

where the Rosseland mean free path, $\bar{\lambda}_R$, is defined by

$$\bar{\lambda}_R = \frac{\int_0^\infty \frac{1}{\sigma_T \nu} \frac{\partial B^\nu}{\partial T} d\nu}{\int_0^\infty \frac{\partial B^\nu}{\partial T} d\nu}$$

V. SPACE AND TIME DEPENDENCE

A. Construction of Approximating Difference Equations

The only known approach to the solution of a system of equations such as (4), (5), and (6) is to approximate the differential equations by finite difference equations on a net of points covering the region in which the solution is required. The difference equations must be so constructed that the approximate solution can be made to approach the true solution as closely as desired by refinement of the net. This requirement is met when the difference equations have the properties of consistency, convergence, and stability. A discussion of the necessary and sufficient conditions for these properties in systems of equations with constant coefficients can be found in Richtmyer (1957).

In general there is no unique procedure by which to derive the most appropriate difference equations for any given calculation. From a practical standpoint, however, the difference equations must be constructed so as to reflect as many properties of the differential equations as possible in the low orders of approximation. Thus the critical features of the system are realized with any net spacing – and not just in the limit as the net spacing approaches zero.

One such feature is energy conservation. Obviously in a nonlinear calculation, where the equations of transport (4) and energy balance (5) are used together, their difference forms must be consistent. Another highly desirable feature is accuracy of the differencing procedure, independent of the size of the net spacing relative to the mean free path.

In Chapter IV, we have seen that the form of the moment equations is such that the wave equation is obtained as $\sigma \rightarrow 0$, and the diffusion formulation results when σ becomes large. In general, the obvious difference procedures in the discrete ordinate representation do not have this property.¹⁰ However, we can insure the correct limiting forms for the discrete ordinate equations by requiring consistency with the difference equations of the moment representation.

B. An Implicit Difference Method

Pursuant to the above remarks we suggest the following method which combines transport and diffusion in a natural way. We further restrict our considerations to plane geometry.

¹⁰ For a review of such procedures refer to Wendroff (1961).

In the following discussion the intensity is denoted by

$$I^{\nu k}(r_j, \mu_\ell, t^n) = I_j^n(\ell, k),$$

although some of the indices may not be written out explicitly. The calculation requires two sets of intensities, one set defined on the zone boundaries, I_j^n , and one set defined at the zone centers, $I_{j+1/2}^n$. The temperatures and densities are zone-centered. At each time step all the quantities are given at t^n and t^{n-1} , and the calculation proceeds as follows:

1. The intensities and temperatures are predicted at t^{n+1} by linear extrapolation.
2. The boundary intensities at t^{n+1} are calculated from the relation

$$\frac{I_j^{n+1} - I_j^n}{c\Delta t} + \mu_\ell \frac{I_{j+1/2}^{n+1} + I_{j+1/2}^n - I_{j-1/2}^{n+1} - I_{j-1/2}^n}{(r_{j+1} - r_{j-1})} + \sigma_T \frac{1}{2} (I_j^{n+1} + I_j^n) = \sigma_a B(T_j^{n+1/2}) + \sigma_s S_j^{n+1/2}$$

where

$$T_j^{n+1/2} = \frac{1}{4} (T_{j+1/2}^{n+1} + T_{j+1/2}^n + T_{j-1/2}^{n+1} + T_{j-1/2}^n),$$

and

$$S_j^{n+1/2} = \sum_{\ell'} \frac{1}{2} [I_j^{n+1}(\ell') + I_j^n(\ell')] A_{\ell, K}(\mu_\ell, \mu_{\ell'}).$$

From the calculated intensities the boundary fluxes are obtained by means of the quadrature formula

$$F_j^{n+1/2} = 2\pi \sum_{\ell} A_{\ell} \mu_\ell \frac{1}{2} [I_j^{n+1}(\ell) + I_j^n(\ell)].$$

3. Knowledge of the boundary fluxes now permits the calculation of temperatures.
 - a. For each zone the $E^{n+1}(k)$, $k = 1, 2, \dots, K$, are calculated from (5a),

$$\frac{E_{j+1/2}^{n+1} - E_{j+1/2}^n}{\Delta t} + \frac{F_{j+1}^{n+1/2} - F_j^{n+1/2}}{r_{j+1} - r_j} + c\sigma_a \frac{1}{2} (E_{j+1/2}^{n+1} + E_{j+1/2}^n) = 4\pi\sigma_a B(T_{j+1/2}^*),$$

together with the Planck mean at the approximate temperature,

$$T_{j+1/2}^* = \frac{1}{2} (T_{j+1/2}^{n+1} + T_{j+1/2}^n):$$

$$\bar{\sigma}_p(T_{j+1/2}^*) = \frac{4\pi}{c} \sum_k A_k' \sigma_a^{\nu k} B^{\nu k}(T_{j+1/2}^*) / a(T_{j+1/2}^*)^4.$$

