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NUCLEAR EXPLOSION INTERACTION STUDIES

Volume I

Methods for Analysis of Radiative Transfer

K. D. Pyatt, Jr., et al.

**General Atomic Division
General Dynamics Corporation
Special Nuclear Effects Laboratory
San Diego, California
Contract AF 29(601)-7035**

TECHNICAL REPORT NO. AFWL-TR-66-108, Vol. I

May 1967

**AIR FORCE WEAPONS LABORATORY
Research and Technology Division
Air Force Systems Command
Kirtland Air Force Base
New Mexico**

Research and Technology Division
AIR FORCE WEAPONS LABORATORY
Air Force Systems Command
Kirtland Air Force Base
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FOREWORD

This report was prepared by General Atomic Division, General Dynamics Corporation, San Diego, California, under Contract AF29(601)-7035. The research was funded by DASA under Program Element 6.16.46.01D, Project 5710, Subtask 07.002, and by ARPA Order 313, Program Element 6.25.03.01.R.

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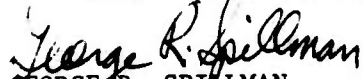
This final report on Nuclear Explosion Interaction Studies is being published in four volumes. The volume titles are as follows: Volume I, Methods for Analysis of Radiative Transfer; Volume II, Methods for Analysis of Thermal Phenomena; Volume III, Miscellaneous Code Development; and Volume IV, Phenomenology Studies (classified SECRET/RESTRICTED DATA).

The first three volumes are devoted, respectively, to theoretical studies and computer code development in radiative transfer, thermal phenomena, and miscellaneous efforts related to various other aspects of the work. The fourth volume, which is classified, contains the results of applications of these techniques, and of those previously developed, to the study of fireball growth and the interaction of laser radiation with materials.

The NEIS program is long-range, and most of the projects described in this report are in an incomplete state of development. This is due in part to the nature of the existing computer programs themselves, which continue in a state of development as long as they are in use, and in part to the time scale involved in bringing new programs to a state of capability for solving real problems.

General Atomic staff personnel contributing to the research include J.H. Alexander, C.R. Dismukes, R. Durstenfeld, R.S. Engelmores, B.E. Freeman, W.B. Lindley, J.T. Palmer, K.D. Pyatt, L.L. Reed, L.M. Schalit, J.R. Triplett, and numerous others. The cooperation of Col R.H. Pennington, Maj G.R. Spillman, Lt B.S. Chambers, III, Lt N.D. Morgan, Lt R.A. Howerton, Dr. P.V. Avizonis, and Mr. D.W. Lane of the Air Force Weapons Laboratory is gratefully acknowledged.

This report has been reviewed and is approved.


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ABSTRACT

The non-equilibrium diffusion approximation to the radiative-transfer equation is developed. The first two moments of the radiative transfer equation, including Thomson scattering and pure absorption, are formed, and the equations are closed by a relation between the radiation energy and pressure. Applications of SPUTTER non-equilibrium diffusion subroutines to several simple radiative-transfer problems are described and compared with results from other numerical radiative-transfer codes. Subroutines are also described which calculate the effect of Thomson scattering in TAMALE. The method of moments, the method of discrete ordinates or characteristics, and the Monte Carlo method are described with special reference to the calculation of radiative transport in two dimensions. Their relative merits are discussed, and considerations bearing on the choice of which to use in various applications are given. The non-equilibrium diffusion approximation, which is the variant of the moments method used in DRADTN and ERADTN, has been extended to axially symmetric configurations of two dimensions in a new program, TDRAD. The method of characteristics has been programmed for the same geometry as that treated by TDRAD. The new code, TRAN2, extends TDRAD to situations in which the radiation is too anisotropic to be described by only two moments. The problem of averaging absorption coefficients and scattering cross sections is a basic one in any calculation of radiative transport. A proposed solution is formulated, and transmission functions are derived for the case where opacities may be considered piecewise constant in space and frequency.

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CONTENTS

I. NON-EQUILIBRIUM DIFFUSION METHODS FOR SPUTTER . . .	1
1.1. Introduction	1
1.2. Differential Equations of Non-equilibrium Diffusion	3
1.3. Difference Equations and Boundary Conditions	7
1.4. How to Use Non-equilibrium Diffusion Subroutines	24
1.5. Test Problems	34
1.6. Appendix: Stability Analysis	41
1.7. Appendix: Listing of ERADTN and DRADTN	49
References	72
II. SCATTERING METHODS FOR TAMALE	73
2.1. Introduction	73
2.2. Analysis of the Transport Equation with Compton Scattering	73
2.3. Numerical Solution of the Transport Equation with Thomson Scattering	77
2.4. The TAMALE Code	79
References	81
III. TWO-DIMENSIONAL RADIATION TRANSPORT TECHNIQUES: A SURVEY OF METHODS	82
3.1. Introduction	82
3.2. The Method of Moments	84
3.3. Discrete Ordinates	87
3.4. The Monte Carlo Method	95
3.5. Conclusions	96
References	98
IV. NON-EQUILIBRIUM DIFFUSION METHODS FOR HECTIC	99
4.1. Introduction	99
4.2. The Finite Difference Approximation	100
4.3. Boundary Conditions	102
4.4. Methods for Solving the System	105
4.5. Procedure for Solving the System	105
4.6. The Subprogram TDRAD	107
4.7. Outline of TDRAD	113
4.8. Review of the Code Development	113
4.9. Appendix: Listing of TDRAD	117

CONTENTS (Continued)

V.	THE METHOD OF CHARACTERISTICS IN CYLINDRICAL GEOMETRY	126
5.1.	Introduction.....	126
5.2.	The Local Coordinate System.....	126
5.3.	Distribution of Rays	127
5.4.	Calculation of Intensities.....	131
5.5.	Thick Zones	132
VI.	FREQUENCY-AVERAGED TRANSMISSION FUNCTIONS	134
6.1.	Introduction.....	134
6.2.	Frequency Averaging for the Transport Equation.....	137
6.3.	Parametric Representation of Transmission Functions ...	143
	References.....	146
	Distribution	147

Figures

1.	Slab Penetration Fluxes	36
2.	Slab Penetration Temperature Profiles	37
3.	Spherical Emission Test Problem, $\Delta t = 0.03$, $\kappa_R = \kappa_P = 0.2$	39
4.	Spherical Emission Test Problem, $\Delta t = 0.03$, $\kappa_R = \kappa_P = 0.1$	39
5.	Spherical Emission Test Problem, $\Delta t = 0.03$, $\kappa_R = \kappa_P = 0.5$	40
6.	Flux Versus Time for Spherical Emission Test Problem, $t = 0.03$	40
7.	Typical Distribution of Directions.....	88
8.	Typical Short Characteristic	92
9.	Hydrodynamic Mesh	100
10.	Typical Cell of Mesh	100
11.	Configuration of Test Problem	115
12.	Coordinate Vectors	127
13.	Components of Ω	129
14.	Long Characteristic	129
15.	Coordinates μ and λ	129

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SECTION I

NONEQUILIBRIUM DIFFUSION METHODS FOR SPUTTER

1.1. INTRODUCTION

Solutions of the radiation transport equation are required in a substantial number of problems involving the transport of energy in high-temperature gases. In this report, numerical solutions to some sample problems are obtained by a method known as the non-equilibrium diffusion approximation. Comparison with numerical solutions gives an indication of the usefulness of the method.

An explicit formulation of the non-equilibrium diffusion equations for slab geometry and pure absorption has been tested (Ref. 1)* and found to constitute a useful approximation to slab penetration problems in the grey atmosphere approximation. Additional tests of the time independent diffusion equations have been made (Ref. 2) by comparison with transport solutions of Milne problems. Independently, the differential non-equilibrium diffusion equations have been derived for the case of radiation interaction through Compton scattering (Ref. 3). The possibility of using the Rosseland and Planck mean opacities, of performing multigroup calculations, and of formulating the difference equations in partially implicit and fully implicit (unconditionally stable) forms has also been noted (Ref. 4). Consequently, the method can be expected to provide generally applicable approximate equations that can be solved economically for one-dimensional geometries and ultimately two-dimensional geometries.

In this report, derivation of the differential equations is presented (Section 1.2), and then these equations are formulated in difference form (Section 1.3) for the one-dimensional geometries (slabs, cylinders, spheres). The code has been incorporated as a subroutine into the SPUTTER code, a one-dimensional, radiation transport — hydrodynamics

*References appear at the end of each section.

code applicable to many high-energy flow phenomena. The subroutine can perform either grey or multifrequency group problems and contains options for determining whether partially or fully implicit equations are solved. The nonlinear coefficients of the equations may be formed more accurately by exercising the option to iterate the equations to time-center the coefficients. At the outside boundaries of the mesh, the following options can be selected: (1) zero net flux (reflection), (2) zero backward current (vacuum), and (3) prescribed backward current (frequently the blackbody boundary condition). Two versions of the code are available as separate subroutines. The DRADTN subroutine (see Section 1.7 for the FORTRAN listing) includes the effects of radiation retardation (energy stored in the radiation field and the propagation of light waves), and is particularly applicable to problems involving temperatures in the kev range, where temperature waves propagate at near light speed. For problems involving temperatures in the ev range, in which changes are slow compared with the light speed, a more economical and accurate code is the ERADTN version (see Section 1.7 for the FORTRAN listing), which omits the retardation terms.

In Section 1.4, features of the codes of special interest to the user are discussed. A glossary of terms appearing in the code is also presented in that section, and particular attention is given to the quantities which must be supplied to control the code. Values for the control quantities are recommended, and the effects of deviations from them are discussed.

In the slab and spherical geometry, radiation transport subroutines for SPATTER are available (Ref. 5). Two of these subroutines, called PRADTN (for plane radiation) and SRADTN (for spherical radiation), have been used to perform a series of test problems (see Section 1.5) having relatively simple initial conditions and material properties. Comparison with the solution of the corresponding problem using DRADTN and ERADTN indicates the error to be expected when similar problems are calculated.

An attempt is made to isolate the effects of the form of the difference equations from the different treatments of the frequency dependence.

1.2. DIFFERENTIAL EQUATIONS OF NON-EQUILIBRIUM DIFFUSION

The equations of non-equilibrium diffusion are the first two moment equations of the radiation transport equation. In this section, these equations are derived independently of the coordinate system. They are thus applicable to two- and three-dimensional radiation flow problems, but will be specialized to the one-dimensional geometries.

The point of departure is the radiation transport equation for the intensity I at position $\vec{r}$ at time t in the direction specified by the unit vector $\vec{\Omega}$. Interaction of the radiation with the material is characterized by the coefficient for pure absorption μ_a and the scattering coefficient μ_s . When the source function is approximated by the local thermodynamic equilibrium assumption in terms of the Planck function B , and scattering is given by the Thomson limit of the Compton cross section, the transport equation is as follows:

$$\frac{1}{c} \frac{\partial I}{\partial t} + \vec{\Omega} \cdot \nabla I = \mu_a (B - I) - \mu_s I + \frac{3\mu_s}{16\pi} \int d\Omega' \left[1 + (\vec{\Omega} \cdot \vec{\Omega}')^2 \right] I' \quad (1)$$

where I' is the intensity in the direction $\vec{\Omega}'$. The frequency dependence has been suppressed, since in the Thomson limit in which scattering occurs without frequency shift, Eq. (1) applies to a single frequency. The polarization of the photons has also been neglected by averaging the scattering integral over polarization in the supposedly unpolarized incident beam.

On the boundaries of the system, the transport equation must be supplemented with a specification of the intensity of all rays passing through the boundary from outside to inside. That is, $I(\vec{\Omega}) = I_0$ if $\vec{\Omega} \cdot \vec{N} < 0$, where $\vec{N}$ is a vector normal to the surface directed outward.

Moments of the radiation intensity are obtained by integrating powers of $\vec{\Omega}$ over the entire solid angle. The radiation energy scalar E , the

approximation employed above depends on temperature only through the density of free electrons,

$$\mu_s = \frac{8\pi}{3} r_o^2 N_e \text{ (cm}^{-1}\text{)}$$

where r_o is the classical electron radius ($= 2.8 \times 10^{-13}$ cm) and N_e is the free electron density (cm^{-3}). In practice, μ_s is negligible compared with μ_a if temperatures are not sufficiently large to produce substantially complete ionization. Consequently, the assumption of the temperature independence of μ_s is an excellent approximation. Changes in material temperature are assumed to take place under the combined effects of radiation absorption or emission, hydrodynamic motions of the material, and energetic sources within the material.

1.3. DIFFERENCE EQUATIONS AND BOUNDARY CONDITIONS

By specializing the equations given in Section 1.2 to one spatial dimension, the one-dimensional non-equilibrium diffusion equations are obtained:

$$\begin{aligned} \frac{\partial E}{\partial t} + \frac{\partial}{\partial r} (\alpha r^{\alpha-1} F) &= c \mu_a (4\pi B - E) \\ \frac{1}{c} \frac{\partial F}{\partial t} + \frac{c}{3} \frac{\partial E}{\partial r} &= -\frac{F}{\lambda} \end{aligned} \tag{10}$$

where the geometry coefficient α takes the value 1, 2, or 3, corresponding to slab, cylinder, or sphere, respectively.

1.3.1. Spatial Difference Equations

These equations are to be replaced by approximating difference equations in a way dictated by accuracy, stability, and ease of computing. The quantities in Eq. (10) are associated with zonal boundaries or interiors as suggested by an integration of the first equation over the zone. The resulting equation describing the conservation of energy is given by

$$\frac{\partial E_{i+1/2}}{\partial t} + \frac{1}{r_{i+1}^\alpha - r_i^\alpha} (\tilde{F}_{i+1} - \tilde{F}_i) = c (\mu'_a)_{i+1/2} (4\pi B_{i+1/2} - E_{i+1/2}) \quad (11)$$

where $\tilde{F}_i = \alpha r_i^{\alpha-1} F_i$, corresponds to the flux at the i^{th} zone boundary integrated over the surface area. Difference equation (11) is formulated in a conservative fashion; i. e., radiation flux out of one zone enters the neighboring zone undiminished. The quantities with half-integral subscripts, $E_{i+1/2}$ and $B_{i+1/2}$, are averages over the zone and are weighted by the zone volume. The second equation for the interface flux is obtained by approximating the derivative by a centered difference

$$\frac{1}{c} \frac{\partial \tilde{F}_i}{\partial t} + \frac{2c}{3} \alpha r_i^{\alpha-1} \frac{(\tilde{E}_{i+1/2} - \tilde{E}_{i-1/2})}{r_{i+1} - r_{i-1}} = - \frac{\tilde{F}_i}{\lambda_i} \quad (12)$$

The material internal energy E_m (erg/g) is taken to be a zone-centered quantity to retain the centering of the third equation,

$$\frac{d(E_m)_{i+1/2}}{dt} = - \frac{c}{\rho} \int_0^\infty d\nu (\mu'_a)_{i+1/2} (4\pi B_{i+1/2} - E_{i+1/2}) - P \frac{d\tau}{dt} + q \quad (13)$$

This equation contains the pressure P , the specific volume τ , the density ρ , and the source q (erg/g sec).

Since the right-hand terms of Eqs. (11) and (13) represent the coupling between radiation and material energies, it is important, in order to ensure energy conservation, that the identical form be used in each equation. Through the equation of state, the material temperature of the zone is related to the internal energy. In turn, the Planck function B and absorption coefficient μ'_a (being zone quantities) are evaluated as functions of the zone temperature. The mean free path λ (an interface quantity) must be obtained by interpolation between the adjacent zonal quantities.

1.3.2. Temporal Difference Equations

The form of the difference equations in time has far-reaching effects on the stability and ease of numerical solution of the system, as well as on its accuracy. Related to the accuracy of solution are considerations of smoothness of the solution in time (avoidance of bounded but slightly damped oscillations) and positivity of the radiation energy. In view of the importance of the time dependence, several alternatives have been tested, and options for some of them are provided in the subroutines.

One of the most important choices is governed by the physical regime in which the problem lies. The equations are substantially simplified and their centering is changed when the time dependent terms of Eqs. (11) and (12) can be neglected, which corresponds to omitting the $\partial I / \partial t$ term of the transport equation. The equations are sufficiently different that separate subroutines have been written. The ERADTN subroutine (see Section 1.7) contains the code without retardation, in a form applicable to problems in which the radiation energy is considerably smaller than the material energy and in which the light propagation is unimportant. The DRADTN subroutine (see Section 1.7) includes the retardation effects.

The equations for the radiation energy E in both of these codes have the form of linear equations, in each of which three neighboring zones are represented. These simultaneous equations can be solved by a well-known algorithm (Ref. 7) with very little labor. The stability of the resulting equations depends, however, on whether Eq. (13), the material energy equation, has been solved simultaneously with the two equations for the radiation quantities. In turn, the feasibility of obtaining a fully implicit system of equations depends on whether the grey approximation is made or several frequency groups are evaluated. In the latter case, partially implicit equations are obtained with an associated stability restriction (see Section 1.7). The fully implicit equations are presumed to be unconditionally stable.

The distinction between these two cases will be made more precise when the equations are formulated in the next section. These equations are nonlinear through the dependence of absorption coefficients and source functions on temperature.

Since the method of solution outlined above requires a linearization of the equations, the time dependence of the coefficients is not taken into account within the time interval of one time cycle. To improve the accuracy, an iteration may be performed in which the estimate of the temperature change in the first step of the calculation is used to re-evaluate the coefficients for a second calculational step. Further iterations of this cycle are not desirable since second order accuracy is obtained in the first iteration (Ref. 8). In Section 1.3.3 the equations discussed above are presented in detail. The ERADTN equations are given first in both the partially implicit and fully implicit forms. The steps required for iteration are also discussed. The same format is then followed for the DRADTN equations.

1.3.3. Difference Equations for ERADTN (No Retardation)

Without retardation terms, Eqs. (11) and (12) can be written at a particular time instant. Denoting the index of the time by superscript n , where $t^n = \sum \Delta t^n$, the first two equations are centered in time at $t^{n+1/2}$, the midpoint of the interval, $\Delta t^n = t^{n+1} - t^n$:

$$P_i (\tilde{F}_{i+1}^{n+1/2} - \tilde{F}_i^{n+1/2}) = c \mu_i (b_j \varphi_i - E_i^{n+1/2})$$

$$R_i (E_i^{n+1/2} - E_{i-1}^{n+1/2}) - \frac{\tilde{F}_i^{n+1/2}}{4\lambda_i}$$
(14)

where $P_i = 1/(\tau_{i+1}^\alpha - \tau_i^\alpha)$, $\varphi_i = a \theta_i^4$, and $R_i = c \alpha r_i^{\alpha-1}/6(r_{i+1} - r_{i-1})$. In the above equations spatial indices have all been made integral by subtracting 1/2 from the half-integral indices. This is the same convention as is

practiced in the SPUTTER code. The source function and coefficients depend on temperature and, for accuracy, should be evaluated as a function of $\theta_i^{n+1/2}$, the temperature at $t^{n+1/2}$.

The frequency dependence has been suppressed except in the source term. Equations (14) result from integration over frequency groups. As is discussed more fully in Section 1.4, absorption coefficients are averaged over the frequency interval, and the source function is

$$\int_{\nu_j}^{\nu_{j+1}} 4\pi B d\nu = b_j \varphi_i$$

where b_j is the normalized partial Planck function.

1.3.4. Partially Implicit Equations for ERADTN

In the partially implicit solution, the two equations (14) are solved for E and F with the source function and coefficients considered as known quantities. Since in this approximation the equations are linear with non-zero values for three neighboring terms, the equations for E become (suppressing time indices):

$$A_i E_{i-1} + B_i E_i + C_i E_{i+1} + D_i = 0 \quad (15)$$

where

$$\begin{aligned} A_i &= -4\lambda_i R_i P_i \\ C_i &= -4\lambda_{i+1} R_{i+1} P_i \\ B_i &= c\mu_i - A_i - C_i \\ D_i &= -c\mu_i b_j \varphi_i \end{aligned} \quad (16)$$

The energy equation (13) can be solved for the temperature change using the equation of state

$$\frac{d\theta_i}{dt} = \left(\frac{dE_m}{dt} - \frac{\partial E_m}{\partial \tau} \frac{d\tau}{dt} \right) / C_v \quad (17)$$

where the specific heat C_v (ergs/(g ev)) has been introduced, to obtain

$$\theta_i^{n+1} = \theta_i^n + \frac{\Delta t^n}{(C_v)_i} \left[q_i - \left(P_i + \frac{\partial E_m}{\partial \tau} \right) \frac{d\tau}{dt} - \frac{c}{\rho} \sum_j \mu_{ij} (b_j \varphi_i - E_{ij}^{n+1/2}) \right] \quad (18)$$

In Eq. (18) the frequency dependence of the source function is denoted by the index j , which stands for a partitioning of the spectrum into frequency groups.

The order of the solution of these equations is as follows: First, Eq. (16) for the coefficients is evaluated as a function of θ_i^n ; second, Eq. (15) is solved for $E_{ij}^{n+1/2}$ for all frequency groups (see Section 1.7); third, Eq. (18) is used to find θ_i^{n+1} . In the event that rapid changes of temperature occur or the coefficients depend strongly on temperature, an iteration can be performed. The centered temperature is estimated to be $\theta^{n+1/2} = (\theta^n + \theta^{n+1})/2$, which is used to re-evaluate Eq. (16). The second and third steps of the calculation are repeated as above. The iteration is terminated after the second pass.

The partially implicit equations can be employed for the grey atmosphere (one frequency group) approximation but are generally inferior to the method discussed below. For the multigroup approximation, however, they are required.

1.3.5. Fully Implicit Equations for ERADTN

For a single frequency group ($b_j = 1$), it is possible to solve simultaneously for the temperature from Eq. (18) and the radiation energy. This is desirable because the stability condition required by the partially implicit equations can thereby be relaxed. First, it is necessary to

linearize Eq. (18). Since $\theta_i^4 \equiv \varphi_i$ appears in Eq. (14), it is also chosen for the linearization variable of Eq. (18):

$$\varphi_i^{n+1} = \varphi_i^n + \frac{4a\theta_i^3 \Delta t^n}{(C_v)_i} \left[q_i - \left(P_i + \frac{\partial E_m}{\partial \tau} \right) \frac{d\tau}{dt} - \frac{c\mu_i}{2\rho} (\varphi_i^{n+1} + \varphi_i^n - 2E_i^{n+1/2}) \right] \quad (19)$$

Second, the first equation of Eqs. (14) is rewritten to maintain the parallelism between the energy exchange terms and to introduce φ_i^{n+1} :

$$P_i (\tilde{F}_{i+1}^{n+1/2} - \tilde{F}_i^{n+1/2}) = \frac{c\mu_i}{2} (\varphi_i^{n+1} + \varphi_i^n - 2E_i^{n+1/2}) \quad (20)$$

By substituting for $\tilde{F}^{n+1/2}$ and φ^{n+1} , an equation of the form of Eq. (15) is obtained in which

$$A_i = -4\lambda_i R_i P_i, \quad C_i = -4\lambda_{i+1} R_{i+1} P_i \quad (21)$$

$$B_i = A_i - C_i + \frac{1}{\frac{1}{c\mu_i} + \frac{2a\theta_i^3 \Delta t^n}{\rho(C_v)_i}}$$

$$D_i = \frac{\left[\left(P_i + \frac{\partial E_m}{\partial \tau} \right) \rho \frac{d\tau}{dt} - \rho q_i \right] \frac{2a\theta_i^3 \Delta t^n}{\rho(C_v)_i} - \varphi_i^n}{\frac{1}{c\mu_i} + \frac{2a\theta_i^3 \Delta t^n}{\rho(C_v)_i}}$$

Solution of the fully implicit equations requires evaluation of the coefficients as functions of θ^n in Eq. (21) and the radiation energies in Eq. (15). The temperature is obtained last (Eq. (19)) and can be used for improving the accuracy of solution by iteration. An estimate of the centered temperature $\theta^{n+1/2} = (\theta^n + \theta^{n+1})/2$ is used to evaluate the coefficients a second time; then a second evaluation of the radiation energies is performed. Since the time dependence of the source term is taken more fully into account in the fully implicit equations than in the partially implicit ones,

the former should be more accurate. Hence, for grey problems there appear to be no reasons (aside from code intercomparisons) for performing partially implicit calculations.