- b. The temperature equation is iterated to convergence using the Newton-Raphson method, while holding the Planck mean constant at the approximate value $\bar{\sigma}_p(T_{j+1/2}^*)$:

$$\rho \frac{(c_v T)_{j+1/2}^{n+1} - (c_v T)_{j+1/2}^n}{c \Delta t} = \sum_k A'_k \sigma_a \nu_k \frac{1}{2} \left[E_{j+1/2}^{n+1}(k) + E_{j+1/2}^n(k) \right] - \bar{\sigma}_p(T^*) a \left[\frac{1}{2} (T_{j+1/2}^{n+1} + T_{j+1/2}^n) \right]^4$$

- c. The procedure is then repeated from 3a using the improved temperatures until the whole process converges to within one part in 10^4 , usually within two or three iterations.

4. Knowledge of the temperatures and zone boundary intensities allows the zone-centered intensities to be calculated from the relation

$$\frac{I_{j+1/2}^{n+1} - I_{j+1/2}^n}{c \Delta t} + \mu_\ell \frac{I_{j+1}^{n+1} + I_{j+1}^n - I_j^{n+1} - I_j^n}{2(r_{j+1} - r_j)} + \sigma_T \frac{1}{2} (I_{j+1/2}^{n+1} + I_{j+1/2}^n) = \sigma_a B(T_{j+1/2}^{n+1/2}) + \sigma_s S_{j+1/2}^{n+1/2}$$

where

$$T_{j+1/2}^{n+1/2} = \frac{1}{2} (T_{j+1/2}^{n+1} + T_{j+1/2}^n)$$

and

$$S_{j+1/2}^{n+1/2} = \sum_{\ell'} \frac{1}{2} \left[I_j^{n+1}(\ell') + I_j^n(\ell') \right] A_{\ell'} \nu_k(\mu_\ell; \mu_{\ell'})$$

This relation is consistent with the difference form of (5a), thereby assuring the conservation of energy.

5. The whole process may be repeated from 1, but it is usually more economical to reduce the time step, Δt , if the calculation is not sufficiently accurate.

C. Discussion

The difference method described in the foregoing section is constructed so as to reproduce the limiting forms developed in Chapter IV. Thus when the cross section is large, the nonequilibrium diffusion equations are obtained with Crank-Nicholson differencing.¹¹ When the cross section goes to zero, the corresponding difference form¹² for the wave equation results.

In the following chapter we illustrate this method in actual numerical calculations. Although the stability of the method has not been rigorously analyzed, it is found experimentally to be subject to the restriction $c \Delta t < \Delta r$.

VI. SAMPLE CALCULATIONS

We consider the problem of the radiative heating of a semi-infinite slab of uniform density which extends from $r = 0$ to $r = R$. The material is characterized by an absorption cross section σ_a , a scattering cross section σ_s , and a constant specific heat c_v .

¹¹ See Richtmyer (1957), p. 93.

¹² See Richtmyer (1957), p. 169.

The radiation and material energy densities are initially zero. At $t = 0$ the slab is exposed to a uniform blackbody radiation field at temperature T_0 which fills the half-space $r < 0$. There are no radiation sources in the region $r > R$.

We seek the distribution of temperature and radiant energy in the slab as a function of time. The calculations were performed on an IBM 7094 using the difference method described in Chapter V, coded in FORTRAN. A typical execution requires 0.1 sec per cycle per frequency group.

A. Constant Cross Sections

We first restrict our attention to the simple case of constant cross sections. Figure 1 illustrates the distribution of temperature and radiant energy density for $\sigma_a = \lambda^{-1}$, $\sigma_s = 0$, and Fig. 2 shows the angular distribution at the boundary. Different treatments of the angular distribution are represented. It is clear that the double Gaussian division of the μ interval is superior to Newton-Cotes division for the same number of points. Figure 2 illustrates clearly the error which would result with an interpolating function that did not take the discontinuity into account.

In Figs. 3 and 4 we illustrate the method in two problems with absorption cross sections which differ by a factor of 10^4 . The Monte Carlo method of Campbell and Nelson (1964) and the diffusion similarity solution of Barfield *et al.* (1954) are used for comparison. As expected, the method of Chapter V exhibits the correct behavior for both large and small cross sections.

An interesting feature of the method is that the scattering integral is not iterated but evaluated in terms of the extrapolated intensities. Since the predicted and corrected intensities do not agree precisely, energy will not be strictly conserved. However, Fig. 5 shows good agreement between this procedure and the Monte Carlo method in a scattering calculation, with overall energy conservation better than one part in 10^4 .