1.3.6. Difference Equations for DRADTN (Retardation Included)

The spatial dependence of the DRADTN equations remains the same as for the ERADTN equations, i. e., as given by Eqs. (11) and (12). However, retention of the time derivative terms in the moment equations imposes additional requirements on the difference equations. First, the possibility of instabilities associated with the streaming of radiation and with the exchange of radiation energy and material energy requires care in formulating the difference equations. Even stable difference forms may be undesirable due to small damping of oscillations. Second, the occurrence of $\partial E / \partial t$ and $\partial F / \partial t$ in Eq. (10) suggests that, in order to center the equations at $t^{n+1/2}$, quantities at $t^n (E^n, F^n)$ be introduced. With them, first differences in time centered at $t^{n+1/2}$ can be formed. Third, the consideration of the conservation of energy must now take account of the radiation energy. As is the case for the ERADTN equations, it is highly desirable that a difference analogue of total energy be conserved exactly by the DRADTN equations.

With centered first differences in time for the first derivatives introduced in Eqs. (11) and (12), the DRADTN equations corresponding to Eq. (14) are given by

$$\frac{E_i^{n+1} - E_i^n}{\Delta t^n} + \frac{P_i}{2} (\tilde{F}_{i+1}^{n+1} - \tilde{F}_i^{n+1} + \tilde{F}_{i+1}^n - \tilde{F}_i^n) = \frac{c\mu_i}{2} (2b_j \phi_i - E_i^{n+1} - E_i^n) \quad (22)$$

$$\frac{\tilde{F}_i^{n+1} - \tilde{F}_i^n}{c\Delta t^n} + 2R_i (E_i^{n+1} - E_{i-1}^{n+1} + E_i^n - E_{i-1}^n) = - \frac{\tilde{F}_i^{n+1} + \tilde{F}_i^n}{2\lambda_i}$$

These equations employ the definitions following Eq. (14). Equations (22) have the following properties: (1) they are linear in E and F for case in

solution, (2) they are centered at $t^{n+1/2}$ for accuracy, (3) they conserve energy in the sense discussed above, and (4) they are expected to be stable against oscillations of the radiation field.

These equations, which are further analyzed below, were the first equations to be coded. As noted in Section 1.6, their solutions are subject to oscillations which, in some cases, are very slightly damped. The equations currently in use are discussed later in this section.

1.3.7. Partially Implicit Equations for DRADTN

For multifrequency problems and as an option for grey problems, the partially implicit form of the equations is solved. In these equations, the source function and the coefficients are evaluated from the available temperatures, θ_i^n . When solved for the unknown quantities E_i^{n+1} , Eq. (22) again have the form of Eq. (15), in which the coefficients are

$$A_i = -Q_i R_i P_i$$

$$C_i = -Q_{i+1} R_{i+1} P_i$$

$$B_i = \frac{1}{\Delta t^n} - A_i - C_i + \frac{c\mu_i}{2} \quad (23)$$

$$D_i = \left(-\frac{1}{\Delta t^n} + \frac{c\mu_i}{2} \right) E_i^n + A_i (E_{i-1}^n - E_i^n) + C_i (E_{i+1}^n - E_i^n) \\ + \frac{P_i}{c\Delta t^n} (Q_{i+1} \tilde{F}_{i+1}^n - Q_i \tilde{F}_i^n) - c\mu_i b_j \phi_i$$

where

$$Q_i = \frac{1}{\frac{1}{c\Delta t^n} + \frac{1}{2\lambda_i}}$$

The partially implicit formulation makes use of E_i^{n+1} obtained above in an energy equation similar to Eq. (18). By using Eq. (17), but paralleling the formulation of the radiation-material exchange term of Eq. (22), the equation for the new temperature becomes

$$\theta_i^{n+1} = \theta_i^n + \frac{\Delta t^n}{(C_v)_i} \left[q_i - \left(P_i + \frac{\partial E_m}{\partial \tau} \right) \frac{d\tau}{dt} - \frac{c}{2\rho} \sum_j \mu_{ij} (2b_j \varphi_i - E_{ij}^n - E_{ij}^{n+1}) \right] \quad (24)$$

As in the case of the ERADTN equations, an iteration may be performed in which the equations are solved a second time using coefficients formed with $\theta^{n+1/2} = (\theta^n + \theta^{n+1})/2$.

1.3.8. Fully Implicit Equations for DRADTN

When the grey atmosphere approximation is suitable, the coupling between radiation and material can be made implicit, thereby relaxing the associated stability condition. The energy equation linearized in φ and the zeroth moment equation are similar to Eqs. (19) and (20).

$$\varphi_i^{n+1} = \varphi_i^n + \frac{4a\theta_i^3 \Delta t^n}{(C_v)_i} \left[q_i - \left(P_i + \frac{\partial E_m}{\partial \tau} \right) \frac{d\tau}{dt} - \frac{c\mu_i}{2\rho} (\varphi_i^{n+1} + \varphi_i^n - E_i^{n+1} - E_i^n) \right] \quad (25)$$

$$\frac{E_i^{n+1} - E_i^n}{\Delta t^n} + \frac{P_i}{2} (\tilde{F}_{i+1}^{n+1} - \tilde{F}_i^n + \tilde{F}_{i+1}^n - \tilde{F}_i^n) = \frac{c\mu_i}{2} (\varphi_i^{n+1} + \varphi_i^n - E_i^{n+1} - E_i^n)$$

The coefficients of Eq. (15) are then

$$A_i = -Q_i R_i P_i$$

$$C_i = -Q_{i+1} R_{i+1} P_i$$

$$B_i = -A_i - C_i + \frac{1}{\frac{2}{c\mu_i} + \frac{4a\theta_i^3 \Delta t^n}{\rho(C_v)_i}} \quad (26)$$

$$D_i = \left(-\frac{1}{\Delta t^n} + \frac{1}{\frac{2}{c\mu_i} + \frac{4a\theta_i^3 \Delta t^n}{\rho(C_v)_i}} \right) E_i^n + A_i (E_{i-1}^n - E_i^n) + C_i (E_{i+1}^n - E_i^n) \\ + \frac{P_i}{c\Delta t^n} (Q_{i+1} \tilde{F}_{i+1}^n - Q_i \tilde{F}_i^n) - \frac{\varphi_i^n + \frac{2a\theta_i^3 \Delta t^n}{(C_v)_i} \left[q_i - \left(P_i + \frac{\partial E_m}{\partial \tau} \right) \frac{d\tau}{dt} \right]}{\frac{1}{c\mu_i} + \frac{2a\theta_i^3 \Delta t^n}{\rho(C_v)_i}}$$

If desired Eq. (25) can be solved for the temperature θ^{n+1} to perform an iteration of the implicit equations.

1.3.9. Modified DRADTN Equations

The difference equations of Eq. (22), although accurate to second order in time and stable, are subject to oscillations which under some circumstances are very slightly damped, as shown in Section 1.6. The equations were reformulated in order to remedy these oscillations, which arise from the centering of terms in time and are manifested by periodic exchange of energy between radiation field and material when the time interval greatly exceeds the characteristic relaxation time of the radiation field.

After several experiments, the equations were written in the following form:

$$\frac{E_i^{n+1} - E_i^n}{\Delta t^n} + P_i \left(\tilde{F}_{i+1}^{n+1} - \tilde{F}_i^{n+1} \right) = \frac{c\mu_i}{2} \left(2b_j \varphi_i - 2E_i^{n+1} \right) \quad (27)$$

$$\frac{\tilde{F}_i^{n+1} - \tilde{F}_i^n}{4c\Delta t^n} + R_i \left(E_i^{n+1} - E_{i-1}^{n+1} \right) = - \frac{\tilde{F}_i^{n+1}}{4\lambda_i}$$

These equations have overcome the oscillation difficulties at the expense of loss in accuracy. It is likely that further experimentation in the form of these equations is warranted. In particular, the equations might take the more accurate, centered form in regions where oscillation cannot occur; but in regions where oscillations are possible, the modified equations could be employed.

1.3.10. Boundary Conditions for Difference Equations

The computation in the above equations is assumed to apply to a finite interval, $r_1 \leq r \leq r_I$, at the ends of which boundary currents F_R and F_L are specified as in Eq. (8). These, in turn, relate the flux and energy at the boundary. The difference equations, however, call only for a boundary flux; the radiation energy is a zone centered quantity at best a half zone removed from the surface. It is proposed to close these equations by performing an extrapolation so that the radiation energy at the boundary introduced by Eq. (9) is related to the interior values of energy. The system of equations can then be solved for the energy by the tri-diagonal matrix inversion algorithm.

For illustration, the left boundary condition is derived. It is assumed, just for the purpose of extrapolating the radiation energy through a half zone, that the geometry is planar, that the solution is time independent, and that the source is constant in the half space to the right of $x = 0$. Then the moment equations can be combined to give

$$\frac{\lambda}{3} \frac{d^2 E}{dx^2} - \mu(E - a\theta^4) = 0$$

having the solution $E = a\theta^4 + Ae^{-\alpha x}$, where $\alpha = \sqrt{3\mu/\lambda}$. To determine the constant A, the boundary condition,

$$F(x=0) = 2F_R - E(x=0) = -\frac{\lambda c}{3} \frac{\partial E}{\partial x} \Big|_{x=0}$$

is imposed. The solution,

$$E = a\theta^4 + \frac{2F_R - \frac{ca}{2}\theta^4}{\frac{c\lambda\alpha}{3} + \frac{c}{2}} e^{-\alpha x}$$

gives a boundary flux of

$$F(x=0) = \frac{F_R - \frac{ca}{4}\theta^4}{\frac{3}{4\lambda\alpha} + \frac{1}{2}}$$

The correct solution, giving $F(x=0) = F_R - (ca/4)\theta^4$, is obtained if $2\lambda\alpha/3 = 1$; consequently, to improve the accuracy of the boundary condition, this substitution is also made in E:

$$E = a\theta^4 + \left(\frac{2}{c}F_R - \frac{a}{2}\theta^4\right)e^{-\alpha x}$$

In order to relate the energy at the boundary $E(x=0)$ to the energy at the first zone center E_1 , the source is eliminated:

$$E(x=0) = \frac{\frac{4}{c}F_R(1 - e^{-\alpha\Delta x_1/2}) + E_1}{2 - e^{-\alpha\Delta x_1/2}}$$

The corresponding value of the boundary flux is

$$F(x=0) = \left(2F_R - \frac{c}{2}E_1\right)\beta_R \quad (28)$$

in which $\beta_R = \frac{1}{2 - e^{-\alpha \Delta x_1/2}}$ and $\alpha = \sqrt{3\mu/\lambda}$. For the right-hand boundary the condition is similar:

$$F(x_1) = \left(-2F_L + \frac{c}{2} E_{I-1} \right) \beta_L \quad (29)$$

where $\beta_L = 1/(2 - e^{-\alpha \Delta x_{I-1}/2})$

In Eq. (28), the thickness of the first zone is $\Delta x_1 = r_2 - r_1$ and the quantity α is evaluated as a function of temperature and density in the first zone. Similarly in Eq. (29), for the right-hand boundary condition the last zone thickness is $\Delta x_{I-1} = r_I - r_{I-1}$, the last zone energy is E_{I-1} , and the quantity α is evaluated from the last zone variables.

The expressions for flux at the boundary, Eqs. (28) and (29), after correction for geometry factors, are to be substituted into the zeroth moment equation. The result is a modification of the coefficients of Eq. (15), the linear equation for the unknown radiation energy densities. At the left-hand boundary $i = 1$, for example, the coefficient $A_1 = 0$, as must be the case to terminate the equations. In addition, the coefficients B_1 and D_1 are modified in a way depending on which form of the equations is being used. To illustrate, the ERADTN coefficients become

$$\begin{aligned} B_1 + \frac{c}{2} \alpha r_1^{\alpha-1} P_1 \beta_R &\rightarrow B_1, \\ D_1 - 2\alpha r_1^{\alpha-1} P_1 F_R \beta_R &\rightarrow D_1 \end{aligned} \quad (30)$$

The boundary equations for DRADTN, as currently formulated, are the same as Eq. (30).

1.3.11. Iteration

The coefficients of the linear equations depend on the temperature and, consequently (in a time dependent problem), on the time. In each of

the subroutines an option is provided to use the estimate of the temperature resulting from the first calculation to recalculate the coefficients. The calculation is then repeated. In principle, this iteration could be repeated until a convergence criterion is satisfied. However, the equations are at best no more than second order accurate. Since a single iteration is sufficient to achieve second order accuracy, it is doubtful that further iteration is warranted. Improved accuracy can be better achieved by a reduced time step. The modified DRADTN equations are only first order accurate in time. Consequently, it is doubtful that the iteration option should be exercised for the DRADTN equations.

1.3.12. Solution of E - equations

The equations for the radiation energy at the advanced time, Eqs. (15), form a set of linear equations in which the coefficient matrix of the E-vector is tridiagonal. These equations are solved by factoring the coefficient matrix into upper and lower matrices. The solution is obtained by solving a recurrence relation

$$E_i = g_i E_{i+1} + h_i \quad (31)$$

in which $g_I = 0$ (resulting from $C_I = 0$) and $g_i = -C_i/d_i$, $h_i = -(D_i + A_i h_{i-1})/d_i$, and $d_i = B_i + A_i g_{i-1}$. The condition $A_I = 0$ suffices to terminate the equations for h_I and d_I .

These equations have been found to suffer from figure loss when the mean free path in the medium is long. To avoid this loss of figures due to the finite precision of the computer, new quantities are defined:

$$A'_i = A_i, \quad C'_i = C_i, \quad D'_i = D_i \quad (32)$$

$$B'_i = B_i + A_i + C_i; \quad g'_i = g_i - 1$$

In terms of these quantities, the above equations can be written

$$\begin{aligned} E_i &= E_{i+1}(g_i' + 1.) + h_i, \\ g_i' &= (-D_i - A_i g_i')/d_i, \quad h_i = -(D_i + A_i h_{i-1})/d_i \\ d_i &= B_i' - C_i + A_i g_i', \quad g_1' = -1 \end{aligned} \quad (33)$$

The modified B_i' is a small quantity when the mean free path is long. The previous equations required the subtraction of the large quantities A_i and C_i from B_i to give the correct result. In addition, under the above circumstances the modified g_i' becomes very small, a result previously achieved by subtraction of quantities near 1 in size.

The flux calculation can also suffer from figure loss. The form of the relation between flux and radiation energy, which is solved for the flux after the radiation energy has been obtained, is given by the first moment equation and is different for DRADTN and ERADTN. Without retardation the result, derived from Eq. (14), is

$$\tilde{F}_i^{n+1} = 4\lambda_i R_i \left(E_{i-1}^{n+1/2} - E_i^{n+1/2} \right) \quad (34)$$

To avoid the subtraction, the flux equation is rewritten

$$\tilde{F}_i^{n+1} = 4\lambda_i R_i \left(h_{i-1} + g_{i-1}' E_i^{n+1/2} \right)$$

Some problems involving temperatures of several kev resulted in overflow of quantities in the fully implicit equations. This overflow was eliminated by forming intermediate quantities in different order, albeit at the cost of less efficient coding.

1.3.13. Time Interval

The control of the time interval reflects two considerations: accuracy and stability. The accuracy criterion is based on limiting the radiation contribution to the energy change in each zone to less than a prescribed fraction of the energy in the zone:

$$\Delta t_R \leq \left(\min_i \frac{E_i}{ER_i} \right) * \text{SLUG} \quad (35)$$

where E_i is the zone internal energy, ER_i is the radiation energy change rate per zone, and the input quantity controlling the accuracy criterion is SLUG. In order to avoid control of the time interval by zones having very small internal energy, the test of Eq. (35) is applied only to zones having greater than a prescribed fraction (given by the input quantity TELM (37)) of the total internal energy.

For problems in which the fully implicit equations are solved, the accuracy criterion affords the only radiative control of the time interval. When the partially implicit equations are solved, however, additional stability criteria are required. The full equations have not yet been subjected to stability analysis. However, the stability analyses given in

Section 1.6 suggest that two criteria be applied. These two conditions must be observed in order that small oscillations will not be amplified when energy is exchanged between radiation and material. The first condition represents stability in the exchange in a single zone between radiation and material:

$$\Delta t_R \leq \min_i \frac{(C_v)_i}{8 \times 10^{12} \theta_i^3 (\kappa_p)_i} \quad (36)$$

where the Planck mean opacity κ_p (cm^2/g) appears. This condition is undoubtedly a conservative one, since some stabilization results from the implicit treatment of the radiation energy. The second condition arises from the requirement that energy flowing between adjacent zones not result in growing oscillations of energy between zones:

$$\Delta t_R \leq \min_i \frac{(\rho \Delta R_i)^2 (\kappa_R)_i (C_v)_i}{1.07 \times 10^{13} \theta_i^3} \quad (37)$$

where κ_R (cm^2/g) is the Rosseland mean opacity and ΔR is the zone thickness. This condition is the explicit stability condition for the (equilibrium) radiation diffusion equation. Again, the condition may be somewhat conservative (perhaps even superfluous), since part of the exchange takes place via the stable radiation energy equation.

1.4. HOW TO USE NON-EQUILIBRIUM DIFFUSION SUBROUTINES

This section contains information useful to the person who desires to perform calculations with the non-equilibrium diffusion subroutines in the SPUTTER code. Criteria are presented for choosing between DRADTN and ERADTN subroutines, code variables are related to variables of the derivations of Section 1.3, input quantities are discussed, and comments are made regarding how to control the problem and what difficulties may be encountered during the calculation.

1.4.1. Differences Between ERADTN and DRADTN

Radiation in equilibrium with material at temperature θ has a density of energy $E = a\theta^4$ which, under conditions of sufficiently high temperature or of low matter density, may become comparable with or greater than the material energy density. If such is the case, it is necessary to take into account this radiation energy in transit through the system in order properly to account for the energy balance of the problem. In the transport equation the radiation energy corresponds to the $1/c \partial I_v / \partial t$ term (sometimes called the retardation term) and gives rise to the time derivative terms in the non-equilibrium diffusion equation (Eq. 16).

As indicated in Section 1.3, the non-equilibrium diffusion equations have a substantially different form requiring more computation when the retardation terms are retained. Consequently, for problems in which radiation energy is negligible, as is the case when

$$\theta (\text{ev}) \ll 2 \times 10^3 [\rho (\text{g/cm}^3)]^{1/3}$$

and when the light speed of propagation of radiation waves can be neglected, it was deemed desirable to solve the equations without considering the retardation terms. These equations are incorporated into a separate subroutine, ERADTN, which should be used for low-temperature problems. For problems in which the radiation energy is not small or in which it is of interest to take account of light speed with which radiation waves

propagate through vacuum, the equations including the retardation terms are solved in the DRADTN subroutine. The user must choose which of these two subroutines to incorporate into his code with the remaining desired SPUTTER subroutines. Fortunately, most of the control quantities are the same for the two codes. Exceptions are noted below, in particular the DRADTN dump tape.

1. 4. 2. Glossary of Code Variables

In Table I the variable quantities used in the DRADTN and ERADTN subroutines are correlated with the quantities defined in Section 1. 3, where the equations are derived. In addition, a brief word description of the variable is given. Only those variables which have a use which is unique to the non-equilibrium diffusion subroutines (there are a few exceptions) are included. Consequently, a number of quantities appearing in these routines but also used in other parts of SPUTTER are not found in Table I; reference should be made to the SPUTTER report for these quantities. Most of the entries in the table are used in both routines; the few appearing only in DRADTN are distinguished by an asterisk (*).

1. 4. 3. Glossary of Input Quantities

Table II contains the quantities needed to control the calculations of the non-equilibrium diffusion subroutines, and information on how to establish their values. The first column contains the decimal location in common storage of the quantity, as required for card input. The second column contains the variable FORTRAN name. The third column contains a description of the quantity. Finally, the fourth column contains a typical value of the quantity. In some cases this value represents a recommended one, (e. g., AC); in other cases, merely a typical one (e. g., GA).

After having chosen between the DRADTN and ERADTN subroutines, it is necessary to make additional selections to determine the values of input quantities. Some comments regarding these selections follow.

Table I
GLOSSARY OF CODE VARIABLES

<u>Code</u>	<u>Symbol</u>	<u>Quantity</u>	<u>Units</u>
RHO(I)	E_i^{n+1}	Radiation energy density	erg/cm ³
X2(I)	$\tilde{F}_i^{n+1}$	Area-integrated flux (per volume factor)	erg/sec
ER(I)	---	Material radiative heating rate (per zone and per volume factor)	erg/sec
PDFU(I)	P_i	Coefficient of flux difference in first moment equation	cm ⁻¹
RUC(I)	R_i	Coefficient of energy difference in second moment equation	cm ⁻¹ /sec
H2(I)	$1/4\lambda_i$	0.25 over diffusion mean free path (Rosseland av.)	cm ⁻¹
H(I)	$c\mu_i/2$	Absorption coefficient times half light speed (Planck av.)	sec ⁻¹
X6(I)	$b_j \theta_i^4$	Integral of Planck function over j th frequency group.	(ev) ⁴
SU(I)	$c\mu_i b_j \phi_i$	Radiation source function	erg/cm ³ sec
Q1(I)	θ_i^4	Fourth power of temperature	(ev) ⁴
Q37(I)	$\ln \theta_i$	Logarithm of temperature	---
Q38(I)	$\ln \tau_i$	Logarithm of specific volume	---
SUMX2(I)	$\sum_j \tilde{F}_i^{n+1}$	Sum over frequency groups of flux	erg/sec
SUMRHO(I)	$\sum_j E_i^{n+1}$	Sum over frequency groups of radiation energy	erg/sec
GU(I)	g_i	Coefficient of E_{i+1} in recurrence for E_i	---
HU(I)	h_i	Inhomogeneous term in recurrence for E_i	erg/cm ³

Table I (Continued)

<u>Code</u>		<u>Symbol</u>	<u>Quantity</u>	<u>Units</u>
OSX2(I)	*	$\sum_j \tilde{F}_i^n$	Sum over frequency groups of old flux	erg/sec
FLUX(I)	---	---	Value of left-hand boundary flux for $GL > 0.5$. Formed in the TQUE4 subroutine.	(ev) ⁴
OLDTH(I)		θ_i^n	"Old" temperature stored during iteration	ev
OLDE(I, IHNU) *		E_i^n	"Old" radiation energy for use in DRADTN	erg/cm ³
OLDF(I, IHNU) *		$\tilde{F}_i^n$	"Old" flux for use in DRADTN	erg/sec
WSB	---	---	Total internal energy; used in time interval criterion	erg
WSBB	---	---	Zone internal energy, used in time interval criterion	erg
THTAMX		$\theta_{\max}$	Largest of zone and boundary temperatures	ev
RDTR		$1/\Delta t_R$	Reciprocal of radiation time interval	sec ⁻¹
RCDT	*	$1/4c\Delta t_R$	Reciprocal of distance light travels during time interval	cm ⁻¹
TSLH		$\alpha_r^{\alpha-1}$	Area factor for left-hand flux boundary condition	cm ^{$\alpha-1$}
TSRH		$\alpha_r^{\alpha-1}$	Area factor for right-hand flux boundary condition	cm ^{$\alpha-1$}
BBSL		$b_j \theta_L^4$	Left-hand boundary Planck integral	ev ⁴
BBR		$b_j \theta_R^4$	Right-hand boundary Planck integral	ev ⁴
BETA1		β_1	Extrapolation coefficient for left-hand boundary energy	---
BETA2		β_2	Extrapolation coefficient for right-hand boundary energy	---
HNU		$h\nu_j$	Lower photon energy boundary of group j	ev

Table I (Continued)

<u>Code</u>	<u>Symbol</u>	<u>Quantity</u>	<u>Units</u>
HNUP	$h\nu_{j+1}$	Upper photon energy boundary of group j	ev
HNU4	$h\nu_j^4$	Fourth power of $h\nu_j$	ev ⁴
HNU4P	$h\nu_{j+1}^4$	Fourth power of $h\nu_{j+1}$	ev ⁴
H3M	$(\kappa\rho\Delta r)_-$	Optical depth of zone to left of interface; used in flux gradient	---
H3P	$(\kappa\rho\Delta r)_+$	Optical depth of zone to right of interface; used in flux gradient	---
BNTH	θ_i^{n+1}	Estimate of new temperature; used in iteration	ev
AU	A_i	Coefficient of E_{i-1} in radiation energy linear equation	---
BU	B_i	Coefficient of E_i in radiation energy linear equation	---
CU	C_i	Coefficient of E_{i+1} in radiation energy linear equation	---
DU	D_i	Inhomogeneous term in radiation energy linear equation	---
*		DRADTN only	

Table II
GLOSSARY OF INPUT QUANTITIES

<u>Common Location</u>	<u>Variable Name</u>	<u>Description</u>	<u>Typical Value</u>
26	LMDA(26)	DRADTN only. Upon restart, the second data packet must contain a card setting LMDA(26) = 0.0. This causes the tape containing OLDE and OLDF to be read to obtain starting values.	0.0
44	KMAX	Frequency group indicator. Zero gives grey, nonzero, multifrequency.	0.0
75	BOILB	Maximum number of radiation sub-cycles permitted. Set to NTIMES in subroutine.	10.0
77	CVB	Iteration control. Zero gives single pass, nonzero, double pass with time-centered coefficients. Used to set the flag NVEZ.	0.0
78	SLUG	Time interval criterion. Maximum permissible fractional zone energy change per cycle.	0.1
79	ALPHA	Geometry selector. All values permissible for non-equilibrium diffusion: 1, slab; 2, cylinder; 3, sphere.	1.0
81	HVB	Implicit selector. When KMAX = 0.0, a nonzero value gives fully implicit equations; otherwise partially implicit equations with time step subject to stability.	1.0
87	CB	Used to minimize the number of frequency groups calculated for multifrequency problems. Merges into one group all groups having lower frequency boundary greater than THTAMX. Too many groups merged will lead to call UNCLE unless CB is half-integral. Operative only in ERADTN.	10.0

Table II (Continued)

<u>Common Location</u>	<u>Variable Name</u>	<u>Description</u>	<u>Typical Value</u>
88	GA	Left boundary condition indicator. Operative only if no pusher. (Pusher present prescribes blackbody flux.) GA < 0 gives zero net flux; GA = 0 gives vacuum to the left; GA > 0 gives UNCLE call.	0.0
90	GL	Right boundary condition indicator. GL < 0 gives zero net flux; GL = 0 gives vacuum to the right; GL = 0.5 gives blackbody flux specified by THETA(IM+1); GL > 0.5 gives flux specified via FLUX(I) in the TQUE4 subroutine.	0.5
126	AC	Criterion in diffusion mean free path (H2(I)) calculation. If optical depth is greatly different in adjacent zones, the optically thinner zone is used instead of forming an average.	0.3
147	EDITMF	Same as S12. Nonzero value gives multifrequency print which also serves as a debug print.	0.0
152	S17	Old implicit switch which sets S9. Note changed from previous usage.	---
8466	TELM(25)	Multiplied to change radiation time interval after all criteria have been applied.	1.0
8478	TELM(37)	Fraction of internal energy of the entire mesh which each zone must exceed before energy change of that zone is tested (see SLUG) in the time interval calculation.	0.003
8858	SOLID(10)	Switch to permit Rosseland mean to be substituted for Planck mean if value is not zero.	0.0

The frequency treatment decided on is very important for the speed and accuracy of the calculation. Two situations permit a monofrequency, or grey, calculation. If the medium is optically thick it is usually permissible to perform a grey calculation. However, it is necessary that the medium be thick to all relevant frequencies, i. e., those which transport appreciable energy. Exceptions occur when sharp temperature changes exist in the medium, such as at radiation or shock fronts and at boundaries. If they are transient or localized, it is usually permissible to perform the grey calculation. At the other extreme, if the medium is optically thin in all important parts of the spectrum, the grey calculation can be performed. In both of these situations it is sometimes desirable to find the spectrum of the radiation in or, more commonly, emerging from the material. It is not necessary to run the calculation with frequency groups through the entire problem history in this case. Instead, the grey calculation can be edited with a "snapshot" multifrequency calculation at desired times. When the material is intermediate between these situations, the multifrequency calculation is necessary. However, it is under these conditions of intermediate optical thickness that the non-equilibrium diffusion approximation is least reliable.

The grey calculation with $KMAX = 0.0$ permits the implicit indicator HVB to be set to a nonzero value, thereby releasing the time interval from the control of stability criteria and leaving it subject only to accuracy considerations. The implicit option should be exercised when possible (the option exists only to permit test investigations of the code). When a multifrequency calculation is required, the partially implicit solution is mandatory. Consequently, multifrequency calculations are lengthy not only because the calculation is repeated for each frequency group, but because the time interval may be reduced substantially below the value for implicit calculation. When there is doubt about the necessity for groups, one can first calculate a grey solution and then compare the resulting radiation fluxes with those obtained with a few "snapshot" multifrequency

calculations. Substantial differences indicate that the multifrequency calculation is required ab initio. Frequently, the grey calculation is not wasted, since the information about zoning of the problem can be incorporated into the subsequent calculation.

No good criterion for the decision about iteration exists. In general, iteration almost doubles the computing time. Iteration may be warranted if the increased accuracy of the solution permits a time interval which is more than twice as large as that used in the solution without iteration. Whether the accuracy is substantially affected depends on both the variability of the coefficients of the radiation equations (which is different for the implicit and partially implicit forms of the equations) and the rapidity of change of the solution with time. When iteration is performed, the accuracy criterion (SLUG) should be relaxed.

The optical depth between zone centers required in the gradient term of the radiation flux is difficult to evaluate accurately in regions where the mean free path changes rapidly in space, as near the front of a radiation wave. No completely satisfactory prescription is yet available, but a method containing the variable AC is available in the subroutines. This quantity, which controls the transition from using an average of optical depths of neighboring zones when the optical depths do not differ greatly to using the smaller optical depth when the difference is large, has been found to give accurate results for a diffusion test problem when $AC = 0.3$. Further improvement would result from a prescription incorporating the effect of temperature gradient on mean free path within a zone.

Boundary conditions at the two faces of the shell of material being calculated are determined from several options. When the spherical or cylindrical shell is not hollow, the boundary condition at the origin is irrelevant, but $GA \leq 0$ should be set. When no pusher exists, the left boundary can be made to give zero net flux to simulate a perfectly reflective region on the left or to permit radiation to flow unimpeded from the material to simulate a vacuum on the left. Similar options are available

for the right boundary with the addition of a blackbody boundary condition and a boundary flux. The blackbody condition simulates the effect of a hohlraum at temperature $THETA(IM+1)$ shining on the right boundary. The boundary flux condition is a special-purpose feature, making use of the TQUE4 routine. With it the frequency dependent flux found in a fireball can be applied to the right surface of the material. Quite small modifications of the subroutines could make these last two options applicable also to the left boundary. An alternative method of applying an external radiation boundary condition is through a source routine which forms an energy source in the material as determined by the rate of energy absorption at various depths. An example is the QUE4 subroutine for incident X-rays.

The time interval of the calculation is determined by both accuracy and stability criteria. The calculation of radiation flow can be performed at a smaller time interval than the hydrodynamics, so that a number of subcycles of the radiation limited by BOILB are calculated every cycle. It is not desirable to allow the number of subcycles to become very large. First, the calculation time for other parts of the cycle is not large compared with the radiation, so no appreciable saving results. Second, substantial radiation flow during subcycles may induce other changes which, when finally calculated on the next cycle, may be catastrophically large. Third, a large amount of computation time is spent during which no information is available about the progress of the problem. Consequently, it is desirable to limit the time interval, if necessary, by control cards so that a limited amount of subcycling occurs. When a strong external source is applied to the surface of the material, transients are established which require an unusually small time interval for a few cycles. Control card reduction of the time interval is usually necessary during the first few cycles.

1.4.4. Subroutines Called by DRADTN and ERADTN

Within the subroutine codes it is assumed that two special-function subroutines and dependent subroutines which are an integral part of the radiation calculation are available. These subroutines are described below.

PLNKUT (α_1, α_2). This function returns the partial Planck function defined by

$$\frac{15}{\pi^4} \int_{\alpha_1}^{\alpha_2} \frac{u^3 du}{e^u - 1}$$

It is a function of two variables, $\alpha_1 = h\nu_1/\theta$ and $\alpha_2 = h\nu_2/\theta$ ($\alpha_1 < \alpha_2$). The routine is described in Ref. 9.

KAPPA (i_1, i_2). This routine returns values of the Rosseland opacity κ_R and the Planck opacity κ_P for the temperatures, densities, and materials appropriate to the zones having indices from i_1 to i_2 . For problems specifying more than one frequency group, the appropriate frequency group average coefficients are provided as well as the quantities averaged over the entire spectrum.

In addition, use is made of the subroutines UNCLE, DVCHK, and NONEQ.

Boundary flux values are formed in a special TQUE4 subroutine and used when $GL > 0.5$ via the FLUX(I) array. These values are the result of integrating the frequency group intensities to obtain the radiation current incident on the boundary. The TQUE subroutine processes the AFWL "users tape" to obtain radiation intensities resulting from fireball calculations.

1.5. TEST PROBLEMS

Test calculations have been performed to evaluate the accuracy of the non-equilibrium diffusion method. These calculations are of two

classes. Idealized problems (slab penetration, isothermal sphere cooling) have been compared with corresponding transport solutions. "Real" problems dealing with interaction, slab penetration, and fireball growth have been computed. On the basis of the results, modifications of mean free path averaging and boundary condition formulation have been made.

Solutions for comparison have been calculated with subroutines, for radiation transport from the SPUTTER code (Ref. 5). These routines are applicable only to spherical geometry (SRADTN) and slab geometry (PRADTN), so the comparison calculations have been restricted to these two geometries.

All of the idealized calculations are without hydrodynamics and use a gray and temperature independent absorption coefficient.

The first calculation applies to a semi-infinite absorbing medium initially cold. At $t = 0$ an isotropic source shines on the surface of the medium and progressively heats it. The initial heating phase is followed by a transition to a diffusive solution in which a wave penetrates progressively more slowly into the interior of the slab. Numerical calculations of this problem have also been made by Barfield (Ref. 10). Both the DRADTN and ERADTN equations have been tested on the problem in which there are four zones per mean free path in the medium. In Fig. 1 the fluxes entering the medium versus time are compared for the two. The only appreciable difference occurs at early time. In Fig. 2, plots of temperature profiles for the ERADTN and PRADTN calculations are compared. Largest deviations appear at early time and near the wave front. Results obtained with DRADTN for this problem are substantially the same as those obtained with ERADTN.

The second idealized problem describes the cooling of a sphere of gas in vacuum. Initially, the sphere is isothermal and contains a fixed number of absorption mean free paths in the radius. Calculations have been performed for three thicknesses of sphere: 1, 2, and 5 mean free paths per radius, in each of which 20 radial zones are used. Comparisons

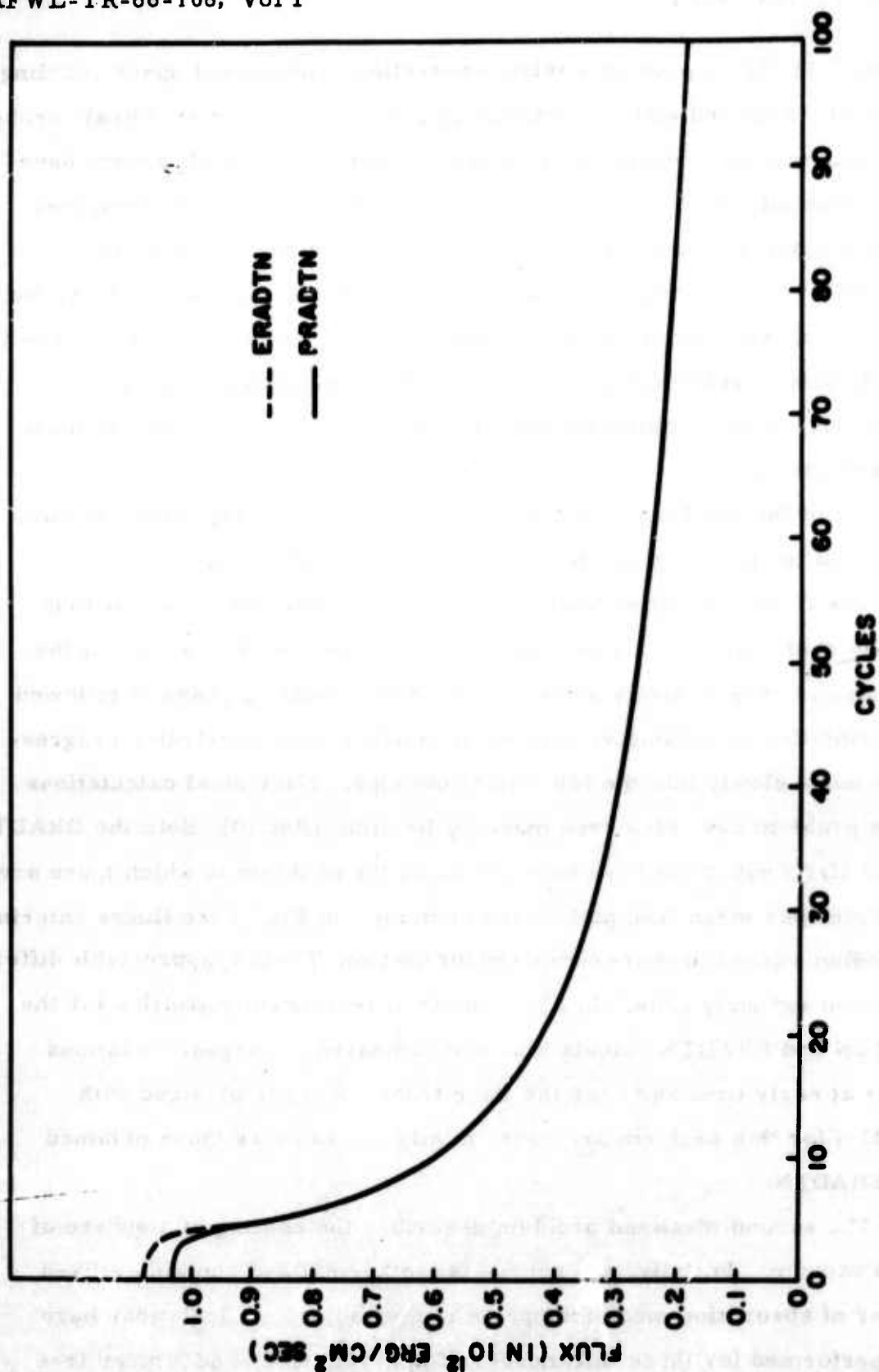


Figure 1. Slab Penetration Fluxes

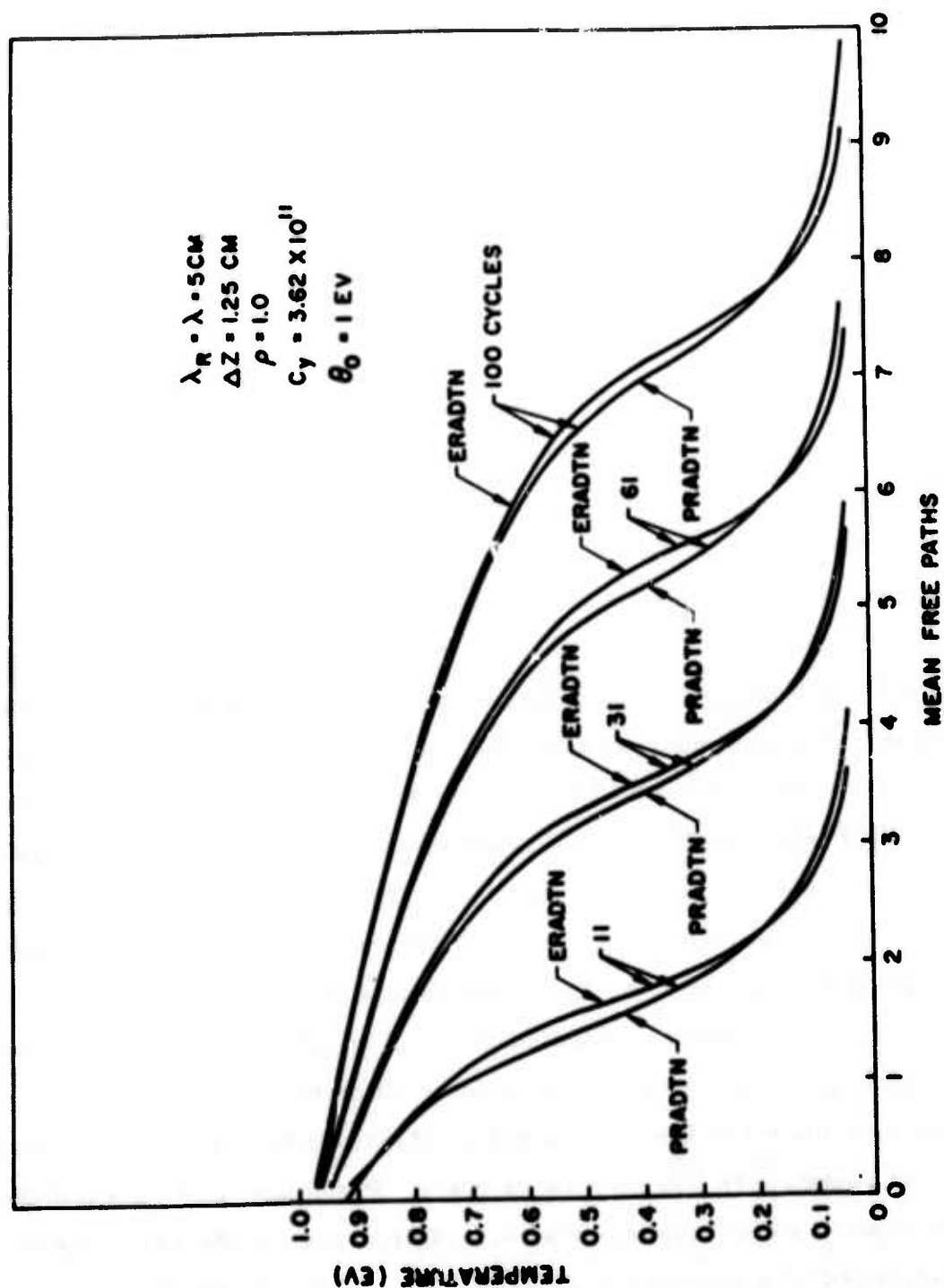


Figure 2. Slab Penetration Temperature Profiles

of ERADTN with SRADTN for these cases are shown in Fig. 3, where the temperature is plotted as a function of time for the 2 mean free path case. In Figs. 4 and 5, the corresponding curves for the 1 and 5 mean free path cases are given. Temperature differences of several percent are found. It is to be expected that both optically thick and optically thin cases will be more accurate. In Fig. 6 the flux at the surface of the sphere is shown as a function of time. The comparison calculations are sufficiently close (never differing by more than 2%) so as to be represented by a single curve for each case. In the one case in which DRADTN was calculated, similar results were obtained but oscillation was observed.

As indicated by the above example, DRADTN presently gives less satisfactory results due to bounded oscillations having small damping. This problem has been improved by recentering in time of the exchange term as indicated in Section 1.3.

Additional test problems corresponding to situations arising in applications of SPUTTER have been run. The ERADTN and PRADTN equations have been compared, and agree well for the problem of radiation impinging on an opaque slab and inducing radiation penetration preceded by a strong shock wave. A cycle of the BLUE GILL fireball problem has been repeated with ERADTN and SRADTN. While results are quite similar in the fireball interior, the fluxes are quite different in the free streaming region outside. The latter appear to point to the failure of the radiation energy to diverge in the Eddington approximation when radiation is emitted from a compact source. This very recently identified problem is still under consideration; incorporating parts of the second moment equation may help solve it. An interaction problem has been compared in which ablation of a target induced by thermal radiation falling on it takes place. Preliminary results indicate agreement after a short transient period. Differences in the early result may be reduced by a modified boundary condition not yet tested for this problem.

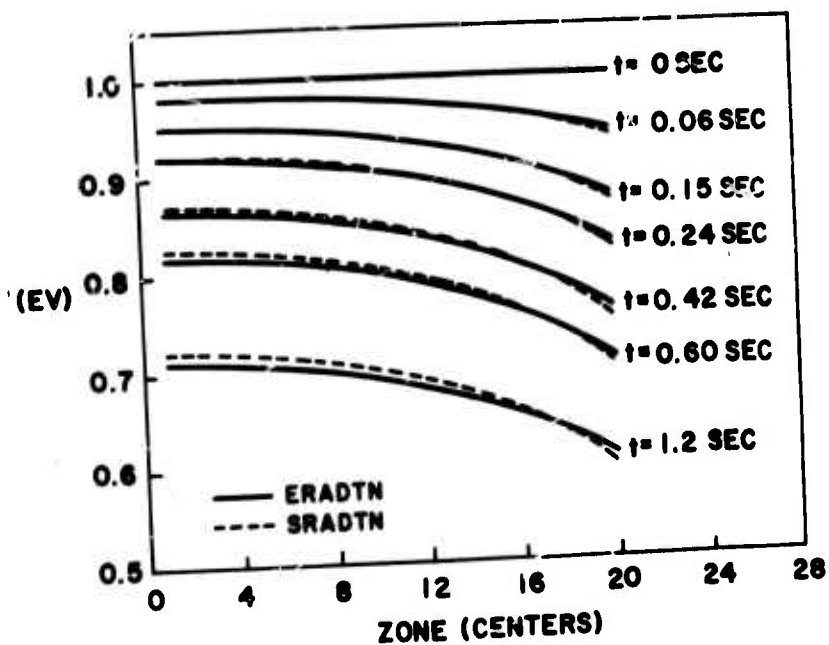


Figure 3. Spherical Emission Test Problem,
 $\Delta t = 0.03$, $\kappa_R = \kappa_P = 0.2$

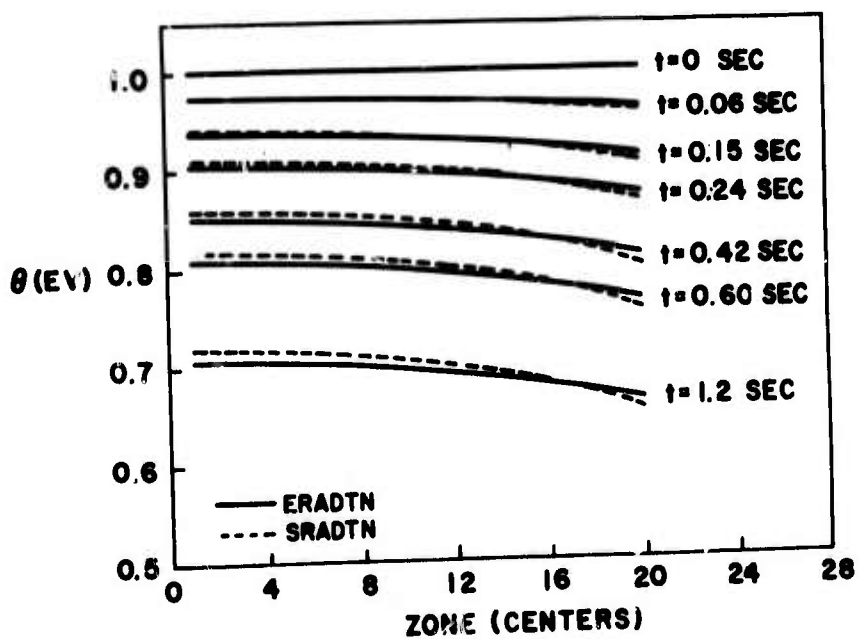


Figure 4. Spherical Emission Test Problem,
 $\Delta t = 0.03$, $\kappa_R = \kappa_P = 0.1$

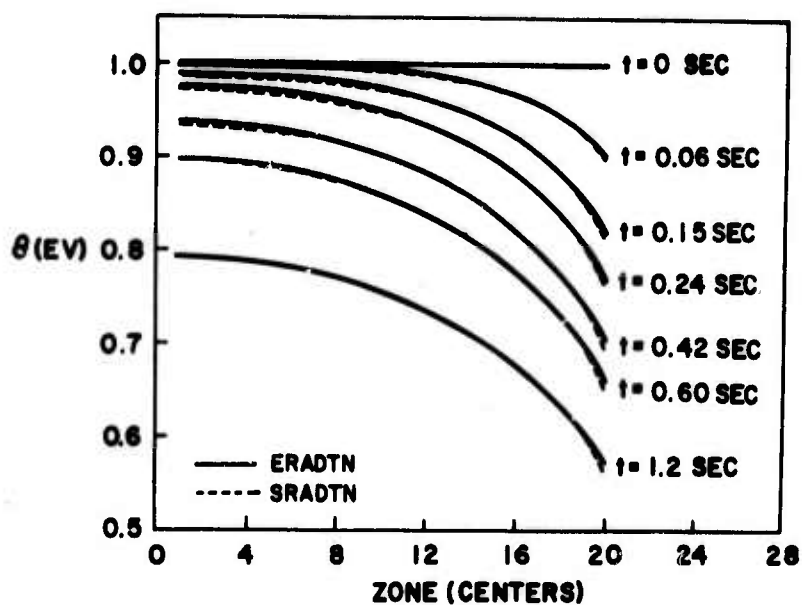


Figure 5. Spherical Emission Test Problem,
 $\Delta t = 0.03$, $\kappa_R = \kappa_P = 0.5$