B. Frequency-Dependent Cross Section

In Fig. 6 we illustrate the temperature and radiation energy density for a simple frequency-dependent cross section

$$\sigma_a^\nu = \sigma_0 \left(\frac{h\nu}{kT_0} \right)^{-3} \left(1 - e^{-h\nu/kT} \right), \quad \sigma_s = 0.$$

The angular distribution was represented by 4 discrete ordinates with double Gaussian divisions and the frequency distribution by 20 groups between $0.1 T_0$ and $10.1 T_0$. The running time for the calculation averaged 3 sec/cycle.

Good agreement with the Monte Carlo method is evident despite the annoying statistical fluctuations – the principal defect of Monte Carlo calculations. The Monte Carlo method required 8 sec/cycle but used a time step double that of the difference method.

Fig. 1. Distribution of temperature and radiation energy density in a slab with constant cross sections ($\sigma_a = \lambda^{-1}$, $\sigma_s = 0$) and constant specific heat. The calculation was performed with $c\Delta t = 0.25\lambda$, $\Delta x = 0.5\lambda$, and both Newton-Cotes and double Gaussian differencing of the angular distribution.

Fig. 2. Angular distribution of radiation at the boundary for the problem illustrated in Fig. 1. Note the discontinuity between incoming and outgoing radiation.

Fig. 3. Comparison with diffusion for very large cross section. The difference calculation was performed with $c\Delta t = 0.05, \Delta x = 0.1$.

Fig. 4. Comparison with Monte Carlo for very small cross section. The difference calculation was performed with $c\Delta t = 0.5, \Delta x = 1.0$.

Fig. 5. The effect of Thompson scattering on energy penetration for constant cross sections. The difference calculation was performed with $c\Delta t = 0.25, \Delta x = 0.5\lambda$, and the Monte Carlo calculation with $c\Delta t = 0.5\lambda, \Delta x = 0.5\lambda$.

Fig. 6. Frequency dependent calculation with $c\Delta t = 0.5\lambda_0$, $\Delta x = 2.0\lambda_0$, and 20 frequency groups with $\Delta h\nu = 0.5 kT_0$. The Monte Carlo calculation was performed with $c\Delta t = 1.0\lambda_0$, $\Delta x = 2.0\lambda_0$.

VII. SUMMARY AND CONCLUSIONS

The last several years have brought an ever growing need for the development of frequency-dependent radiation transport calculations. Not only is the nonlinear transport problem of interest from the standpoint of applications, but it presents a mathematical problem of considerable challenge. The analytical treatment of problems judged quite elementary from a practical standpoint requires some of the most sophisticated techniques of modern analysis.¹³ At the present time, therefore, numerical methods are apparently the only way to get results in problems of practical interest.

In numerical methods the nonlinear character of the problem presents little difficulty. Accuracy of the method in the presence of the large variation and considerable complexity of the cross sections is the critical feature of the problem. The Monte Carlo method is well adapted to deal with complicated cross sections and geometries but usually requires an enormous amount of computing time to reduce statistical fluctuations to reasonable limits. It is therefore necessary to consider other methods, free from statistical effects.

In this report we have considered one approach to the problem presented by the large variation of cross section, although we have avoided the difficulties posed by the complex structure of lines and absorption edges.

¹³ See Wing (1962), Chapter 8.

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* AEC and UCRL documents can be obtained from the Clearinghouse for Federal Scientific and Technical Information, National Bureau of Standards, U. S. Dept. of Commerce, Springfield, Va.

APPENDIX: HALF-RANGE MOMENT EQUATIONS

In order to develop the half-range moment equations we change the notation slightly so that

$$M_\ell(r, t) = 2\pi \int_0^1 I(\mu) \mu^\ell d\mu,$$

$$N_\ell(r, t) = 2\pi \int_{-1}^0 I(\mu) \mu^\ell d\mu,$$

and

$$L_\ell(r, t) = M_\ell + N_\ell.$$

We multiply the transport equation (4) by $2\pi\mu^\ell d\mu$ and integrate over the intervals $[0, 1]$ and $[-1, 0]$ to obtain

$$\begin{aligned} \frac{1}{c} \frac{\partial M_\ell}{\partial t} + \frac{\partial M_{\ell+1}}{\partial r} + \frac{\alpha}{2r} \left[(\ell + 2)M_{\ell+1} - \ell M_{\ell-1} - 2\pi I(0^+) \delta_\ell \right] + \sigma_T M_\ell \\ = -\frac{2\pi}{\ell + 1} \sigma_a B(T) + 2\pi \sigma_s \int_0^1 S(\mu) \mu^\ell d\mu, \end{aligned}$$