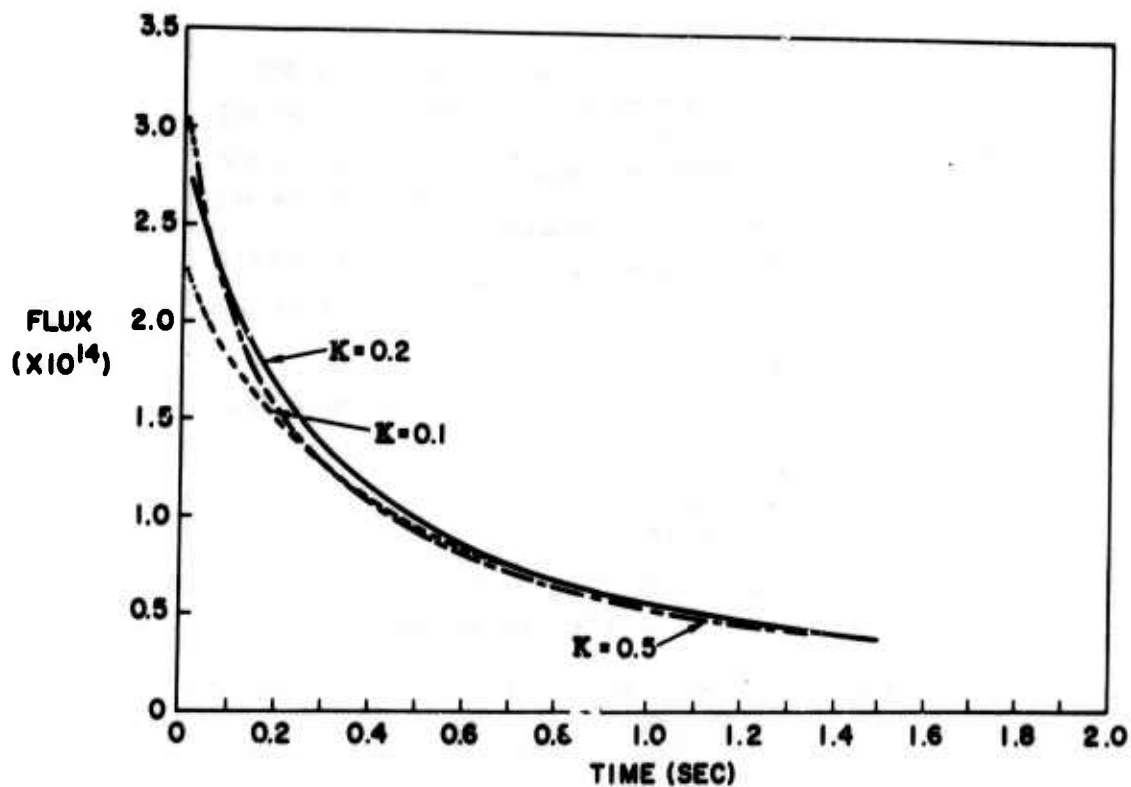


Figure 6. Flux Versus Time for Spherical
 Emission Test Problem, $t = 0.03$

The findings to date show very satisfactory agreement for slab problems and indicate that there are many potential applications of the non-equilibrium diffusion equations. How generally applicable the method can be made is not yet known.

1.6. APPENDIX: STABILITY ANALYSIS

The stability analysis of the difference equations for non-equilibrium diffusion is partially developed in this section. The defining equations for this physical process are given.

The stability theory of finite difference equations is sufficiently stated in a book by Richtmyer (Ref. 11). He gives the following definition of stability:

Definition

If a finite difference scheme is given by

$$u^{n+1} = c(\Delta t)u^n$$

where u^n is an m -column vector and $c(\Delta t)$ is an $m \times m$ array, the system is said to be stable if there exists a τ such that the sequence

$$\left\{ \|c(\Delta t)\|^j \right\}_{j=0}^n \text{ is uniformly bounded, where } 0 < \Delta t < \tau.$$

Consistent with this definition, a sufficient condition for stability is that the spectral radius of $c(\Delta t)$ be less than 1. This theorem is developed and proved by Richtmyer (Ref. 11).

The difference equations proposed for defining non-equilibrium diffusion are

$$(1) \frac{E_i^{n+1} - E_i^n}{\Delta t^n} + \frac{P_i}{2} (F_{i+1}^{n+1} - F_i^{n+1} + F_{i+1}^n - F_i^n) = \frac{c\mu_i}{2} (2b_j \phi_i - E_i^{n+1} - E_i^n)$$

$$(2) \frac{F_i^{n+1} - F_i^n}{c\Delta t^n} + 2R_i (E_i^{n+1} - E_{i-1}^{n+1} + E_i^n - E_{i-1}^n) = \frac{-1}{2\lambda_i} (F_i^{n+1} + F_i^n)$$

$$(3) \phi_i^{n+1} = \phi_i^n + f_i \left[q_i - \left(P_i + \frac{\partial E_m}{\partial \tau} \right) \frac{\partial \tau}{\partial t} - \frac{c}{2\rho} \sum_j \mu_j (2b_j \phi_i - E_i^{n+1} - E_i^n) \right]$$

where the terms are defined as in Section 1.3. The first two equations are the defining relations for the pertinent moments of the intensity. The third equation expresses the conservation of energy.

As the difference equations are now stated, a stability condition cannot be found as a function of the parameters. Various assumptions are employed to reduce the system to one amenable to solution. These assumptions are summarized as follows:

1. Ignore hydrodynamics
2. No energy sources, i.e., $q_i = 0$
3. Monofrequency
4. Plane geometry
5. Scattering is negligible

With these assumptions the system of equations becomes

$$(1) \frac{E_i^{n+1} - E_i^n}{\Delta t} + \frac{1}{2\Delta x} (F_{i+1}^{n+1} - F_i^{n+1} + F_{i+1}^n - F_i^n) = \frac{c\mu}{2} (2\phi_i - E_i^{n+1} - E_i^n)$$

$$(2) \frac{F_i^{n+1} - F_i^n}{c\Delta t} + \frac{c}{6\Delta x} (E_i^{n+1} - E_{i-1}^{n+1} + E_i^n - E_{i-1}^n) = -\frac{\mu}{2} (F_i^{n+1} + F_i^n)$$

$$(3) \phi_i^{n+1} = \phi_i^n - \left(\frac{4a\theta_i^3}{(C_v)_i} \right) \frac{c\Delta t\mu}{2\rho} (2\phi_i - E_i^{n+1} - E_i^n)$$

With this system of equations two possible special cases may be investigated. Consider first that the material energy is much larger than the radiation energy. This requirement is equivalent to $\phi \approx \text{constant}$ for some time interval τ . In this time interval one can investigate the stability of partially implicit equations (1) and (2) above. Expanding E and F into Fourier components, one finds, after some reduction, that the amplification matrix $C(\Delta t)$ is given by

$$C(\Delta t) = \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix}$$

where

$$C_{11} = \frac{(1 + \frac{c\mu\Delta t}{2})(1 - \frac{c\mu\Delta t}{2}) - \frac{c^2}{3}(\frac{\Delta t}{\Delta x})^2 \sin^2 k \frac{\Delta x}{2}}{M}$$

$$C_{12} = - \frac{2 \frac{\Delta t}{\Delta x} i \sin k \frac{\Delta x}{2} e^{i(k\Delta x/2)}}{M}$$

$$C_{21} = - \frac{\frac{2c^2}{3} \frac{\Delta t}{\Delta x} i \sin k \frac{\Delta x}{2} e^{-i(k\Delta x/2)}}{M}$$

$$C_{22} = \frac{(1 - \frac{c\mu\Delta t}{2})(1 + \frac{c\mu\Delta t}{2}) - \frac{c^2}{3}(\frac{\Delta t}{\Delta x})^2 \sin^2 k \frac{\Delta x}{2}}{M}$$

$$\begin{pmatrix} E^{n+1} \\ F^{n+1} \end{pmatrix} = C(\Delta t) \begin{pmatrix} E^n \\ F^n \end{pmatrix}$$

$$M = (1 + \frac{c\mu\Delta t}{2})^2 + \frac{c^2}{3}(\frac{\Delta t}{\Delta x})^2 \sin^2 k \frac{\Delta x}{2}$$

A sufficient condition for stability is that the eigenvalues of $C(\Delta t)$ lie within the unit circle. The eigenvalues are given by

$$\lambda^2 - T\lambda + \Delta = 0 \quad \text{where } T = \text{trace } (C(\Delta t))$$

$$\Delta = \det (C(\Delta t))$$

The conditions that the roots lie within the unit circle can be found from the Routh criterion (Ref. 12) after making the transformation $\lambda = (\omega + 1)/(\omega - 1)$. This

transformation maps the interior of the unit circle into the left half complex plane. Making the substitution, one has

$$\omega^2(1 + \Delta - T) + 2\omega(1 - \Delta) + 1 + T + \Delta = 0$$

For a second order equation the Routh criterion requires that the coefficients of the equation be positive if the roots of the equation are contained within the left half plane. Thus, the conditions are given by

$$\begin{aligned} (1) \Delta &< 1 \\ (2) |T| &< \Delta + 1 \end{aligned}$$

After some algebraic manipulation, one can show that conditions (1) and (2) are always satisfied independent of Δt . Thus, the system is unconditionally stable.

The second case in which the stability can be analyzed is the situation in which spatial homogeneity exists. The difference equations can then be written as

$$(1) E^{n+1} - E^n = g[\alpha \phi^n + (1 - \alpha) \phi^{n+1} - \beta E^{n+1} - (1 - \beta) E^n]$$

$$(2) F^{n+1} - F^n = -g(\gamma F^{n+1} + (1 - \gamma) F^n)$$

$$(3) \phi^{n+1} - \phi^n = -\lambda g[\alpha \phi^n + (1 - \alpha) \phi^{n+1} - \beta E^{n+1} - (1 - \beta) E^n]$$

where $g = c\mu\Delta t$, $\lambda = 4a\theta^3/\rho C_v$, and $0 \leq \alpha \leq 1$, $0 \leq \beta \leq 1$, and $0 \leq \gamma \leq 1$.

One notes that the second equation is always stable if $\gamma \geq 1/2$. For the coupled system of Eqs. (1) and (3), one has the following system:

$$\begin{pmatrix} E^{n+1} \\ \phi^{n+1} \end{pmatrix} = C(\Delta t) \begin{pmatrix} E^n \\ \phi^n \end{pmatrix}$$

where $C(\Delta t)$ is as defined previously.

The elements of the amplification matrix are found to be

$$C_{11} = [[1 - g(1 - \beta)][1 + \lambda g(1 - \alpha)] + \lambda g^2(1 - \alpha)(1 - \beta)] / Q$$

$$C_{21} = [\beta \lambda g[1 - g(1 - \beta)] + [1 + g\beta][\lambda g(1 - \beta)]] / Q$$

$$C_{12} = [g\alpha[1 + \lambda g(1 - \alpha)] + g(1 - \alpha)(1 - \lambda g\alpha)] / Q$$

$$C_{22} = [\beta \lambda g^2 \alpha + (1 + g\beta)(1 - \lambda g\alpha)] / Q$$

where $Q = (1 + g\beta)[1 + \lambda g(1 - \alpha)] - \beta \lambda g^2(1 - \alpha)$.

After some reduction, one finds

$$T = \frac{2 - g(1 - 2\beta) + \lambda g(1 - 2\alpha)}{1 + g\beta + g\lambda(1 - \alpha)}$$

and

$$\Delta = \frac{1 - g(1 - \beta + \lambda\alpha)}{1 + g\beta + \lambda g(1 - \alpha)}$$

It is interesting to note that $T = \Delta + 1$. Thus, the characteristic roots are given by

$$\lambda^2 - (\Delta + 1)\lambda + \Delta = 0$$

or

$$\lambda_{1,2} = \frac{\Delta + 1 \pm \sqrt{(\Delta + 1)^2 - 4\Delta}}{2}$$

$$= \begin{cases} \Delta \\ 1 \end{cases}$$

Therefore, for all parameter variations the roots are real and distinct.

The coefficients α , β determine whether the system of equations is implicit and unconditionally stable. For various parameter variations the stability conditions are listed in Table III. It is clear from Table III that the system of equations is unconditionally stable when the equations are partially or fully implicit in both E and ϕ .

Table III
STABILITY CONDITIONS AND ORDER OF ACCURACY

Case	α	β	Description	Accuracy	Stability Conditions
1	0	1	Fully implicit	1st order	Uncond. stab.
2	1/2	1	Fully imp. in E ; partially imp. in ϕ	1st order	Uncond. stab.
3	0	0	Explicit in E ; fully imp. in ϕ	1st order	$\Delta t < \frac{2}{c\mu \left(1 - \frac{4a\theta^3}{\rho C_v}\right)}$
4	1	1/2	Part. imp. in E ; exp. in ϕ	1st order	$\Delta t < \frac{2\rho C_v}{4c\mu a\theta^3}$
5	1	0	Explicit	1st order	$\Delta t < \frac{2}{c\mu \left(1 + \frac{4a\theta^3}{\rho C_v}\right)}$
6	0	1/2	Part. imp. in E ; fully imp. in ϕ	1st order	Uncond. stab.
7	1/2	1/2	Part. imp. in both E, ϕ	2nd order	Uncond. stab.

For this simplified system of equations another problem of interest is the amount of damping in the system. For the second equation one notes that

$$F^{n+1} = \left(\frac{1 - g(1 - \gamma)}{1 + g\gamma} \right) F^n$$

or

$$F^{n+1} = \left[\frac{1 - g(1 - \gamma)}{1 + g\gamma} \right]^n F^0$$

Thus, the solution for the flux has a damping coefficient given by $[1 - g(1 - \gamma)] / (1 + g\gamma)$ when $\gamma \geq 1/2$.

From matrix theory (Ref. 13) one knows that there exists a similarity transformation P such that

$$P^{-1} C P = \begin{bmatrix} 1 & 0 \\ 0 & \Delta \end{bmatrix}$$

or

$$C = P \begin{bmatrix} 1 & 0 \\ 0 & \Delta \end{bmatrix} P^{-1}$$

Thus, the equations can be rewritten as

$$\begin{pmatrix} E^{n+1} \\ \phi_{n+1} \end{pmatrix} = (P) \begin{pmatrix} 1 & 0 \\ 0 & \Delta \end{pmatrix} (P^{-1}) \begin{pmatrix} E^n \\ \phi^n \end{pmatrix}$$

By successive substitution, one has

$$\begin{pmatrix} E^{n+1} \\ \phi_{n+1} \end{pmatrix} = P \begin{pmatrix} 1 & 0 \\ 0 & \Delta^n \end{pmatrix} P^{-1} \begin{pmatrix} E^0 \\ \phi^0 \end{pmatrix}$$

At this point the significance of the roots 1 and Δ becomes apparent. The root 1 corresponds to the steady state solution, and the root Δ is the transient part of the solution. Hence, the damping in the system can be controlled by varying Δ .