and

$$\begin{aligned} \frac{1}{c} \frac{\partial N_\ell}{\partial t} + \frac{\partial N_{\ell+1}}{\partial r} + \frac{\alpha}{2r} \left[(\ell + 2)N_{\ell+1} - \ell N_\ell + 2\pi I(0^-) \delta_\ell \right] + \sigma_T N_\ell \\ = (-1)^\ell \frac{2\pi}{\ell + 1} \sigma_a B(T) + 2\pi \sigma_s \int_{-1}^0 S(\mu) \mu^\ell d\mu, \end{aligned}$$

where $\delta_\ell = 1$ for $\ell = 0$ and $\delta_\ell = 0$ for $\ell = 1, 2, \dots$

For Thompson scattering we have

$$2\pi \int_0^1 S\mu^\ell d\mu = \frac{0.375}{(\ell + 1)(\ell + 3)} [(\ell + 4)L_0 + (\ell)L_2]$$

and

$$2\pi \int_{-1}^0 S\mu^\ell d\mu = (-1)^\ell \frac{0.375}{(\ell + 1)(\ell + 3)} [(\ell + 4)L_0 + (\ell)L_2].$$

The sequence of moment equations is truncated after n terms by the terminal relations

$$\begin{aligned} \sum_{\ell=0}^n C_\ell N_\ell &= 0, \\ \sum_{\ell=0}^n (-1)^\ell C_\ell M_\ell &= 0, \end{aligned}$$

where the polynomials orthogonal on the half-range are

$$R_n(\mu) \equiv P_n(2\mu + 1) = \sum_{\ell=0}^n C_\ell \mu^\ell, \quad -1 \leq \mu \leq 0,$$

$$Q_n(\mu) \equiv P_n(2\mu - 1) = \sum_{\ell=0}^n (-1)^\ell C_\ell \mu^\ell, \quad 0 \leq \mu \leq 1.$$

For reference the first few polynomials are given in Table I.

Table I. Legendre polynomials for $\ell = 0$ through 4.

ℓ	$P_\ell(\mu)$	$Q_\ell(\mu)$	μ_ℓ^+
0	1	1	None
1	μ	$2\mu - 1$	$1/2$
2	$\frac{1}{2}(3\mu^2 - 1)$	$6\mu^2 - 6\mu + 1$	$\frac{1}{2}(1 \pm 1/\sqrt{3})$
3	$\frac{1}{2}(5\mu^3 - 3\mu)$	$20\mu^3 - 30\mu^2 + 12\mu - 1$	$\frac{1}{2}(1 \pm \sqrt{3/5}), \frac{1}{2}$
4	$\frac{1}{8}(35\mu^4 - 30\mu^2 + 3)$	$70\mu^4 - 140\mu^3 + 90\mu^2 - 20\mu + 1$	$\frac{1}{2}(1 \pm \sqrt{3/7}, \sqrt{1 \pm \sqrt{8/15}})$

$$R_\ell(\mu) = (-1)^\ell Q_\ell(-\mu), \quad \mu_\ell^- = -\mu_\ell^+,$$

$$\int_0^1 Q_\ell(\mu) Q_{\ell'}(\mu) d\mu = \begin{cases} 0, & \ell \neq \ell' \\ \frac{1}{2\ell+1}, & \ell = \ell' \end{cases} = \int_{-1}^0 R_\ell(\mu) R_{\ell'}(\mu) d\mu,$$

$$(\ell+1)Q_{\ell+1} = (2\ell+1)(2\mu-1)Q_\ell - \ell Q_{\ell-1}.$$

In order to evaluate the term $I(0)$ which appears in the zeroth moment equation, we must refer to the equivalence between the discrete ordinate and Legendre polynomial representations. We have the relations

$$M_k = 2\pi \sum_{\ell=0}^n A_\ell I_\ell^+(\mu_\ell^+)^k,$$

$$N_k = 2\pi \sum_{\ell=0}^n A_\ell I_\ell^-(\mu_\ell^-)^k,$$

where μ_ℓ^+ and μ_ℓ^- are respectively the zeros of $Q_n(\mu)$ and $R_n(\mu)$. From these relations we may solve for the I_ℓ^+ in terms of the M_k and the I_ℓ^- in terms of the N_k . We then use

$$I(\mu) = \sum_{\ell=1}^n L_\ell(\mu) I_\ell^+, \quad \mu > 0,$$

$$I(\mu) = \sum_{\ell=1}^n L_\ell(\mu) I_\ell^-, \quad \mu < 0,$$

to obtain $I(0^+)$ and $I(0^-)$. The Lagrangian coefficients, $L_\ell(\mu)$, are given in Chapter III, Sec. C.

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