1.7. APPENDIX: LISTING OF ERADTN AND PRADTN

```

SUBROUTINE RADTN
C*****DRAD0020
C*          S P U T T E R   C O M M O N          **DRAD0060
C
COMMON LMDA(37), NR , NSMLR , IA , IB , ICA , ICR , DRAD0080
1 KMAX , BLANK1, BLANK2, BLANK3, IAP1 , IBP1 , ICAP1 , ICRP1 , DRAD0090
2 II , IG , NRAD , BLANK4, IAM1 , IBM1 , ICAM1 , ICRM1 , DRAD0100
3 IIP1 , IGM1 , IALPHA, BLANK5, TH , TMAX , BLANK6, DELPRT, DRAD0110
4 FREQ , CNTMAX, AR , ASMLR , PUSHA , PUSHB , BOILA , BOILB , DRAD0120
5 CVA , CVB , SLUG , ALPHA , HVA , HVB , HCA , HCB , DRAD0130
6 EMINA , EMINB , CA , CB , GA , GB , GL , GR , DRAD0140
7 RHOL , RHOR , EPIO , EPSI , RIA , RIB , ROIA , ROIB , DRAD0150
8 RPIA , RPIB , RPDIA , RPOIB , TPRINT, TA , TB , TC , DRAD0160
COMMON TD , TE , DTH2 , DTH2P , DTH1 , DTRMIN, DTMAX , DRAD0170
1 DTMAX1, DTMAX2, DTMAX3, DTR , SWITCH, CO , CMIN , DELTA , DRAD0180
2 GAMA , WCRIT , SIGMAQ, AC , ACO3T4, CNVRT , SUMRA , SUMRB , DRAD0190
3 ROIA , ROIAM1, ROIB , ROIBP1, GMS , S1 , S2 , S3 , DRAD0200
4 S4 , S5 , S6 , S7 , S8 , S9 , S10 , S11 , DRAD0210
5 S12 , S13 , S14 , S15 , S16 , S17 , S18 , S19 , DRAD0220
6 S20 , EO , FO , TAU , ZERO , R (152), DELTAR(152), DRAD0230
7 ASQ (152), RD (152), VO (152), RDD (152), SMLR (152), DRAD0240
8 DELR ( 37), P (152), P1 (152), PB (152), PB1 (152), DRAD0250
COMMON P2 (152), SV (152), RHO (152), THETA (152), DRAD0260
1 W (152), E (152), EI (152), EK (152), A (152), DRAD0270
2 V (152), G (152), D (152), C (152), X2 (152), DRAD0280
3 X3 (152), X4 (152), X5 (152), X6 (152), X7 (152), DRAD0290
4 SMLA (152), SMLB (152), SMLC (152), SMLD (152), SMLE (152), DRAD0300
5 EC (152), ER (152), SMLQ (152), SMLH (152), BIGA (152), DRAD0310
6 BIGB (152), CV (152), BC (152), BR (152), CHIC (152), DRAD0320
7 CHIR (152), CAPAC (152), CAPAR (152), CRTC (152), CRTR (152), DRAD0330
8 CRTPC (152), GOFR (152), FEW (152), CAR (152), OKLM ( 37), DRAD0340
COMMON TELM ( 37), EKLM ( 37), ELM ( 37), FCLM ( 37), DRAD0350
1 FRLM ( 37), WLM ( 37), GLM ( 37), AMASNO( 37), CHRNO ( 37), DRAD0360
2 ZP1 ( 37), ZP2 ( 37), SOLID ( 37), ECHCK ( 37), RK (104), DRAD0370
3 RL ( 37), RHOK (104), RDK (104), THETAK(104), TEMP ( 16), DRAD0380
4 HEAD ( 12), MAXL , MAXLM , DRAD0390
C*          **DRAD0400
C*****DRAD0410
C
DIMENSION RUC(1), OSX2(1), H2(1), Q1(1), GU(1), SU(1), HU(1) DRAD0420
DIMENSION PDFU(1), SUMRHO(1), H(1), SUMX2(1), OLDTH(1) DRAD0430
DIMENSION Q37(1), Q38(1) DRAD0440
DIMENSION OLDE(152,3), OLDF(152,3)
COMMON /LINDLY/ HNU,SGNL,IHNU,NHNU,HNU,NT,IM,IN,DHNU,THICK,NY DRAD0450
COMMON/TQ/QINT1(300),QINT2(300),TITLE(12),FLUX(30) DRAD0460
COMMON /CNTRL/ SCYCLE, JMULT DRAD0470
C
EQUIVALENCE (SMLA,PDFU), (SMLD,SUMRHO) DRAD0480
EQUIVALENCE (BC,OSX2), (BIGB,H), (CRTR,SUMX2), (CHIC,SU) DRAD0490
EQUIVALENCE (SMLH,GU), (CAR,Q37), (CHIR,Q38), (SMLC,OLDTH) DRAD0500
EQUIVALENCE (ACO3T4,TROBG), (S12,EDITMF) DRAD0510
EQUIVALENCE (EC,Q1), (X7,H2), (BIGA,HU ), (GOFR,RUC) DRAD0520
DRAD0530
C
DATA ILMDA /0/
C*****DRAD0550
C          **DRAD0560
C          EDITMF SAME AS S12 **DRAD0570
C          H SAME AS BIGB **DRAD0580
C          H2 SAME AS X7 **DRAD0590
C          OLDTH SAME AS SMLC **DRAD0600
C          PDFU SAME AS SMLA **DRAD0610
C          Q1 SAME AS EC **DRAD0620
C          RUC SAME AS GOFR **DRAD0630
C          Q37 SAME AS CAR **DRAD0640
C          Q38 SAME AS CHIR **DRAD0650
C          SUMX2 SAME AS CRTR **DRAD0660
C

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C          SU      SAME AS  CHIC          *DRAD0670
C          HU      SAME AS  HIGA          *DRAD0680
C          TROBG   SAME AS  AC03T4        *DRAD0690
C          GU      SAME AS  SMLH          *DRAD0700
C          SUMRHO  SAME AS  SMLD          *DRAD0710
C                                           *DRAD0720
C*****DRAD0730
C                                           DRAD0780
C
C      NONEQUILIBRIUM RADIATION DIFFUSION AS IN LA-3377
C
C      FOR DRADTN AND ERADTN. NY (IN LINDLEY COMMON) IS TEMPERATURE
C      ITERATION INDEX. THIS IS USED IN A SPECIAL DIANA THAT GOES WITH
C      DRADTN AND ERADTN.
C                                           DRAD0820
C*****DRAD0830
C
C      INITIALIZATION AND CALCULATION FOR NO VAPOR ZONES
C*****
C                                           DRAD0840
C      CALL DVCHK(KDMY)
C      NTIMES=BOILB          DRAD0850
C      IM=IBM1              DRAD0860
C      IN=IA                DRAD0870
C      IDMHNU = 3
C      IF (KMAX .EQ. 0) DHNU = 1.          DRAD0880
C      IF(ZP1(26).EQ.0.) GO TO 15
C
C      SAVE STUFF FROM EIONX FOR NONEQ AND RESET IN OR IM          DRAD0900
C                                           DRAD0910
C                                           DRAD0920
C      IF (PUSHA .LT. 0.0) GO TO 100      DRAD0930
C      IM = NR - 1                      DRAD0940
C      CALL NONEQ(IM+1,4)                DRAD0950
C      GO TO 15                          DRAD0960
C 100 IN = NR                           DRAD0970
C      CALL NONEQ(IN-1,4)                 DRAD0980
C 15  CONTINUE                          DRAD0990
C      IMP1=IM+1                         DRAD1000
C      INM1=IN-1                         DRAD1010
C      INP1 = IN + 1                     DRAD1020
C      IF (IMP1 - IN) 20, 20, 25
C
C      CALCULATE BLACKBODY EMISSION AND EXIT IF NO VAPOR ZONES      DRAD1040
C                                           DRAD1050
C                                           DRAD1060
C 20  X2(IMP1) = 1.0275E12 * A(IMP1) * (THETA(IM)**4 - THETA(IMP1)**4)
C      ER(IM)=-X2(IMP1)                  DRAD1080
C      GO TO 1300                        DRAD1090
C 25  NVEZ = 1
C      NY = NVEZ
C      IF(CYB.EQ.0.0) NVEZ = 2
C      VEZ = NVEZ
C
C      FORM INTERPOLATION QUANTITIES FOR OPACITY SUBROUTINE
C                                           DRAD1170
C                                           DRAD1210
C      DO 1076 I=IN,IM
C      OSX2(I) = 0.
C      Q37(I)=ALOG(THETA(I))
C                                           DRAD1226
C 1076 Q38(I)=ALOG(SV(I))                DRAD1230
C      OSX2(IMP1) = 0.
C
C      OBTAIN ROSSELAND AND PLANCK OPACITIES FOR ENTIRE SPECTRUM
C      (REQUIRES DIANE TAPE HAVING MONOFREQUENCY OPACITIES FIRST)
C
C      IMNU = 0
C      CALL KAPPA(IN,IM)
C                                           DRAD1240
C                                           DRAD1250

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AFWL-TR-66-108, Vol I

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C*****DRAD1260
C                                     DRAD1270
C      M I N I M U M   T I M E   S T E P   C A L C U L A T I O N   DRAD1280
C                                     DRAD1290
C*****DRAD1300
      WSB = 0.0
      DO 1075 I = 1, MAXLM
1075  WSB = WSB + ELM(I)
      DTR1=1.E10
      DTR2=1.E10
1080 DO 1230 I=IN,IM
C                                     DRAD1310
C                                     DRAD1320
C                                     DRAD1330
C      CALL UNCLE IF EITHER KAPPA IS ZERO OR NEGATIVE   DRAD1340
C                                     DRAD1350
C                                     DRAD1360
C      IF (AMIN1(CAPAC(I), CAPAR(I)) .GT. 0.0) GO TO 1120   DRAD1370
C      S1=13.1090   DRAD1380
C      CALL UNCLE   DRAD1390
C
C      SOLID(10) NOT ZERO GIVES ALL ROSSELAND OPTION
C
1120 IF (SOLID(10).EQ.0.0) GO TO 1123
      TEMP(1) = CAPAR(I)
      TEMP(3) = CAPAR(I)
      GO TO 1125
1123 TEMP(1)=SQRT(CAPAR(I)*CAPAC(I))
      TEMP(3) = CAPAC(I)
1125 IF (0.001 - THETA(I)) 1160,1230,1230   DRAD1480
1160 H(I) = 0.5 * TEMP(1) / SV(I) * DELTAR(I)   DRAD1490
      TEMP(1) = 1.E10   DRAD1500
      TEMP(2) = 1.E10   DRAD1510
      IF (TELM(37) .EQ. 0.0 .OR. ER(I) .EQ. 0.0) GO TO 1170
      WSB = E(I) * G(I)   DRAD1530
      IF (WSB - TELM(37) * WSB) 1170, 1165, 1165   DRAD1550
C                                     DRAD1560
C      ACCURACY CRITERION - DONE FOR FULLY AND PARTIALLY IMPLICIT CASES
C                                     DRAD1580
1165 TEMP(1) = SLUG * WSB / ABS(ER(I))
1170 IF (KMAX .EQ. 0 .AND. HVB .NE. 0.0) GO TO 1172   DRAD1600
C                                     DRAD1610
C      STABILITY CRITERION -- BYPASSED IN FULLY IMPLICIT CASE   DRAD1620
C                                     DRAD1630
      TEMP(2) = CV(I) / (2.066E12*TEMP(3)*THETA(I)**3)
      TEMP(3) = TEMP(2)*3.*H(I)**2
      TEMP(2) = AMIN1(TEMP(2),TEMP(3))
1172 TEMP(2) = AMIN1(TEMP(1), TEMP(2))
      TEMP(2) = TEMP(2)*TELM(25)
C
C      FIND MINIMUM TIME STEP   DRAD1680
C
      IF (TEMP(2)) 1230,1230,1190   DRAD1700
1190 IF (TEMP(2)-DTR1) 1200,1210,1210   DRAD1710
1200 DTR2=DTR1   DRAD1720
      IMN2=IMN1   DRAD1730
      DTR1=TEMP(2)   DRAD1740
      IMN1=I   DRAD1750
      GO TO 1230   DRAD1760
1210 IF (TEMP(2)-DTR2) 1220,1230,1230   DRAD1770
1220 DTR2=TEMP(2)   DRAD1780
      IMN2=I   DRAD1790
1230 CONTINUE   DRAD1800
      DTRMIN=DTR1   DRAD1810
      EO=IMN1   DRAD1820
C                                     DRAD1830
C      SET UP MINIMUM TIME STEPS BETWEEN EDITS   DRAD1840
C                                     DRAD1850

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AFWL-TR-66-108, Vol I

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IF (DTR1-TELM(26)) 1240,1250,1250
1240 TELM(26)=DTR1
      TELM(27)=IMN1
      TELM(28)=DTR2
      TELM(29)=IMN2
      TELM(30)=SOLID(18)+1.0
1250 CONTINUE
C
C      DETERMINE IF RADIATION OR HYDRO WILL SUBCYCLE
C
      IF(DTRMIN-DTR) 1280,125,1260
1260 BLANK3=TH+AMIN1(DTRMIN,GR*OTH2)
      IF(S17) 125,1270,125
1270 S9 = 1.0
      GO TO 125
C
C      REDUCE TIME STEP
C
1280 NRAD=ZP1(18)/DTRMIN+1.0
      DTR=ZP1(18)/FLOAT(NRAD)
      IF(NRAD-NTIMES) 125,125,1290
1290 S1=13.1290
      CALL UNCLE
      125 THTAMX=.025
C*****
C
C      CALCULATE GEOMETRY FACTORS AND FIND HIGHEST TEMPERATURE
C*****
      DO 180 I=IN,IM
      GO TO (132, 134, 136), IALPHA
C
C      SLABS
C
132 PDFU(I) = 1. / (C(I+1) - C(I))
      RUC(I+1)=5.0E9 / (C(I+2) - C(I))
      GO TO 138
C
C      CYLINDERS
C
134 PDFU(I) = 1. / (C(I+1)**2 - C(I)**2)
      RUC(I+1)=1.0E10 * C(I+1) / (C(I+2) - C(I))
      GO TO 138
C
C      SPHERES
C
136 PDFU(I) = 1. / (C(I+1)**3 - C(I)**3)
      RUC(I+1)=1.5E10 * C(I+1)**2 / (C(I+2) - C(I))
138 IF (THETA(I) .LE. THTAMX) GO TO 180
      THTAMX=THETA(I)
180 CONTINUE
      IF (THTAMX .LT. THETA(18) .AND. GL .GT. 0.) THTAMX = THETA(18)
      IF (THTAMX .LT. THETA(1A-1) .AND. GA .GT. 0.) THTAMX = THETA(1A-1)
      GO TO (182, 184, 186), IALPHA
C
C      BOUNDARY QUANTITIES
C
182 TSLH = 1.
      TSRH = 1.
      GO TO 188
184 TSLH = C(IN) + C(IN)
      TSRH = C(IMP1) + C(IMP1)
      GO TO 188
186 TSLH = 3. * C(IN)**2
      TSRH = 3. * C(IMP1)**2

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DRAD1860
 DRAD1870
 DRAD1880
 DRAD1890
 DRAD1900
 DRAD1910
 DRAD1920
 DRAD1930
 DRAD1940
 DRAD1950
 DRAD1960
 DRAD1970
 DRAD1980
 DRAD1990
 DRAD2000

 DRAD2020

 DRAD2040
 DRAD2050
 DRAD2060
 DRAD2070
 DRAD2080
 DRAD2090
 DRAD2100
 DRAD2110
 DRAD2120
 DRAD2130
 DRAD2140
 DRAD2150
 DRAD2160
 DRAD2170
 DRAD2180
 DRAD2190
 DRAD2200
 DRAD2210
 DRAD2220
 DRAD2230
 DRAD2240
 DRAD2250
 DRAD2260
 DRAD2270
 DRAD2280
 DRAD2290
 DRAD2300
 DRAD2310
 DRAD2320
 DRAD2330
 DRAD2340
 DRAD2350
 DRAD2360
 DRAD2370
 DRAD2380
 DRAD2390
 DRAD2400

 DRAD2420
 DRAD2430
 DRAD2440
 DRAD2450
 DRAD2460
 DRAD2470
 DRAD2480
 DRAD2490
 DRAD2500

AFWL-TR-66-108, Vol I

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188 CDT = 1.2E11 * DTR
    HCDT = 1. / CDT
    ROTH = 1. / DTR
    CALL DVCHK(KDMY)
    GO TO (190, 200), KDMY
190 S1 = 13.0190
    CALL UNCLE

C
C      ZERO X3, X4, X5, X6 (IN CASE MERGE FREQUENCIES)
C      AND ER, SUMX2, SUMRHO (FOR FREQUENCY INTEGRATION)
C
200 DO 210 I=IN,IM
    X3(I)=0.
    X4(I)=0.
    X5(I)=0.
    X6(I)=0.
    ER(I) = 0.
    SUMX2(I) = 0.
    SUMRHO(I) = 0.

C
C      SET UP FOR KAPPA INTERPOLATION
C
210 Q1(I)=THETA(I)**4
    SUMX2(IMP1) = 0.

C
C      *****
C      BEGIN FREQUENCY LOOP
C      *****
C      SET UP MAX FREQ BOUNDARY
C
    HNUP=1.0E6
    HNUP4=1.0E24
    IF (KMAX.EQ.0) GO TO 280
220 IHNU = IHNU +1
    CALL KAPPA(IN,IM)
    HNU4=HNUP**4
    DHNU = DHNU
    DHNU = HNUP - HNU

C
C      MERGE GROUPS WITH HNU MORE THAN CB TIMES LARGEST THETA
C      DON'T KNOW HOW TO MERGE E AND F. NO MERGE FOR NOW
C
    CB=1.0E10

C
    IF (CB .GT. 0.0) GO TO 225
    S1 = 13.022
    CALL UNCLE
225 IF (TH*AMX - HNU / CB) 240, 230, 230
230 IF (IHNU - 1) 235, 370, 260
235 S1 = 13.0235
    CALL UNCLE

C
C      REJECT TAPE IF MORE THAN HALF OF GROUPS MERGE
C
240 IF (IHNU+IHNU-NHNU) 260,250,250
250 IF (AMOD(CB,1.) .EQ. 0.5) GO TO 260
    S1=13.0250
    CALL UNCLE
260 DO 270 I=IN,IM
    BETA=HNU/THETA(I)

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ORAD2520

ORAD2540

ORAD2550

ORAD2560

ORAD2570

ORAD2580

ORAD2590

ORAD2600

ORAD2610

ORAD2620

ORAD2630

ORAD2640

ORAD2650

ORAD2660

ORAD2670

ORAD2680

ORAD2690

ORAD2700

*ORAD2710

*ORAD2720

*ORAD2730

ORAD2740

ORAD2750

ORAD2760

ORAD2770

ORAD2780

ORAD2790

ORAD2800

ORAD2810

ORAD2820

ORAD2830

ORAD2840

ORAD2850

ORAD2860

ORAD2870

ORAD2880

ORAD2890

ORAD2900

ORAD2910

ORAD2920

ORAD2930

ORAD2940

ORAD2950

ORAD2960

ORAD2970

ORAD2980

ORAD2990

ORAD3000

ORAD3010

ORAD3020

ORAD3030

ORAD3040

<pre> BETAP=HNUP/THETA(I) DFB=PLNKUT(BETA,BETAP) IF (DFB.EQ.0.) GO TO 270 TEMP(1)=DFB*Q1(I) EMB1=EXP(-BETA) EMB2=EXP(-BETAP) TEMP(2)=DFB+0.0384974/Q1(I)*(HNUP/(1.0-EMB1) I*EMB1-HNUP4/(1.0-EMB2)*EMB2) </pre>	<pre> DRAD3050 DRAD3060 DRAD3070 DRAD3080 DRAD3090 DRAD3100 DRAD3110 DRAD3120 DRAD3130 DRAD3140 DRAD3150 DRAD3160 DRAD3170 DRAD3180 DRAD3190 DRAD3200 DRAD3210 DRAD3220 DRAD3230 DRAD3240 DRAD3250 DRAD3260 DRAD3270 DRAD3280 DRAD3290 DRAD3300 DRAD3310 DRAD3320 DRAD3330 DRAD3340 DRAD3350 DRAD3360 DRAD3370 DRAD3380 DRAD3390 DRAD3400 DRAD3410 DRAD3420 DRAD3430 DRAD3440 DRAD3450 DRAD3460 DRAD3470 </pre>
<pre> C C FORM NUMERATORS AND DENOMINATORS OF MERGED KAPPAS C X6(I)=X6(I)+TEMP(1) X4(I)=X4(I)+TEMP(2) X5(I)=X5(I)+CAPAC(I)*TEMP(1) X3(I)=X3(I)+TEMP(2)/CAPAR(I) 270 CONTINUE HNUP=HNU HNUP4=HNUP4 IF (THTAMX- HNUP/CB) 220,310,310 </pre>	<pre> DRAD3490 DRAD3500 DRAD3510 DRAD3520 DRAD3530 DRAD3540 DRAD3550 DRAD3560 DRAD3580 </pre>
<pre> C C FORM MERGED KAPPAS C 310 DO 350 I=IN,IM IF (X6(I)) 320,350,330 320 S1=13.0320 CALL UNCLE 330 CAPAR(I)=X4(I)/X3(I) CAPAC(I)=X5(I)/X6(I) 350 CONTINUE HNUP=1.0E6 HNUP4=1.0E24 DHNU = HNUP - HNU GO TO 480 </pre>	<pre> DRAD3600 DRAD3610 DRAD3620 </pre>
<pre> C C MONOFREQUENCY CALCULATION C 280 NHNU=1 IHNU = 1 DO 290 I=IN,IM 290 X6(I)=Q1(I) HNU = .001 GO TO 480 </pre>	<pre> DRAD3640 </pre>
<pre> C C FREQUENCY GROUP CALCULATION OF SOURCES C 360 IHNU = IHNU +1 CALL KAPPA(IN,IM) DHNU=HNUP-HNU HNU4=HNU**4 370 DO 392 I = IN, IM DFB = PLNKUT(HNU / THETA(I), HNUP / THETA(I)) 392 X6(I)=DFB*Q1(I) </pre>	
<pre> C C SET BOUNDARY CONDITION FOR LEFT HAND SIDE C 480 IF (INM1) 490, 510, 500 490 S1=13.0490 CALL UNCLE 500 IF(KMAX .EQ. 0) GO TO 501 IF (THETA(INM1) .LE. 0.0) THETA(INM1) = 1.0E-5 DFB=PLNKUT(HNU/THETA(INM1),HNUP/THETA(INM1)) GO TO 502 501 DFB=1. 502 CONTINUE HBSL = DFB * THETA(INM1)**4 </pre>	

AFWL-TR-66-108, Vol I

C	GO TO 520	DRAD3650
C		DRAD3660
C	NO BOUNDARY CONDITION FOR GA .GT. 0.0	
C		DRAD3680
C	510 IF (GA .GT. 0.0) GO TO 515	DRAD3690
C	IF (GA .EQ. 0.0) BBSL = 0.	DRAD3700
C	GO TO 520	DRAD3710
C	515 S1 = 13.0515	DRAD3720
C	CALL UNCLE	DRAD3730
C		DRAD3740
C	SET BOUNDARY CONDITION FOR RIGHT HAND SIDE	
C		DRAD3760
C	520 IF (GL .EQ. 0.0) X6(IMP1)=0.0	DRAD3770
C	IF (GL.NE.0.5) GO TO 530	DRAD3780
C	IF (KMAX .NE. 0) GO TO 522	
C	DFB = 1.	
C	GO TO 525	
C	522 DFB = PLNKUT(HNU / THETA(IMP1), HNU / THETA(IMP1))	ERAD3790
C	525 X6(IMP1) = DFB * THETA(IMP1)**4	ERAD3800
C		DRAD3810
C	SPECIAL RIGHT BOUNDARY SOURCE (GL A POSITIVE	DRAD3820
C	INTEGER) NOW INCLUDED	
C		DRAD3840
C	530 IF (GL.GT.0.5) X6(IMP1) = FLUX (IHNU)	DRAD3850
C	LBR=-X6(IMP1)	DRAD3860
C		DRAD3870
C	FORM ROSSELAND AND PLANCK OPTICAL DEPTHS	DRAD3880
C		DRAD3890
C	H3M = CAPAR(IN) / SV(IN) * DELTAR(IN)	DRAD3900
C	DO 580 I=IN,IM	DRAD3910
C	IF (AMIN1(CAPAC(I), CAPAR(I)) .GT. 0.0) GO TO 560	DRAD3920
C	S1=13.0550	DRAD3930
C	CALL UNCLE	DRAD3940
C		DRAD3950
C	FOR NONEQUILIBRIUM DIFFUSION, H AND H2	DRAD3960
C	ARE MU AND (1./(4.*LAMBDA)) RESPECTIVELY.	DRAD3970
C		DRAD3980
C	560 H(I) = CAPAC(I) / SV(I) * 1.5E10	DRAD3990
C	IF (SOLID(10).NE.0.0) H(I) = H(I)*CAPAR(I)/CAPAC(I)	DRAD4000
C	SU(I) = 2.74E2 * H(I) * X6(I)	DRAD4010
C	IF (I .EQ. IM) GO TO 580	DRAD4020
C		DRAD4030
C	WARNING - ASYNCHRONISMS IN SV AND DELTAR LEAD TO	DRAD4040
C	ERRONEOUS FLUCTUATIONS IN H3. THIS CAN BE FIXED	DRAD4050
C	BY SUBSTITUTING G IN PLANES, BUT SPHERES WILL	DRAD4060
C	STILL HAVE THIS TROUBLE.	DRAD4070
C		DRAD4080
C	576 H3P = CAPAR(I+1) / SV(I+1) * DELTAR(I+1)	DRAD4090
C		
C	FOR SHARP CHANGES IN OPTICAL DEPTH, USE THINNER ZONE TO DEFINE H2	
C	CAVEAT. TROUBLE IN SCATTERING PROBLEMS - CODE CHANGES SOON	
C		DRAD4100
C	IF (ABS(H3M-H3P)/(H3M+H3P).LE.AC) GO TO 578	DRAD4110
C	H2(I+1)=.25*AMIN1(H3M/DELTAR(I),H3P/DELTAR(I+1))	DRAD4120
C	GO TO 580	DRAD4130
C	578 H2(I+1) = (H3M + H3P) * 0.25/ (DELTAR(I) + DELTAR(I+1))	DRAD4170
C	580 H3M = H3P	
C		
C	INITIALIZE E SUPER N AND F SUPER N	
C		
C	IF (NVEZ .EQ. 2 .AND. CVB .NE. 0.0) GO TO 592	
C	IF (SOLID(18) .GT. 0.0 .AND. LMDA(26) .EQ. 0) GO TO 585	
C	LMDA(26) = 0	
C	DO 583 I = IN, IM	

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      OLDE(I,IHNU) = 157.0 * X6(I)
583  OLDF(I,IHNU) = 0.0
      OLDF(IMP1,IHNU) = 0.0
      GO TO 592
585  IF (SOLID(18) .GT. 5CYCLE .OR.  ILMDA .EQ. 12345) GO TO 592
587  READ (13)  TESTC, (OLDE(I,IHNU), OLDF(I,IHNU), I=1,152)
      IF (IHNU .GT. 1) GO TO 592
      IF (TESTC - SOLID(18)) 587, 592, 590
590  S1 = 13.0590
      CALL UNCLE

C
C      EXTRAPOLATION COEFFICIENTS TO FORM RADIATION
C      ENERGIES AT BOUNDARIES
C
592  BETA1 = 1.0 / (2.0 - EXP(-DELTAR(IN) * SQRT(CAPAR(IN) * H(IN) *
      2 5.0E-11 / SV(IN))))
      BETA2 = 1.0 / (2.0 - EXP(-DELTAR(IM) * SQRT(CAPAR(IM) * H(IM) *
      2 5.0E-11 / SV(IM))))
      CALL DVCHK(KDUMY)
      GO TO (588, 589), KDUMY
588  S1 = 13.0588
      CALL UNCLE
C*****DRAD4260
C      NONEQUILIBRIUM DIFFUSION TREATMENT
C      FORM COEFFICIENTS OF IMPLICIT EQUATIONS
C*****DRAD4320
589  IF(INP1-IM) 593,593,1500
C      SPECIAL CASE - SINGLE VAPOR ZONE
C
1500 CONTINUE
      BU = 2.*H(IN) +1.5E10*(TSRH*BETA2 +TSLH*BETA1)*PDFU(IN)+RDTR
      DU=2.055E12*PDFU(IN)*(BBSL*TSLH*BETA1-BBR*TSRH*BETA2)
      1  +RDTR*OLDE(IN,IHNU)
      IF(KMAX.EQ.0.AND.HVB.NE.0.0)GO TO 1550
C      PARTIALLY IMPLICIT - MULTIFREQUENCY CASE
C
1530 CONTINUE
      RHO(IN)=(SU(IN)+DU)/BU
      GO TO 669
C      FULLY IMPLICIT TERMS
C
1550 GO TO(1595,1596),NVEZ
C      NO ITERATION
C
1595 T4=G1(IN)
      GO TO 1597
1596 IF(CVB.EQ.0.0)GO TO 1595
C      ITERATION
C
      J4=OLDTH(IN)**4
1597 TEMP(1)=5.48E2*THETA(IN)**3
      TEMP(2)=G(IN)*RDTR*CV(IN)
      DENOM=TEMP(2)/H(IN)+TEMP(1)/PDFU(IN)
      BU=BU-2.*H(IN)/PDFU(IN)*TEMP(1)/DENOM
      SU(IN) = (SMLQ(IN) - (PB1(IN) + P(IN)) * VD(IN)) *(TEMP(1) /
      2 DENOM)- (TEMP(2)/DENOM) * 2.74E2 * T4

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AFWL-TR-66-108, Vol I

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C
C
C
GO TO 1530
LEFT-HAND BOUNDARY CONDITION
593 QU1 = 1. / (RCDT + H2(IN+1))
RU1 = RUC(IN+1) * QU1
CU = -PDFU(IN) * RU1
DU = RDTR + H(IN) + H(IN)
DU = -RDTR*OLDE(IN, IHNU) + PDFU(IN)*QU1*RCDT*OLDF(IN+1, IHNU)
IF (KMAX .EQ. 0 .AND. HVB .NE. 0.0) GO TO 594
DU = DU - SU(IN)
GO TO 598
FULLY IMPLICIT TERMS
594 GO TO (595, 596), NVEZ
NO ITERATION
595 T4 = Q1(IN)
GO TO 597
596 IF (CVB .EQ. 0.0) GO TO 595
ITERATION
T4 = OLDTH(IN)**3
597 TEMP(1) = 5.48E2 * THETA(IN)**3
TEMP(2) = G(IN) * RU1 * CV(IN)
DENOM = TEMP(2) / H(IN) + TEMP(1) / PDFU(IN)
BU = BU - 2.*H(IN)/PDFU(IN) * TEMP(1) / DENOM
DU = DU - (SMLQ(IN) - (PB1(IN) +
2 P(IN)) * VD(IN)) * (TEMP(1) / DENOM) - (TEMP(2)/DENOM)*2.74E2*T4
598 IF (INM1) 490, 600, 610
600 IF (GA .LT. 0.0) GO TO 620
610 TS1 = PDFU(IN) * TSLH * 1.5E10 * BETA1
BU = BU + TS1
DU = DU - TS1 * 137.0 * BBSL
620 GU(IN) = BU / (CU - BU)
HU(IN) = DU / (CU - BU)
IF (INP1-IM) 630, 650, 625
625 S1 = 13.0625
CALL UNCLE
GENERAL CASE -- FORWARD PASS
630 IMM1 = IM - 1
DO 640 I = INP1, IMM1
QU2 = 1. / (RCDT + H2(I+1))
RU2 = RUC(I+1) * QU2
AU = -PDFU(I) * RU2
CU = -PDFU(I) * RU2
BU = RDTR + H(I) + H(I)
DU = -RDTR * OLDE(I, IHNU) + PDFU(I) * RCDT * (QU2 * OLDF(I+1, IHNU)
1 -QU1 * OLDF(I, IHNU))
IF (KMAX .EQ. 0 .AND. HVB .NE. 0.0) GO TO 634
DU = DU - SU(I)
GO TO 638
FULLY IMPLICIT TERMS
634 GO TO (635, 636), NVEZ
NO ITERATION
635 T4 = Q1(I)

```

DRAD4690
DRAD4700
DRAD4710
DRAD4720

DRAD4740

DRAD4770
DRAD4780
DRAD4790
DRAD4800
DRAD4810
DRAD4820
DRAD4830
DRAD4840
DRAD4850
DRAD4860
DRAD4870
DRAD4880
DRAD4890
DRAD4900
DRAD4910
DRAD4920
DRAD4930
DRAD4940
DRAD4950
DRAD4960
DRAD4970

DRAD5000
DRAD5010
DRAD5020
DRAD5030
DRAD5040

DRAD5070
DRAD5080
DRAD5090
DRAD5100
DRAD5110
DRAD5120
DRAD5130
DRAD5140

DRAD5160
DRAD5170

DRAD5200
DRAD5210
DRAD5220
DRAD5230
DRAD5240
DRAD5250
DRAD5260
DRAD5270
DRAD5280
DRAD5290
DRAD5300

```

GO TO 637
636 IF (CVB .EQ. 0.0) GO TO 635
C
C      ITERATION
C
T4 = OLDTH(I)**4
637 TEMP(1) = 5.48E2 * THETA(I)**3
TEMP(2) = G(I) * RDTR * CV(I)
DENOM = TEMP(2) / H(I) + TEMP(1) / PDFU(I)
BU = BU - 2.*H(I)/PDFU(I) * TEMP(1) / DENOM
DU = DU - (SMLQ(I) - (PB1(I) +
2 P(I)) * VD(I)) * (TEMP(1) / DENOM) - (TEMP(2)/DENOM) * 2.74E2 * T4*****
638 DENOM = BU - CU + AU*GU(I-1)
GU(I) = (-BU - AU*GU(I-1)) / DENOM
HU(I) = -(DU + AU * HU(I-1)) / DENOM
QU1 = QU2
RU1 = RU2
640 CONTINUE
C
C      RIGHT-HAND BOUNDARY CONDITION
C
650 AU = -PDFU(IM) * RU1
BU = RDTR + H(IM) + H(IM)
DU = -RDTR * OLDE(IM,IHNU) - PDFU(IM) * RCDT * QU1 * OLDF(IM,IHNU)
IF (KMAX .EQ. 0 AND. HVB .NE. 0.0) GO TO 654
DU = DU - SU(IM)
GO TO 658
C
C      FULLY IMPLICIT TERMS
C
654 GO TO (655, 656), NVEZ
C
C      NO ITERATION
C
655 T4 = Q1(IM)
GO TO 657
656 IF (CVB .EQ. 0.0) GO TO 655
C
C      ITERATION
C
T4 = OLDTH(IM)**4
657 TEMP(1) = 5.48E2 * THETA(IM)**3
TEMP(2) = G(IM) * RDTR * CV(IM)
DENOM = TEMP(2) / H(IM) + TEMP(1) / PDFU(IM)
BU = BU - 2.*H(IM)/PDFU(IM) * TEMP(1) / DENOM
DU = DU - (SMLQ(IM) - (PB1(IM) +
2 P(IM)) * VD(IM)) * (TEMP(1) / DENOM) - (TEMP(2)/DENOM)*2.74E2*T4 *****
658 IF (GL .LT. 0.) GO TO 660
TS1 = PDFU(IM) * TSRH * 1.5E10 * BETA2
BU = BU + TS1
DU = DU + TS1 * 137.0 * BBR
660 GU(IM) = -1.
HU(IM) = -(DU + AU * HU(IM-1)) / (BU + AU * GU(IM-1))
C*****
C
C      FORM RADIATION ENERGY, FLUX AND RADIATION SOURCE ER.
C
C*****
DO 670 I = IN, IM
IBK = IN + IM - I
RHO(IBK) = (GU(IBK) + 1.) * RHO(IBK+1) + HU(IBK)
IF (RHO(IBK) .GE. 0.0) GO TO 670
S1 = 13.0669
CALL UNCLE
670 CONTINUE

```

DRAD5310
 DRAD5320
 DRAD5330
 DRAD5340
 DRAD5350
 DRAD5360
 DRAD5370
 DRAD5380
 DRAD5390
 DRAD5400

 DRAD5450
 DRAD5460
 DRAD5470
 DRAD5480
 DRAD5490
 DRAD5500
 DRAD5510
 DRAD5540
 DRAD5550
 DRAD5560
 DRAD5570
 DRAD5580
 DRAD5590
 DRAD5600
 DRAD5610
 DRAD5620
 DRAD5630
 DRAD5640
 DRAD5650
 DRAD5660
 DRAD5670
 DRAD5680
 DRAD5690
 DRAD5700
 DRAD5710
 DRAD5720
 DRAD5730
 DRAD5740

 DRAD5770
 DRAD5780
 DRAD5790
 DRAD5800
 DRAD5830
 DRAD5840
 DRAD5860
 DRAD5870
 DRAD5880
 DRAD5890
 DRAD5910
 DRAD5920
 DRAD5930
 DRAD5940

AFWL-TR-66-108, Vol I

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C
C      CHECK ON BOUNDARY X2'S BYPASSED FOR NOW
C
669 IF(INM1)490,671,673
671 IF (GA) 672, 673, 673
672 X2(IN) = 0.0
    GO TO 674
673 X2(IN) = (2.055E12*BBSL -1.5E10*RHO(IN))*TSLH*BETA1
674 IF(GL)675,678,678
675 X2(IMP1) = 0.0
    GO TO 679
678 X2(IMP1) = (2.055E12*BBR +1.5E10*RHO(IM))*TSRH*BETA2
    IF(IM-INP1)700,679,679
C
C      FORM FLUXES
C
679 DO 680 I = INP1, IM
680 X2(I) = (RCDT * OLDF(I,IHNU) + RUC(I) * (HU(I-1)
    1 + GU(I-1) * RHO(I))) / (RCDT + H2(I))
    CALL DVCHK(KDMY)
    GO TO (690, 700), KDMY
690 S1 = 13.0690
    CALL UNCLE
C
C      FORM RADIATION CONTRIBUTION TO ZONE ENERGY
C
700 DO 710 I = IN, IM
    ER(I)=ER(I)+X2(I)-X2(I+1)+RDTR/PDFU(I)*(OLDE(I,IHNU)-RHO(I))
    GO TO (710, 704), NVEZ
704 OLDE(I,IHNU) = RHO(I)
    OSX2(I) = OSX2(I) + OLDF(I,IHNU)
    OLDF(I,IHNU) = X2(I)
710 CONTINUE
    IF (NVEZ .NE. 2) GO TO 990
    OSX2(IMP1) = OSX2(IMP1) + OLDF(IMP1,IHNU)
    OLDF(IMP1,IHNU) = X2(IMP1)
C*****
C
C      OPTIONAL EDIT OF X2 ETC.
C
C*****
990 CNT1=SOLID(18)+1.0
    CNT2=AMIN1(TPRINT,CNTMAX)
    IF (CNT1 .LT. CNT2) GO TO 1020
    F (SOLID(18) .EQ. SCYCLE .OR. NVEZ .EQ. 1
    1 .OR. (ZP1(18)/DTR) .GT. 1.5) GO TO 1000
    WRITE (13) CNT1, (OLDE(I,IHNU), OLDF(I,IHNU), I=1,152)
1000 IF (EDITMF .EQ. 0.0) GO TO 1020
    TEMP(1) = TH + DTR
    WRITE (6,3) CNT1, TEMP(1), MHNU, NVEZ
    WRITE (6,4)
    H(IMP1) = 0.
    H2(IMP1) = 0.
    GU(IMP1) = 0.
    HU(IMP1) = 0.
    RHO(IMP1) = 0.
    DO 1010 I = IN, IMP1
1010 WRITE (6,5) I,THETA(I),X6(I),H(I),H2(I),GU(I),HU(I),RHO(I),X2(I)
    3 FORMAT (9H1CYCLE = F7.0, 9H TIME = E13.6, 4X11MHNU(LOWER)=F10.4,
    2 10H PASS NO. 11/)
    4 FORMAT (7X1HI, 9X5HTHETA, 12X2HX6, 13X1HH, 12X2HH2, 12X2HGU,
    2 12X2HHU, 11X3HRHO, 12X2HX2)
    5 FORMAT (18, 1P8E14.7)
C
C      ADVANCE FREQ, STORE EMERGENT FLUX, TEST FOR COMPLETION OF GROUPS
C

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DRAD5950
 DRAD5960
 DRAD5970
 DRAD5980
 DRAD5990
 DRAD6000
 DRAD6010
 DRAD6030
 DRAD6040
 DRAD6050
 DRAD6070
 DRAD6080
 DRAD6090
 DRAD6100
 DRAD6110
 DRAD6130
 DRAD6140
 DRAD6150
 DRAD6160
 DRAD6170
 DRAD6180
 DRAD6190
 DRAD6200
 DRAD6220
 DRAD6230
 DRAD6240
 DRAD6250
 DRAD6260
 DRAD6270
 DRAD6280
 DRAD6290
 DRAD6300
 DRAD6390
 DRAD6400

C		DRAD6410
1020	DO 1030 I=IN,IMP1	DRAD6420
	SUMRHO(I) = SUMRHO(I) + RHO(I)	DRAD6430
	SUMX2(I)=SUMX2(I)+X2(I)	DRAD6440
1030	CONTINUE	DRAD6450
	CALL DVCHK (K000FX)	DRAD6460
	GO TO (1050,1040), K000FX	DRAD6470
1040	IF (IHNU .GT. IDMHNU) GO TO 1050	
	HNUP=HNH	
	HNUP4=HNH4	DRAD6490
	IF (IHNU=HNHNU) 360,1060,1050	DRAD6500
C	*****	DRAD6510
C		*DRAD6520
C	END FREQUENCY LOOP	*DRAD6530
C		*DRAD6540
C	*****	DRAD6550
1050	S1 = 13.1050	DRAD6560
	CALL UNCLE	DRAD6570
C		DRAD6580
C	ITERATE ON TEMPERATURE IF NVEZ EQUALS ONE	DRAD6590
C		DRAD6600
1060	ILMDA=12345	
	GO TO (1061, 1065), NVEZ	
1061	NVEZ = 2	DRAD6620
	VEZ = NVEZ	DRAD6630
	NY = NVEZ	DRAD6640
	IHNU=0	DRAD6650
	DO 1062 I = IN, IM	DRAD6660
	BNTH = THETA(I) + (SMLQ(I) + ER(I) - (PB1(I) + P(I)) * VD(I)) *	DRAD6670
	2 DTR / (G(I) * CV(I))	DRAD6680
	OLDTH(I) = THETA(I)	DRAD6690
	THETA(I) = 0.5 * (OLDTH(I) + BNTH)	DRAD6700
1062	Q37(I)=ALOG(THETA(I))	DRAD6710
	IF (KMAX.EQ. 0) CALL KAPPA(IN,IM)	DRAD6720
	GO TO 200	DRAD6730
1065	IF (CVB .EQ. 0.0) GO TO 1067	DRAD6740
	DO 1066 I = IN, IM	DRAD6750
1066	THETA(I) = OLDTH(I)	DRAD6760
C		DRAD6770
C	SET UP FOR ENCALC	DRAD6780
C		DRAD6790
1067	DO 1070 I = IN, IMP1	DRAD6800
	Q1(I) = 0.	DRAD6810
	RHO(I) = SUMRHO(I)	DRAD6820
1070	X2(I) = SUMX2(I)	DRAD6830
1300	IF (ZP1(26) .EQ. 0.0) GO TO 1400	DRAD6840
C		DRAD6850
C	RESTORE NONEQ QUANTITIES	
C		DRAD6870
	IF (PUSHA .LT. 0.0) GO TO 1350	DRAD6880
	CALL NONEQ(IMP1,5)	DRAD6890
	GO TO 1400	DRAD6900
1350	CALL NONEQ(INM1,5)	DRAD6910
1400	RETURN	DRAD6920
	END	DRAD6921

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SUBROUTINE RADTN
C*****ERAD 0
C*****ERAD 10
C*****ERAD 20
C*      S P U T T E R   C O M M O N          **ERAD 30
C*                                           *ERAD 40
COMMON LMUA(37), NR , NSMLR , IA , IB , ICA , ICB , ERAD 50
1 KMAX , BLANK1, BLANK2, BLANK3, IAP1 , IBP1 , ICAP1 , ICBP1 , ERAD 60
2 II , IG , NRAD , BLANK4, IAM1 , IBM1 , ICAM1 , ICPM1 , ERAD 70
3 IIP1 , IGM1 , IALPHA, BLANK5, TH , TMAX , BLANK6, DFLPRT, ERAD 80
4 FREQ , CNTMAX, AR , ASMLR , PUSHA , PUSHB , BOILA , FOILB , ERAD 90
5 CVA , CVB , SLUG , ALPHA , HVA , HVB , HCA , HCB , ERAD 100
6 EMINA , EMINB , CA , CB , GA , GB , GL , GR , ERAD 110
COMMON TD , TE , DTH2 , DTH2P , DTH1 , DTRMIN, DTMAX , ERAD 140
1 DTMAX1, DTMAX2, DTMAX3, DTR , SWITCH, CO , CMIN , DELTA , ERAD 150
2 GAMA , WCRIT , SIGMAQ, AC , ACO3T4, CNVRT , SUMRA , SUMRB , ERAD 160
3 ROIA , ROIAM1, ROIB , ROIBP1, GMS , S1 , S2 , S3 , ERAD 170
4 S4 , S5 , S6 , S7 , S8 , S9 , S10 , S11 , ERAD 180
5 S12 , S13 , S14 , S15 , S16 , S17 , S18 , S19 , ERAD 190
6 S20 , EO , FO , TAU , ZERO , R (152), DELTAR(152), ERAD 200
7 ASQ (152), RD (152), VD (152), RDD (152), SMLR (152), ERAD 210
8 DELR ( 37), P (152), P1 (152), PB (152), PB1 (152) ERAD 220
COMMON P2 (152), SV (152), RHO (152), THETA (152), ERAD 230
1 W (152), E (152), EI (152), EK (152), A (152), ERAD 240
2 V (152), G (152), D (152), C (152), X2 (152), ERAD 250
3 X3 (152), X4 (152), X5 (152), X6 (152), X7 (152), ERAD 260
4 SMLA (152), SMLB (152), SMLC (152), SMLD (152), SMLE (152), ERAD 270
5 EC (152), Ek (152), SMLQ (152), SMLH (152), BIGA (152), ERAD 280
6 BIGB (152), CV (152), BC (152), BR (152), CHIC (152), ERAD 290
7 CHIR (152), CAPAC (152), CAPAR (152), CRTC (152), CRTR (152), ERAD 300
8 CRTPC (152), GOFR (152), FEY (152), CAR (152), OKLM ( 37) ERAD 310
COMMON TELM ( 37), EKLM ( 37), ELM ( 37), FCLM ( 37), ERAD 320
1 FRLM ( 37), WLM ( 37), QLM ( 37), AMASNO( 37), CHRNO ( 37), ERAD 330
2 ZP1 ( 37), ZP2 ( 37), SOLID ( 37), ECHCK ( 37), RK (104), ERAD 340
3 RL ( 37), RHOK (104), RDK (104), THETAK(104), TEMP ( 16), ERAD 350
4 HEAD ( 12), MAXL , MAXLM , ERAD 360
C*                                           **ERAD 370
C*****ERAD 380
C*****ERAD 390
DIMENSION RUC(1), OSX2(1), H2(1), Q1(1), GU(1), SU(1), HU(1) ERAD 400
DIMENSION PDFU(1), SUMRHO(1), H(1), SUMX2(1), OLDTH(1) ERAD 410
DIMENSION Q37(1), Q38(1) ERAD 420
COMMON /LINDLY/ HNUN,SGNL,IHNU,NHNU,HNUP,NT,IM,IN,DHNU,THICK,NY ERAD 430
COMMON/TQ/QINT1(300),QINT2(300),TITLE(12),FLUX(30) ERAD 440
COMMON/CNTRL/ SCYCLE, JMULTE ERAD 450
C*                                           ERAD 460
EQUIVALENCE (SMLA,PDFU), (SMLD,SUMRHO) ERAD 470
EQUIVALENCE (BC,OSX2),(BIGB,H),(CRTR,SUMX2),(CHIC,SU) ERAD 480
EQUIVALENCE (SMLH,GU),(CAR,Q37),(CHIR,Q38),(SMLC,OLDTH) ERAD 490
EQUIVALENCE (ACO3T4,TROBG),(S12,EDITMF) ERAD 500
EQUIVALENCE (EC,Q1),(X7,H2),(BIGA,HU ),(GOFR,RUC) ERAD 510
C*                                           ERAD 520
C*****ERAD 530
C*                                           *ERAD 540
C*                                           *ERAD 550
C*           EDITMF SAME AS S12 *ERAD 560
C*           H SAME AS HIGB *ERAD 570
C*           H2 SAME AS X7 *ERAD 580
C*           OLDTH SAME AS SMLC *ERAD 590
C*           PDFU SAME AS SMLA *ERAD 600
C*           Q1 SAME AS EC *ERAD 610
C*           RUC SAME AS GOFR *ERAD 620
C*           Q37 SAME AS CAR *ERAD 630
C*           Q38 SAME AS CHIR *ERAD 640
C*           SUMX2 SAME AS CRTR *ERAD 650
C*           SU SAME AS CHIC *ERAD 660
C*           HU SAME AS BIGA *ERAD 670
C*           TROBG SAME AS ACO3T4

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C          GU      SAME AS  SMLH
C          SUMRHO  SAME AS  SMLD
C
C*****ERAD 680
C          ERAD 690
C          ERAD 700
C          ERAD 710
C          ERAD 720
C          ERAD 730
C          ERAD 740
C          ERAD 750
C          ERAD 760
C          ERAD 770
C          ERAD 780
C          ERAD 790
C*****ERAD 800
C          ERAD 810
C          ERAD 820
C          ERAD 830
C*****ERAD 840
C          ERAD 850
C          ERAD 860
C          ERAD 870
C          ERAD 880
C          ERAD 890
C          ERAD 900
C          ERAD 910
C          ERAD 920
C          ERAD 930
C          ERAD 940
C          ERAD 950
C          ERAD 960
C          ERAD 970
C          ERAD 980
C          ERAD 990
C          ERAD1000
C          ERAD1010
C          ERAD1020
C          ERAD1030
C          ERAD1040
C          ERAD1050
C          ERAD1060
C          ERAD1070
C          ERAD1080
C          ERAD1090
C          ERAD1100
C          ERAD1110
C          ERAD1120
C          ERAD1130
C          ERAD1140
C          ERAD1150
C          ERAD1160
C          ERAD1170
C          ERAD1180
C          ERAD1190
C          ERAD1200
C          ERAD1210
C          ERAD1220
C          ERAD1230
C          ERAD1240
C          ERAD1250
C          ERAD1260
C          ERAD1270
C          ERAD1280
C          ERAD1290
C          ERAD1300
C          ERAD1310
C          ERAD1320
C*****
C          NONEQUILIBRIUM RADIATION DIFFUSION AS IN LA-3377
C
C          FOR DRADTN AND ERADTN. NY (IN LINDLEY COMMON) IS TEMPERATURE
C          ITERATION INDEX. THIS IS USED IN A SPECIAL DIANA THAT GOES WITH
C          DRADTN AND ERADTN.
C*****
C          INITIALIZATION AND CALCULATION FOR NO VAPOR ZONES
C*****
C          CALL DVCHK (K000FX)
C          NTIMES=BOILB
C          IM=IBM1
C          IN=IA
C          IF (KMAX .EQ. 0) DHNU = 1.
C          10 IF (ZP1(26).EQ.0.) GO TO 30
C
C          SAVE STUFF FROM EIONX FOR NONEQ AND RESET IN OR IM
C
C          IF (PUSHA.LT.0.0) GO TO 20
C          IM = NR - 1
C          CALL NONEQ(IM+1,4)
C          GO TO 30
C          20 IN = NR
C          CALL NONEQ(IN-1,4)
C          30 CONTINUE
C          IMP1=IM+1
C          INM1=IN-1
C          IMP1 = IN + 1
C          40 IF (IMP1-IN) 50,50,60
C
C          CALCULATE BLACKBODY EMISSION AND EXIT IF NO VAPOR ZONES
C
C          50 X2(IMP1) = 1.0275E12 * A(IMP1) * (THETA(IM)**4 - THETA(IMP1)**4)
C          ER(IM)=-X2(IMP1)
C          GO TO 1310
C          60 NVEZ = 1
C          NY = NVEZ
C          IF(CVB.EQ.0.0) NVEZ = 2
C          VEZ = NVEZ
C
C          FORM INTERPOLATION QJANTITIES FOR OPACITY SUBROUTINE
C
C          DO 70 I=IN,IM
C          Q37(I)=ALOG(THETA(I))
C          70 Q38(I)=ALOG(SV(I))
C
C          OBTAIN ROSSELAND AND PLANCK OPACITIES FOR ENTIRE SPECTRUM
C          (REQUIRES DIANE TAPE HAVING MONOFREQUENCY OPACITIES FIRST)
C
C          IMNU = 0
C          CALL KAPPA(IN,IM)
C*****
C          MINIMUM TIME STEP CALCULATION
C*****
C          WSB = 0.0

```

DO 40 I=1,MAXLM	ERAD1330
80 WSB = WSB + ELM(I)	ERAD1340
DTR1=1.E10	ERAD1350
DTR2=1.E10	ERAD1360
90 DO 210 I=IN,IM	ERAD1370
C	ERAD1380
C	ERAD1390
C	ERAD1400
CALL UNCLE IF EITHER KAPPA IS ZERO OR NEGATIVE	ERAD1410
IF (AMIN1(CAPAC(I),CAPAR(I)).GT.0.0) GO TO 100	ERAD1420
95 S1=13.0095	ERAD1430
CALL UNCLE	ERAD1440
C	ERAD1450
C	ERAD1460
C	ERAD1470
SOLID(10) NOT ZERO GIVES ALL ROSSELAND OPTION	ERAD1480
100 IF (SOLID(10).EQ.0.0) GO TO 110	ERAD1490
TEMP(1) = CAPAR(I)	ERAD1500
TEMP(3) = CAPAR(I)	ERAD1510
GO TO 120	ERAD1520
110 TEMP(1)=SQRT(CAPAR(I)*CAPAC(I))	ERAD1530
TEMP(3) = CAPAC(I)	ERAD1540
120 IF (0.001-THETA(I)) 130,210,210	ERAD1550
130 H(I) = 0.5 * TEMP(1) / SV(I) * DELTAR(I)	ERAD1560
TEMP(1) = 1.E10	ERAD1570
TEMP(2) = 1.E10	ERAD1580
IF (TELM(37).EQ.0.0.OR.ER(I).EQ.0.0) GO TO 150	ERAD1590
WSBB = E(I) * G(I)	ERAD1600
IF (WSBB-TELM(37)*WSB) 150,140,140	ERAD1610
C	ERAD1620
C	ERAD1630
C	ERAD1640
ACCURACY CRITERION - DONE FOR FULLY AND PARTIALLY IMPLICIT CASES	ERAD1650
140 TEMP(1) = SLUG * WSBB / ABS(ER(I))	ERAD1660
150 IF (KMAX.EQ.0.AND.HVB.NE.0.0) GO TO 160	ERAD1670
C	
C	
C	
STABILITY CRITERION -- BYPASSED IN FULLY IMPLICIT CASE	
TEMP(2) = .5*CV(I)/(4.1132E12*TEMP(3)*THETA(I)**3)	
TEMP(3) = TEMP(2)*3.*H(I)**2	
TEMP(2) = AMIN1(TEMP(2),TEMP(3))	
160 TEMP(2) = AMIN1(TEMP(1),TEMP(2))	
TEMP(2)=TEMP(2)*TELM(25)	
C	ERAD1690
C	ERAD1700
C	ERAD1710
C	ERAD1720
FIND MINIMUM TIME STEP	ERAD1730
IF (TEMP(2)) 210,210,170	ERAD1740
170 IF (TEMP(2)-DTR1) 180,190,190	ERAD1750
180 DTR2=DTR1	ERAD1760
IMN2=IMN1	ERAD1770
DTR1=TEMP(2)	ERAD1780
IMN1=I	ERAD1790
GO TO 210	ERAD1800
190 IF (TEMP(2)-DTR2) 200,210,210	ERAD1810
200 DTR2=TEMP(2)	ERAD1820
IMN2=I	ERAD1830
210 CONTINUE	ERAD1840
DTRMIN=DTR1	ERAD1850
EO=IMN1	ERAD1860
C	ERAD1870
C	ERAD1880
C	ERAD1890
SET UP MINIMUM TIME STEPS BETWEEN EDITS	ERAD1900
IF (DTR1-TELM(26)) 220,230,230	ERAD1910
220 TELM(26)=DTR1	ERAD1920
TELM(27)=IMN1	ERAD1930
TELM(28)=DTR2	ERAD1940
TELM(29)=IMN2	ERAD1950
TELM(30)=SOLID(10)+1.0	

230 CONTINUE	ERAD1960
C	ERAD1970
C DETERMINE IF RADIATION OR HYDRO WILL SUBCYCLE	ERAD1980
C	ERAD1990
IF (UTRMIN-UTR) 260,280,240	ERAD2000
240 BLANK3=TH+AMIN1(UTRMIN,GR*OTH2)	ERAD2010
IF (S17) 280,250,280	ERAD2020
250 S9 = 1.0	ERAD2030
GO TO 280	ERAD2040
C	ERAD2050
C REDUCE TIME STEP	ERAD2060
C	ERAD2070
260 NRAU=ZP1(18)/UTRMIN+1.0	ERAD2080
OTH=ZP1(18)/FLOAT(NRAU)	ERAD2090
IF (NRAU-NTIMES) 280,280,270	ERAD2100
270 S1=13.0270	ERAD2110
CALL UNCLE	ERAD2120
280 THTAMX=.025	ERAD2130
C*****	ERAD2140
C	ERAD2150
C CALCULATE GEOMETRY FACTORS AND FIND HIGHEST TEMPERATURE	ERAD2160
C	ERAD2170
C*****	ERAD2180
DO 330 I=IN,IM	ERAD2190
GO TO (290,300,310), IALPHA	ERAD2200
C	ERAD2210
C SLABS	ERAD2220
C	ERAD2230
290 PDFU(I) = 1. / (C(I+1) - C(I))	ERAD2240
RUC(I+1)=5.0E9 / (C(I+2) - C(I))	ERAD2250
GO TO 320	ERAD2260
C	ERAD2270
C CYLINDERS	ERAD2280
C	ERAD2290
300 PDFU(I) = 1. / (C(I+1)**2 - C(I)**2)	ERAD2300
RUC(I+1)=1.0E10 * C(I+1) / (C(I+2) - C(I))	ERAD2310
GO TO 320	ERAD2320
C	ERAD2330
C SPHERES	ERAD2340
C	ERAD2350
310 PDFU(I) = 1. / (C(I+1)**3 - C(I)**3)	ERAD2360
RUC(I+1)=1.5E10 * C(I+1)**2 / (C(I+2) - C(I))	ERAD2370
320 IF (THETA(I).LE.THTAMX) GO TO 330	ERAD2380
THTAMX=THETA(I)	ERAD2390
330 CONTINUE	ERAD2400
IF (THTAMX .LT. THETA(1B) .AND. GL .GT. 0.) THTAMX = THETA(1B)	ERAD2410
IF (THTAMX .LT. THETA(1A-1) .AND. GA .GT. 0.) THTAMX = THETA(1A-1)	ERAD2420
GO TO (340,350,360), IALPHA	ERAD2430
C	ERAD2440
C BOUNDARY QUANTITIES	ERAD2450
C	ERAD2460
340 TSLH = 1.	ERAD2470
TSRH = 1.	ERAD2480
GO TO 370	ERAD2490
350 TSLH = C(IN) + C(IN)	ERAD2500
TSRH = C(IMP1) + C(IMP1)	ERAD2510
GO TO 370	ERAD2520
360 TSLH = 3. * C(IN)**2	ERAD2530
TSRH = 3. * C(IMP1)**2	ERAD2540
370 HOTH = 1. / UTH	ERAD2550
CALL DVCHK(KDMY)	ERAD2560
GO TO (380,390), KDMY	ERAD2570
380 S1 = 13.0380	ERAD2580
CALL UNCLE	ERAD2590
C	ERAD2600

AFWL-TR-66-108, Vol I

C	ZERO X3, X4, X5, X6 (IN CASE MERGE FREQUENCIES)	ERAD2610
C	AND ER, SUMX2, SUMH0 (FOR FREQUENCY INTEGRATION)	ERAD2620
C		ERAD2630
	390 DO 400 I=IN,IM	ERAD2640
	X3(I)=0.	ERAD2650
	X4(I)=0.	ERAD2660
	X5(I)=0.	ERAD2670
	X6(I)=0.	ERAD2680
	ER(I) = 0.	ERAD2690
	SUMX2(I) = 0.	ERAD2700
	SUMH0(I) = 0.	ERAD2710
C		ERAD2720
C	SET UP FOR KAPPA INTERPOLATION	ERAD2730
C		ERAD2740
	400 Q1(I)=THETA(I)**4	ERAD2750
	SUMX2(IMP1) = 0.	ERAD2760
C		ERAD2770
C		ERAD2780
C	*****	ERAD2790
C		*ERAD2800
C	BEGIN FREQUENCY LOOP	*ERAD2810
C		*ERAD2820
C	*****	ERAD2830
C		ERAD2840
C	SET UP MAX FREQ BOUNDARY	ERAD2850
C		ERAD2860
	HNUP=1.0E6	ERAD2870
	HNUP4=1.0E24	ERAD2880
	IF (KMAX.EQ.0) GO TO 530	ERAD2890
	410 IHNU = IHNU +1	ERAD2900
	CALL KAPPA(IN,IM)	ERAD2910
	HNU4=HNUP**4	ERAD2920
	DHNU = DHNU	ERAD2930
	HNU = HNUP - HNU	ERAD2940
C		ERAD2950
C	MERGE GROUPS WITH HNU MORE THAN CB TIMES LARGEST THETA	ERAD2960
C		ERAD2970
	IF (CB.GT.0.0) GO TO 420	ERAD2980
	415 S1 = 13.0415	ERAD2990
	CALL UNCLE	ERAD3000
	420 IF (THTAMX-HNU/CB) 450,430,430	ERAD3010
	430 IF (IHNU-1) 440,560,470	ERAD3020
	440 S1 = 13.0440	ERAD3030
	CALL UNCLE	ERAD3040
C		ERAD3050
C	REJECT TAPE IF MORE THAN HALF OF GROUPS MERGE	ERAD3060
C		ERAD3070
	450 IF (IHNU+IHNU-NHNU) 470,460,460	ERAD3080
	460 IF (AMOD(CB,1.).EQ.0.5) GO TO 470	ERAD3090
	S1=13.0460	ERAD3100
	CALL UNCLE	ERAD3110
	470 DO 480 I=IN,IM	ERAD3120
	BETA=HNU/THETA(I)	ERAD3130
	BETAP=HNUP/THETA(I)	ERAD3140
	DFB=PLNKUT(BETA,BETAP)	ERAD3150
	IF (DFB.EQ.0.) GO TO 480	ERAD3160
	TEMP(1)=DFB*Q1(I)	ERAD3170
	EMB1=EXP(-BETA)	ERAD3180
	EMB2=EXP(-BETAP)	ERAD3190
	TEMP(2)=DFB*0.0384974/Q1(I)*(HNU4/(1.0-EMB1)	ERAD3200
	1*EMB1-HNUP4/(1.0-EMB2)*EMB2)	ERAD3210
C		ERAD3220
C	FORM NUMERATORS AND DENOMINATORS OF MERGED KAPPAS	ERAD3230
C		ERAD3240
	X6(I)=X6(I)+TEMP(1)	ERAD3250

	X4(I)=X4(I)+TEMP(2)	ERAD3260
	X5(I)=X5(I)+CAPAC(I)*TEMP(1)	ERAD3270
	X3(I)=X3(I)+TEMP(2)/CAPAR(I)	ERAD3280
480	CONTINUE	ERAD3290
	HNUP=HNU	ERAD3300
	HNUP4=HNUP	ERAD3310
	IF (THTAMX-HNU/CB) 410,490,490	ERAD3320
C		ERAD3330
C	FORM MERGED KAPPAS	ERAD3340
C		ERAD3350
490	DO 520 I=IN,IM	ERAD3360
	IF (X6(I)) 500,520,510	ERAD3370
500	S1=13.0500	ERAD3380
	CALL UNCLE	ERAD3390
510	CAPAR(I)=X4(I)/X3(I)	ERAD3400
	CAPAC(I)=X5(I)/X6(I)	ERAD3410
520	CONTINUE	ERAD3420
	HNUP=1.0E6	ERAD3430
	HNUP4=1.0E24	ERAD3440
	DHNU = HNUP - HNU	ERAD3450
	GO TO 580	ERAD3460
C		ERAD3470
C	MONOFREQUENCY CALCULATION	ERAD3480
C		ERAD3490
530	NHNU=1	ERAD3500
	IHNU = 1	ERAD3510
	DO 540 I=IN,IM	ERAD3520
540	X6(I)=Q1(I)	ERAD3530
	HNU = .001	ERAD3540
	GO TO 580	ERAD3550
C		ERAD3560
C	FREQUENCY GROUP CALCULATION OF SOURCES	ERAD3570
C		ERAD3580
550	IHNU = IHNU +1	ERAD3590
	CALL KAPPA(IN,IM)	ERAD3600
	DHNU=HNUP-HNU	ERAD3610
	HNUP4=HNUP**4	ERAD3620
560	DO 570 I=IN,IM	ERAD3630
	DFB = PLNKUT(HNU / THETA(I), HNUP / THETA(I))	ERAD3640
570	X6(I)=DFB*Q1(I)	ERAD3650
C		ERAD3660
C	SET BOUNDARY CONDITION FOR LEFT HAND SIDE	ERAD3670
C		ERAD3680
580	IF (INM1) 590,630,600	ERAD3690
590	S1=13.0590	ERAD3700
	CALL UNCLE	ERAD3710
600	IF (KMAX.NE.0) GO TO 610	ERAD3720
	DFB = 1.	ERAD3730
	GO TO 620	ERAD3740
610	IF (THETA(INM1) .LE. 0.0) THETA(INM1) = 1.0E-5	ERAD3750
	DFB = PLNKUT (HNU/THETA(INM1),HNUP/THETA(INM1))	ERAD3760
620	BBSL = DFB * THETA(INM1)**4	ERAD3770
	GO TO 650	ERAD3780
C		ERAD3790
C	NO BOUNDARY CONDITION FOR GA .GT. 0.0	ERAD3800
C		ERAD3810
630	IF (GA.GT.0.0) GO TO 640	ERAD3820
	IF (GA .EQ. 0.0) BBSL = 0.	ERAD3830
	GO TO 650	ERAD3840
640	S1 = 13.0640	ERAD3850
	CALL UNCLE	ERAD3860
C		ERAD3870
C	SET BOUNDARY CONDITION FOR RIGHT HAND SIDE	ERAD3880
C		ERAD3890
650	IF (GL .EQ. 0.0) X6(IMP1)=0.0	ERAD3900

```

IF (GL.NE.0.5) GO TO 680
IF (KMAX.NE.0) GO TO 660
UFB = 1.
GO TO 670
660 UFB = PLNKUT(HNU / THETA(IMP1), HNUP / THETA(IMP1))
670 X6(IMP1) = UFB * THETA(IMP1)**4
C
C      SPECIAL RIGHT BOUNDARY SOURCE (GL A POSITIVE
C      INTEGER) NOW INCLUDED
C
680 IF(GL.GT.0.5) X6(IMP1) = FLUX (IHNU)
    UBR=-X6(IMP1)
C
C      FORM ROSSELAND AND PLANCK OPTICAL DEPTHS
C
H3M = CAPAR(IN) / SV(IN) * DELTAR(IN)
DO 720 I=IN,IM
IF (AMIN1(CAPAC(I),CAPAR(I)).GT.0.0) GO TO 690
685 S1=13.0685
    CALL UNCLE
C
C      FOR NONEQUILIBRIUM DIFFUSION, H AND H2
C      ARE MU AND (1./(4.*LAMBDA)) RESPECTIVELY.
C
690 H(I) = CAPAC(I) / SV(I) * 1.5E10
    IF(SOLID(10).NE.0.0) H(I) = H(I)*CAPAR(I)/CAPAC(I)
    SU(I) = 2.74E2 * H(I) * X6(I)
    IF (I.EQ.IM) GO TO 720
C
C      WARNING - ASYNCHRONISMS IN SV AND DELTAR LEAD TO
C      ERRONEOUS FLUCTUATIONS IN H3. THIS CAN BE FIXED
C      BY SUBSTITUTING G IN PLANES, BUT SPHERES WILL
C      STILL HAVE THIS TROUBLE.
C
700 H3P = CAPAR(I+1) / SV(I+1) * DELTAR(I+1)
C
C      FOR SHARP CHANGES IN OPTICAL DEPTH, USE THINNER ZONE TO DEFINE H2
C
CAVEAT. TROUBLE IN SCATTERING PROBLEMS - CODE CHANGES SOON
C
IF (ABS(H3M-H3P)/(H3M+H3P).LE.AC) GO TO 710
H2(I+1)=.25*AMIN1(H3M/DELTAR(I),H3P/DELTAR(I+1))
GO TO 720
710 H2(I+1) = (H3M + H3P) * 0.25/ (DELTAR(I) + DELTAR(I+1))
720 H3M = H3P
C
C      EXTRAPOLATION COEFFICIENTS TO FORM RADIATION
C      ENERGIES AT BOUNDARIES
C
BETA1 = 1.0 / (2.0 - EXP(-DELTAR(IN) * SQRT(CAPAR(IN) * H(IN) *
2 5.0E-11 / SV(IN))))
BETA2 = 1.0 / (2.0 - EXP(-DELTAR(IM) * SQRT(CAPAR(IM) * H(IM) *
2 5.0E-11 / SV(IM))))
C*****
C      NONEQUILIBRIUM DIFFUSION TREATMENT
C
C      FORM COEFFICIENTS OF IMPLICIT EQUATIONS
C*****
C      CALL DVCHK(KDMY)
C      GO TO (730,740), KDMY
730 S1 = 13.0730
    CALL UNCLE

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ERAD3910
 ERAD3920
 ERAD3930
 ERAD3940
 ERAD3950
 ERAD3960
 ERAD3970
 ERAD3980
 ERAD3990
 ERAD4000
 ERAD4010
 ERAD4020
 ERAD4030
 ERAD4040
 ERAD4050
 ERAD4060
 ERAD4070
 ERAD4080
 ERAD4090
 ERAD4100
 ERAD4110
 ERAD4120
 ERAD4130
 ERAD4140
 ERAD4150
 ERAD4160
 ERAD4170
 ERAD4180
 ERAD4190
 ERAD4200
 ERAD4210
 ERAD4220
 ERAD4230
 ERAD4240
 ERAD4250
 ERAD4260
 ERAD4270
 ERAD4280
 ERAD4290
 ERAD4300
 ERAD4310
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 ERAD4370
 ERAD4380
 ERAD4390
 ERAD4400
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 ERAD4470
 ERAD4480
 ERAD4490
 ERAD4500
 ERAD4510
 ERAD4520
 ERAD4530
 ERAD4540
 ERAD4550

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740 IF (INP1-IM) 810,810,750
C
C      SPECIAL CASE - SINGLE VAPOR ZONE
C
750 CONTINUE.
  BU = 2.*H(IN) + 1.5E10*(TSRH*BETA2 + TSLH*BETA1)*PDFU(IN)
  DU = 2.055E12*PDFU(IN)*(HBSL*TSLH*BETA1-HBR*TSRH*BETA2)
  IF (KMAX.EQ.0.AND.HVB.NE.0.0) GO TO 770
C
C      PARTIALLY IMPLICIT - MULTIFREQUENCY CASE
C
760 CONTINUE
  RHO(IN)=(SU(IN)+DU)/BU
  GO TO 1000
C
C      FULLY IMPLICIT TERMS
C
770 GO TO (780,790), NVEZ
C
C      NO ITERATION
C
780 T4=Q1(IN)
  GO TO 800
790 IF (CVB.EQ.0.0) GO TO 780
C
C      ITERATION
C
  T4=OLDTH(IN)**4
800 TEMP(1)=5.48E2*THETA(IN)**3
  TEMP(2)=G(IN)*RDTR*CV(IN)
  DENOM=TEMP(2)/H(IN)+TEMP(1)/PDFU(IN)
  BU=BU-2.*H(IN)/PDFU(IN)*TEMP(1)/DENOM
  SU(IN) = (SMLQ(IN) - (PB1(IN) + P(IN)) * VD(IN)) * (TEMP(1) /
2 DENOM) - (TEMP(2)/DENOM) * 2.74E2 * T4
  GO TO 760
C
C      LEFT-HAND BOUNDARY CONDITION
C
810 RU1=RUC(IN+1)/H2(IN+1)
  CU = -PDFU(IN) * RU1
  BU = H(IN) + H(IN)
  DU = 0.
  IF (KMAX.EQ.0.AND.HVB.NE.0.0) GO TO 820
  UU = DU - SU(IN)
  GO TO 860
C
C      FULLY IMPLICIT TERMS
C
820 GO TO (830,840), NVEZ
C
C      NO ITERATION
C
830 T4 = Q1(IN)
  GO TO 850
840 IF (CVB.EQ.0.0) GO TO 830
C
C      ITERATION
C
  T4 = OLDTH(IN)**4
850 TEMP(1) = 5.48E2 * THETA(IN)**3
  TEMP(2) = G(IN) * RDTR * CV(IN)
  UENOM = TEMP(2) / H(IN) + TEMP(1) / PDFU(IN)
  BU = BU - 2.*H(IN)/PDFU(IN) * TEMP(1) / DENOM
  UU = DU - (SMLQ(IN) - (PB1(IN) +
2 P(IN)) * VD(IN)) * (TEMP(1) / DENOM) - (TEMP(2)/DENOM)*2.74E2*T4

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ERAD4560
ERAD4570
ERAD4580
ERAD4590
ERAD4600
ERAD4610
ERAD4620
ERAD4630
ERAD4640
ERAD4650
ERAD4660
ERAD4670
ERAD4680
ERAD4690
ERAD4700
ERAD4710
ERAD4720
ERAD4730
ERAD4740
ERAD4750
ERAD4760
ERAD4770
ERAD4780
ERAD4790
ERAD4800
ERAD4810
ERAD4820
ERAD4830
ERAD4840
ERAD4850
ERAD4860
ERAD4870
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ERAD4900
ERAD4910
ERAD4920
ERAD4930
ERAD4940
ERAD4950
ERAD4970
ERAD4980
ERAD4990
ERAD5000
ERAD5010
ERAD5020
ERAD5030
ERAD5040
ERAD5050
ERAD5060
ERAD5070
ERAD5080
ERAD5090
ERAD5100
ERAD5110
ERAD5120
ERAD5130
ERAD5140
ERAD5150
ERAD5160
ERAD5170
ERAD5180
*****
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AFWL-TR-66-108, Vol I

860 IF (INM1) 590,870,880	ERAD5210
870 IF (GA.LT.0.0) GO TO 890	ERAD5220
880 TS1 = PDFU(IN) * TSLH * 1.5E10 * BETA1	ERAD5230
BU = BU + TS1	ERAD5240
DU = DU - TS1 * 137.0 * HUSL	ERAD5250
890 GU(IN)=BU/(CU-BU)	
HU(IN)=-DU/(BU-CU)	
IF (INP1-IM) 910,980,900	ERAD5280
900 S1 = 13.0900	ERAD5290
CALL UNCLE	ERAD5300
C	ERAD5310
C	ERAD5320
C	ERAD5330
910 IMM1 = IM - 1	ERAD5340
DO 970 I=INP1,IMM1	ERAD5350
HU2=RUC(I+1)/H2(I+1)	ERAD5360
AU = -PDFU(I) * HU1	ERAD5370
CU = -PDFU(I) * HU2	ERAD5380
BU = H(I) + H(I)	
DU = 0.	ERAD5400
IF (KMAX.EQ.0.AND.HVB.NE.0.0) GO TO 920	ERAD5410
DU = DU - SU(I)	ERAD5420
GO TO 960	ERAD5430
C	ERAD5440
C	ERAD5450
C	ERAD5460
920 GO TO (930,940), NVEZ	ERAD5470
C	ERAD5480
C	ERAD5490
C	ERAD5500
930 T4 = Q1(I)	ERAD5510
GO TO 950	ERAD5520
940 IF (CVB.EQ.0.0) GO TO 930	ERAD5530
C	ERAD5540
C	ERAD5550
C	ERAD5560
T4 = OLDTH(I)**4	ERAD5570
950 TEMP(1) = 5.48E2 * THETA(I)**3	ERAD5580
TEMP(2) = G(I) * ROTR * CV(I)	ERAD5590
DENOM = TEMP(2) / H(I) + TEMP(1) / PDFU(I)	ERAD5600
BU = BU - 2.*H(I)/ PDFU(I) * TEMP(1) / DENOM	ERAD5610
DU = DU - (SMLQ(I) - (PB1(I) +	*****
2 P(I)) * VD(I)) * (TEMP(1) / DENOM) - (TEMP(2)/DENOM) * 2.74E2 * T4*****	
960 DENOM = BU - CU + AU * GU(I-1)	
GU(I) = (-BU - AU*GU(I-1)) / DENOM	
HU(I) = -(DU + AU * HU(I-1)) / DENOM	ERAD5660
RU1 = RU2	ERAD5670
970 CONTINUE	ERAD5680
C	ERAD5690
C	ERAD5700
C	ERAD5710
980 AU = -PDFU(IM) * RU1	ERAD5720
BU=H(IM)+H(IM)	ERAD5730
DU = 0.	ERAD5740
IF (KMAX.EQ.0.AND.HVB.NE.0.0) GO TO 990	ERAD5750
DU = DU - SU(IM)	ERAD5760
GO TO 1030	ERAD5770
C	ERAD5780
C	ERAD5790
C	ERAD5800
990 GO TO (1000,1010), NVEZ	ERAD5810
C	ERAD5820
C	ERAD5830
C	ERAD5840
1000 T4 = Q1(IM)	ERAD5850

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        GO TO 1020
1010 IF (CVU.EQ.0.0) GO TO 1000
C
C          ITERATION
C
        T4 = OLDTM(IM)**4
1020 TEMP(1) = 5.48E2 * THETA(IM)**3
        TEMP(2) = G(IM) * KUTH * CV(IM)
        DENOM = TEMP(2) / H(IM) + TEMP(1) / PDFU(IM)
        BU = BU - 2.*H(IM)/PDFU(IM) * TEMP(1) / DENOM
        DU = DU - (SMLQ(IM) - (PB1(IM) +
        2 P(IM)) * VD(IM)) * (TEMP(1) / DENOM) - (TEMP(2)/DENOM)*2.74E2*T4
1030 IF (GL.LT.0.) GO TO 1040
        TS1 = PDFU(IM) * TSKH * 1.5E10 * HETA2
        BU = BU + TS1
        DU = DU + TS1 * 137.0 * BBR
1040 GU(IM) = -1.
        HU(IM) = -(DU+AU*HU(IM-1))/(BU+AU*GU(IM-1))
C*****
C          FORM RADIATION ENERGY, FLUX AND RADIATION SOURCE ER.
C
C*****
        DO 1050 I=IN,IM
        IBK = IN + IM - 1
        RHO(IBK) = (GU(IBK) + 1.)*RHO(IBK+1) + HU(IBK)
        IF (RHO(IBK).GE.0.0) GO TO 1050
1045 S1 = 13.1045
        CALL UNCLE
1050 CONTINUE
C
C          CHECK ON BOUNDARY X2'S BYPASSED FOR NOW
C
1060 IF (INM1) 590,1070,1090
1070 IF (GA) 1080,1090,1090
1080 X2(IN) = 0.0
        GO TO 1100
1090 X2(IN) = (2.055E12*BBSL -1.5E10*RHO(IN))*TSLH*BETA1
1100 IF (GL) 1110,1120,1120
1110 X2(INP1) = 0.0
        GO TO 1130
1120 X2(INP1) = (2.055E12*BBR +1.5E10*RHO(IM))*TSRH*BETA2
        IF (IM-INP1) 1160,1130,1130
C
C          FORM FLUXES
C
1130 DO 1140 I=INP1,IM
1140 X2(I) = HUC(I)*(HU(I-1)+GU(I-1)*RHO(I))/H2(I)
        CALL DVCHK(KOMY)
        GO TO (1150,1160), KOMY
1150 S1 = 13.1150
        CALL UNCLE
C
C          FORM RADIATION CONTRIBUTION TO ZONE ENERGY
C
1160 DO 1170 I=IN,IM
        ER(I) = ER(I) + X2(I) - X2(I+1)
1170 CONTINUE
C*****
C          OPTIONAL EDIT OF X2 ETC.
C
C*****
1180 CNT1=SOLID(18)+1.0
        CNT2=AMIN1(TPRINT,CNTMAX)

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ERAD5860
 ERAD5870
 ERAD5880
 ERAD5890
 ERAD5900
 ERAD5910
 ERAD5920
 ERAD5930
 ERAD5940
 ERAD5950

 ERAD5980
 ERAD5990
 ERAD6000
 ERAD6010
 ERAD6040
 ERAD6050
 ERAD6060
 ERAD6070
 ERAD6080
 ERAD6090
 ERAD6100
 ERAD6120
 ERAD6130
 ERAD6140
 ERAD6150
 ERAD6160
 ERAD6170
 ERAD6180
 ERAD6190
 ERAD6200
 ERAD6210
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 ERAD6240
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 ERAD6270
 ERAD6280
 ERAD6290
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 ERAD6370
 ERAD6380
 ERAD6390
 ERAD6400
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 ERAD6420
 ERAD6430
 ERAD6440
 ERAD6450
 ERAD6460
 ERAD6470
 ERAD6480
 ERAD6490
 ERAD6500

IF (CNT1.LT.CNT2) GO TO 1200	ERAD6510
1190 IF (EDITMF.EQ.0.0) GO TO 1200	ERAD6520
TEMP(1) = TH + DTR	ERAD6530
WRITE (6,3) CNT1, TEMP(1), HNU, NVEZ	
WRITE (6,4)	
H(IMP1) = 0.	
H2(IMP1) = 0.	
GU(IMP1) = 0.	
HU(IMP1) = 0.	
RHO(IMP1) = 0.	
DO 1196 I = IN, IMP1	
1196 WRITE (6,5) I, THETA(I), X6(I), H(I), H2(I), GU(I), HU(I), RHO(I), X2(I)	
3 FORMAT (9H1CYCLE = F7.0, 9H TIME = E13.6, 4X11HNU(LOWER)=F10.4,	
2 10H PASS NO. 11/)	
4 FORMAT (7X1H1, 9X5HTHETA, 12X2HX6, 13X1HH, 12X2HH2, 12X2HGU,	
2 12X2HHU, 11X3HH40, 12X2HX2)	
5 FORMAT (18, 1P8E14.7)	
C	ERAD6620
C ADVANCE FREQ, STORE EMERGENT FLUX, TEST FOR COMPLETION OF GROUPS	ERAD6630
C	ERAD6640
1200 DO 1210 I=IN,IMP1	ERAD6650
SUMRHO(I) = SUMRHO(I) + RHO(I)	ERAD6660
SUMX2(I)=SUMX2(I)+X2(I)	ERAD6670
1210 CONTINUE	ERAD6680
CALL DVCHK (K000FX)	ERAD6690
GO TO (1230,1220), K000FX	ERAD6700
1220 HNU4=HNU	ERAD6710
HNU4=HNU4	ERAD6720
IF (IHNU-NHNU) 550,1240,1230	ERAD6730
C*****	ERAD6740
C	*ERAD6750
C END FREQUENCY LOOP	*ERAD6760
C	*ERAD6770
C*****	ERAD6780
1230 S1 = 13.1230	ERAD6790
CALL UNCLE	ERAD6800
C	ERAD6810
C ITERATE ON TEMPERATURE IF NVEZ EQUALS ONE	ERAD6820
C	ERAD6830
1240 GO TO (1250,1270), NVEZ	ERAD6840
1250 NVEZ = 2	ERAD6850
VEZ = NVEZ	ERAD6860
NY = NVEZ	ERAD6870
IHNU=0	ERAD6880
DO 1260 I=IN,IM	ERAD6890
BNTH = THETA(I) + (SMLQ(I) + ER(I) - (PB1(I) + P(I)) * VD(I)) *	ERAD6900
2 DTR / (G(I) + CV(I))	ERAD6910
OLDTH(I) = THETA(I)	ERAD6920
THETA(I) = 0.5 * (OLDTH(I) + BNTH)	ERAD6930
1260 Q37(I)=ALOG(THETA(I))	ERAD6940
IF (KMAX.EQ. 0) CALL KAPPA(IN,IM)	ERAD6950
GO TO 390	ERAD6960
1270 IF (CVB.EQ.0.0) GO TO 1290	ERAD6970
DO 1280 I=IN,IM	ERAD6980
1280 THETA(I) = OLDTH(I)	ERAD6990
C	ERAD7000
C SET UP FOR ENCALC	ERAD7010
C	ERAD7020
1290 DO 1300 I=IN,IMP1	ERAD7030
Q1(I) = 0.	ERAD7040
RHO(I) = SUMRHO(I)	ERAD7050
1300 X2(I) = SUMX2(I)	ERAD7060
1310 IF (ZP1(26).EQ.0.0) GO TO 1330	ERAD7070
C	ERAD7080
C RESTORE NONEQ QUANTITIES	ERAD7090
C	ERAD7100
IF (PUSHA.LT.0.0) GO TO 1320	ERAD7110
CALL NONLQ(IMP1,5)	ERAD7120
GO TO 1330	ERAD7130
1320 CALL NONEQ(INM1,5)	ERAD7140
1330 RETURN	ERAD7150
END	ERAD7160

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SECTION II

SCATTERING METHODS FOR TAMALE2.1. INTRODUCTION

The TAMALE code (Ref. 1) is a one-dimensional, multifrequency, thermal-radiation, transport code that allows for the finite transit time of photons through the system. (This "retardation" version of the code is currently under development.) This report describes an approach for extending capability of the code to include Thomson scattering, i. e., the scattering of low-energy photons by free electrons.

2.2. ANALYSIS OF THE TRANSPORT EQUATION WITH COMPTON SCATTERING

The calculation of the contribution to radiant energy transfer due to the scattering of photons by free electrons is based on the numerical solution of the relevant radiation transport equation along a selection of sampling rays through the sphere. A discussion of the analysis and logic of the parent code, SPUTTER, is presented in Ref. 2.

The radiation transport equation for the intensity $I(\nu, \vec{\Omega}, r, t)$ with units of energy per unit of frequency, solid angle, time, and area is given by (Ref. 3)

$$\begin{aligned} \frac{1}{c} \frac{\partial}{\partial t} I(\nu_1, \Omega_1, r, t) + \Omega_1 \cdot \nabla I(\nu_1, \Omega_1, r, t) = \mu_a (1 - e^{-h\nu_1/\theta}) [B_{\nu_1}(\theta) \\ - I(\nu_1, \Omega_1)] - N_e I(\nu_1, \Omega_1) \int d\Omega_2 \frac{d\sigma}{d\Omega_2} \left[1 + \frac{c^2}{2h\nu_2^3} I(\nu_2, \Omega_2) \right] \\ + N_e \left[1 + \frac{c^2}{2h\nu_1^3} I(\nu_1, \Omega_1) \right] \int d\Omega_3 \frac{d\sigma}{d\Omega_1} \frac{\nu_1}{\nu_3} \frac{d\nu_3}{d\nu_1} I(\nu_3, \Omega_3) \end{aligned}$$

The first term on the right side represents the quantity of radiant energy absorbed and emitted at frequency ν_1 in direction Ω_1 . The second term represents loss of energy by scattering out of the beam Ω_1, ν_1 , and the third term the gain by scattering into the beam Ω_1, ν_1 . The coefficient N_e is the number of free electrons per unit volume, and μ_a is the absorption coefficient at r for frequency ν_1 . The assumptions necessary to derive this equation are as follows:

1. Polarization of photons is neglected.
2. The average kinetic energy of electrons is so small that Doppler effects may be ignored.
3. Local thermodynamic equilibrium (LTE) exists.
4. The electron states are nondegenerate.

Before arriving at an analytical expression for the intensity that is amenable to computer solution, several more assumptions must be made.

The event of a photon being scattered from an electron at rest causes the photon to change frequency. From quantum mechanics one has the Compton formula for the new frequency:

$$\nu_f = \frac{\nu_i}{1 + \gamma_i(1-\mu)}$$

where ν_i, ν_f are the incident and scattered photon frequencies, respectively,

$$\gamma_i = \frac{h\nu_i}{m_0 c^2}$$

where m_0 is the mass of the electron and c is the speed of light, and

$$\mu = \Omega_f \cdot \Omega_i.$$

A major difficulty in solving the transport equation is that the solid-angle integrations appearing in the scattering terms cannot be performed even if the differential cross sections for scattering, $d\sigma/d\Omega$, are assumed to be simple functions. The reason for this is that the intensity I depends

upon Ω both directly and through the frequency ν , which by the above Compton formula is also a function of Ω through the scattering cosine, μ . To avoid this difficulty, the following assumptions are made:

1. $\gamma < 0.2$
2. $I(\nu_2, \Omega) \approx I(\nu_1, \Omega) + \left(\frac{\partial I}{\partial \gamma}\right)_1 (\gamma_2 - \gamma_1)$.

The first assumption requires that the photon energies under consideration be small relative to the rest mass of an electron (i.e., $h\nu < 100$ kev). The second assumption requires that the intensity be a smooth function of ν . This approximation is equivalent to the "age" approximation of neutron transport theory. With these approximations the resulting transport equation for Compton scattering in plane or spherically symmetric systems through first order in γ is given by

$$\begin{aligned} \frac{1}{c} \frac{\partial I}{\partial t} + \vec{\Omega}_1 \cdot \vec{\nabla} I = \mu'_a (B - I) - \mu_s \left\{ I - \frac{3}{16} \int_{-1}^1 d\mu_3 I(\mu_3) \left[3 - \mu_1^2 \right. \right. \\ \left. \left. + (3\mu_1^2 - 1)\mu_3^2 \right] + \gamma \left[-2I + \frac{3}{16} \left(1 + \frac{c^2 I}{h\nu_1^3} \right) \int_{-1}^1 d\mu_3 \left[1 - \gamma \left(\frac{\partial I}{\partial \gamma} \right)_3 \right] \right. \right. \\ \left. \left. \cdot \left[3 - \mu_1^2 + \mu_1 \mu_3 (3\mu_1^2 - 5) + (3\mu_1^2 - 1)\mu_3^2 + \mu_1 (3 - 5\mu_1^2)\mu_3^3 \right] \right] \right\} \\ + O(\gamma^2) \end{aligned}$$

where $\mu_s = (8/3)\pi r_o^2 N_e$ and $\mu'_a = \mu_a (1 - e^{h\nu/\theta})$. Terms of order γ^2 are derived in Ref. 3. The above equation can be further simplified by assuming that stimulated scattering is negligible, i.e., $c^2 I / h\nu_1^3 \ll 1$.

The present development of scattering in TAMALE takes into account only the terms of order zero in γ , which are dominant at low energy, and correspond to restriction of the Compton effect to the limiting case of Thomson scattering. With this approximation, the transport equation for spherical geometry becomes

$$\frac{1}{c} \frac{\partial I}{\partial t} + \mu \frac{\partial I}{\partial r} + \frac{1 - \mu^2}{r} \frac{\partial I}{\partial \mu} = \mu'_a (B - I) - \mu_s I + \frac{3}{16} \mu_s \left[(3 - \mu^2) \int_{-1}^1 I(\mu') d\mu' \right. \\ \left. + (3\mu^2 - 1) \int_{-1}^1 I(\mu') \mu'^2 d\mu' \right]$$

Under the transformation

$$x = r\mu \text{ and } y = r\sqrt{1 - \mu^2}$$

the above equation reduces to the standard form:

$$\frac{1}{c} \frac{\partial I}{\partial t} + \frac{\partial I}{\partial x} = \mu'_a (B - I) - \mu_s I + \frac{3}{16} \mu_s \left[(3 - \mu^2) \int_{-1}^1 I(\mu') d\mu' \right. \\ \left. + (3\mu^2 - 1) \int_{-1}^1 I(\mu') \mu'^2 d\mu' \right]$$

In the present TAMALE code the capability exists for solving the transport equation with retardation effects but without scattering, or solving the transport equation with scattering but without retardation effects. The treatment of retardation is discussed in Ref. 4 and in Ref. 5 and is not further considered in this report.

With the retardation term $1/c \partial I / \partial t$ discarded, the equation to be solved becomes

$$\frac{\partial I}{\partial x} + (\mu'_a + \mu_s) I = \mu'_a B + \frac{3}{16} \mu_s \left[(3 - \mu^2) \int_{-1}^1 I(\mu') d\mu' \right. \\ \left. + (3\mu^2 - 1) \int_{-1}^1 I(\mu') \mu'^2 d\mu' \right] \quad (38)$$

or

$$I(x_2) = I(x_1)e^{-(\mu'_a + \mu_s)(x_2 - x_1)} + \int_{x_1}^{x_2} \mu'_a B(x')e^{-(\mu'_a + \mu_s)(x_2 - x')} dx' + F_s(x_2) \quad (39)$$

where

$$F_s(x_2) = \frac{3}{16} \mu_s \int_{x_1}^{x_2} \left[(3 - \mu^2) \int_{-1}^1 I(\mu') d\mu' + (3\mu^2 - 1) \int_{-1}^1 I(\mu') \mu'^2 d\mu' \right] e^{-(\mu'_a + \mu_s)(x_2 - x')} dx'$$

2.3. NUMERICAL SOLUTION OF THE TRANSPORT EQUATION WITH THOMSON SCATTERING

The numerical solution to Eq. (39) above has been developed in Ref. 6. The salient features of this development will be repeated for continuity and ease of reference.

The first two terms on the right side have already been considered in Ref. 2. In evaluating the third term, $F_s(x_2)$, two numerical approximations are made:

1. The radiation energy and pressure vary linearly with x .
2. $\mu^2 \cong x^2/(a^2 + y^2)$, where $a^2 = (x_2 + x_1)^2/4$ and $x_1 \leq x \leq x_2$.

With these assumptions the scattering source contribution can be developed in the following manner:

$$F_s(x_2) = \frac{3}{16} \mu_s \left\{ \left(\frac{1 - e^{\bar{\mu} \Delta}}{\bar{\mu} \Delta} \right) \left[T_0(x_2) + \left(\frac{x_2^2}{a^2} \right) T_2(x_2) \right] \Delta \right.$$

$$\begin{aligned}
& + \left[\frac{e^{-\bar{\mu}\Delta}(1 + \bar{\mu}\Delta) - 1}{(\bar{\mu}\Delta)^2} (T_o(x_2) - T_o(x_1)) + \frac{x_2}{a^2} (2T_2(x_2)\Delta + x_2(T_2(x_2) - T_2(x_1))) \right] \\
& + \left(\frac{2 - e^{-\bar{\mu}\Delta}[(\bar{\mu}\Delta)^2 + 2\bar{\mu}\Delta + 2]}{(\bar{\mu}\Delta)^3} \right) (T_2(x_2)\Delta + 2x_2(T_2(x_2) - T_2(x_1))) \frac{\Delta^2}{a^2} \\
& + \left(\frac{e^{-\bar{\mu}\Delta}[(\bar{\mu}\Delta)^3 + 3(\bar{\mu}\Delta)^2 + 6\bar{\mu}\Delta + 6] - 6}{(\bar{\mu}\Delta)^4} \right) (T_2(x_2) - T_2(x_o)) \frac{\Delta^3}{a^2} \quad (40)
\end{aligned}$$

where

$$\Delta = x_2 - x_1$$

$$\bar{\mu} = \mu'_a + \mu_s$$

$$I_k = \int_{-1}^1 I(\mu) \mu^k d\mu$$

$$T_o(x_i) = 3I_o(x_i) - I_2(x_i)$$

$$T_2(x_i) = 3I_2(x_i) - I_o(x_i)$$

To avoid loss of numerical significance when $\bar{\mu}\Delta < 0.1$, the following approximations are used:

$$\left(\frac{1 - e^{-\bar{\mu}\Delta}}{\bar{\mu}\Delta} \right) \approx 1 - \frac{\bar{\mu}\Delta}{2}$$

$$\frac{e^{-\bar{\mu}\Delta}(1 + \bar{\mu}\Delta) - 1}{(\bar{\mu}\Delta)^2} \approx \frac{\bar{\mu}\Delta}{3} - 1/2$$

$$\frac{2 - e^{-\bar{\mu}\Delta}[(\bar{\mu}\Delta)^2 + 2\bar{\mu}\Delta + 2]}{(\bar{\mu}\Delta)^3} \approx 1/3 - \frac{\bar{\mu}\Delta}{4}$$

$$\frac{e^{-\bar{\mu}\Delta}[(\bar{\mu}\Delta)^3 + 3(\bar{\mu}\Delta)^2 + 6\bar{\mu}\Delta + 6] - 6}{(\bar{\mu}\Delta)^4} \approx \frac{\bar{\mu}\Delta}{5} - 1/4$$

2.4. THE TAMALE CODE

The coding to incorporate Thomson scattering into TAMALE is contained completely within the subroutines RADTN, TRANS, and RETARD.

The logic of the calculation proceeds exactly as before in the TAMALE code. Three new quantities, μ_s , $T_0(x_i)$, and $T_2(x_i)$ must be available in the RETARD subroutine to complete the calculation. The scattering coefficient μ_s is defined as $K_S \rho$, where K_S is an input number CAPAC(52) and ρ is the material density. In the applications considered, the quantity K_S has been set to .2, corresponding to $Z/2$ free electrons per atom, where Z is the atomic number. The other two quantities, $T_0(x_i)$ and $T_2(x_i)$, are stored in arrays FI0(IHNU, x_i) and FI2(IHNU, x_i). These arrays are located in CHUCK common.

An iteration feature has been added to the transport calculation. In solving Eq. (40), the assumption had been made that the intensity $I(x_i, t_n)$ could be evaluated from the moments of the intensity $I_0(x, t_{n-1})$ and $I_2(x, t_{n-1})$ at an earlier time step. This assumption is not valid in general; in particular, on a restart or an initial start the values in the arrays FI0 and FI2 are zero, so that there will initially be a decrease in the intensity due to scattering out of the beam but no corresponding increase due to scattering into the beam, and conservation of photons is violated. This problem is alleviated by an implicit iteration procedure. The user has at his disposal two parameters. One parameter is the maximum number of iterations (CAPAC(50)) and the other is the convergence criterion which the functions FI0(IHNU, x_i) and FI2(IHNU, x_i) must satisfy before continuing the calculation (CAPAC(51)).

The input quantities specifically used when Thomson scattering is employed are summarized below (these are also the values used for a sample problem that was solved on the AFWL computer):

<u>Card No.</u>	<u>Quantity</u>	<u>Value</u>	<u>Purpose</u>
77	CVB	1	Specifies all y-lines
2638	CAPAC(50)	10.	Number of iterations
2639	CAPAC(51)	.1	Gives 10% accuracy criterion
2640	CAPAC(52)	.2	Specifies K_S

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SECTION III
TWO-DIMENSIONAL RADIATION TRANSPORT TECHNIQUES
A SURVEY OF METHODS

3.1. INTRODUCTION

Several methods for calculating the effects of radiation in hydrodynamical problems have been proposed and tried. In this section, a few of the better methods are compared.

The quantity of interest is the rate of deposition of radiant energy as a function of time and position. The methods to be discussed relate the deposition to the radiant intensity I , which is defined by

$$dE = I(\vec{x}, \vec{\Omega}, \nu, t) \vec{\Omega} \cdot d\vec{a} d\Omega d\nu dt$$

where dE is the amount of radiant energy in a band $d\nu$ of frequencies that flows through an element of area $d\vec{a}$ at $\vec{x}$ in directions contained in the solid angle $d\Omega$ during time interval dt (polarization being neglected). Two related quantities of first importance are the density E and the flux $\vec{F}$ of radiant energy, which are defined as

$$E(\vec{x}, \nu, t) = \frac{1}{c} \int I d\Omega$$

$$\vec{F}(\vec{x}, \nu, t) = \int \vec{\Omega} I d\Omega$$
(41)

The rate of deposition of radiant energy is

$$A = c \int \sigma_d(\vec{x}, \nu, t) E(\vec{x}, \nu, t) d\nu$$
(42)

where σ_d is a coefficient that depends on the properties of matter at $\vec{x}$, t .

The material will, of course, be radiating energy at some rate $R(\vec{x}, t)$, so that the net rate at which it gains energy from the radiation field is $A - R$.

The equation for transport of radiation is

$$\frac{1}{c} \frac{\partial I}{\partial t} + \vec{\Omega} \cdot \nabla I + \sigma_t I = S \quad (43)$$

where $\sigma_t(\vec{x}, \nu, t)$ is the reciprocal of the mean free path (corrected for induced emission) of photons of frequency ν near $\vec{x}$ at time t , and S is the source, which is defined by

$$dE' = S(\vec{x}, \vec{\Omega}, \nu, t) dV d\Omega d\nu dt$$

where dE' is the amount of radiant energy leaving the element of volume dV around $\vec{x}$ in directions contained in the solid angle $d\Omega$ in the frequency band $d\nu$ during time interval dt . The two contributions to the source are emission

$$S_e(\vec{x}, \vec{\Omega}, \nu, t) = \frac{\chi(\vec{x}, \nu, t) R(\vec{x}, t)}{4\pi}$$

where χ is the spectrum, and scattering

$$S_s(\vec{x}, \vec{\Omega}, \nu, t) = \iint \sigma_s(\vec{x}, \vec{\Omega}' \rightarrow \vec{\Omega}, \nu' \rightarrow \nu, t) I(\vec{x}, \vec{\Omega}', \nu', t) d\Omega' d\nu'$$

where σ_s is a coefficient of scattering. Near local thermodynamic equilibrium (LTE),

$$S_e(\vec{x}, \vec{\Omega}, \nu, t) = \sigma_a(\vec{x}, \nu, t) B(\theta(\vec{x}, t), \nu)$$

where σ_a is the coefficient of absorption, corrected for induced emission, and B is the Planck function. When departures from LTE are significant, S_e takes a more complicated form, but the problem of how best to calculate it is beyond the scope of this report. The significant point is that S_e is isotropic and strongly temperature dependent.

The methods that are discussed below for finding numerical solutions of the transport equation are of three types: (1) methods that use a finite set of directions, (2) methods that involve the calculation of moments, and (3) Monte Carlo. Methods of the first two types are designed to calculate the intensity I for a given distribution of the source S . But wherever scattering is an important effect, the source depends on the intensity. It then becomes necessary either to iterate to obtain consistency between I and S , or, if sufficiently small time steps are being taken, to use the S from one time step for calculating I at the next time step, or something of this sort. In fact, at frequencies where Compton scattering is important, the calculation of the source may become a major part of the total effort.

In order to keep the discussion as simple and as explicit as possible, only applications using an Eulerian technique to calculate hydrodynamics in an r - z coordinate system (cylindrical coordinates without the angular variable) will be considered. It will further be assumed that the hydrodynamical calculation will advance material properties from time $t = t_{n-1/2}$ to $t = t_{n+1/2}$, assuming that the rates of transfer of radiant energy are held constant at values computed for $t = t_n$. Then radiant intensities and transfer rates are calculated at time t_{n+1} , assuming temperatures, densities, and opacities during the interval $t_n \leq t \leq t_{n+1}$ are as calculated for $t = t_{n+1/2}$.

3.2. THE METHOD OF MOMENTS

The method of moments consists in multiplying the vanishing quantity

$$\mathcal{L} = \frac{1}{c} \frac{\partial I}{\partial t} + \bar{\Omega} \cdot \nabla I + \sigma I - S$$

by each of a set of weighting functions and integrating the products over the domain of $\bar{\Omega}$. Thus,

$$\begin{aligned}\int \mathbf{I} \cdot \mathbf{Z} d\Omega &= \frac{1}{c} \frac{\partial}{\partial t} \int \mathbf{I} d\Omega + \nabla \cdot \int \vec{\Omega} \mathbf{I} d\Omega + \sigma \int \mathbf{I} d\Omega - \int \mathbf{S} d\Omega \\ &= -\frac{\partial \mathbf{E}}{\partial t} + \nabla \cdot \vec{\mathbf{F}} + c\sigma \mathbf{E} - \int \mathbf{S} d\Omega = 0\end{aligned}$$

and

$$\begin{aligned}\int \vec{\Omega} \mathbf{Z} d\Omega &= \frac{1}{c} \frac{\partial}{\partial t} \int \vec{\Omega} \mathbf{I} d\Omega + \nabla \cdot \int \vec{\Omega} \vec{\Omega} \mathbf{I} d\Omega + \sigma \int \vec{\Omega} \mathbf{I} d\Omega - \int \vec{\Omega} \mathbf{S} d\Omega \\ &= \frac{1}{c} \frac{\partial \vec{\mathbf{F}}}{\partial t} + \nabla \cdot \int \vec{\Omega} \vec{\Omega} \mathbf{I} d\Omega + \sigma \vec{\mathbf{F}} - \int \vec{\Omega} \mathbf{S} d\Omega = 0\end{aligned}$$

where $\mathbf{E}$ and $\vec{\mathbf{F}}$ are as defined by Eq. (41). The next step would be to calculate $\int \vec{\Omega} \vec{\Omega} \mathbf{Z} d\Omega$, but for present purposes, the calculation will stop with the first moment. It is characteristic of the method that each equation is coupled with the next through the moment of the streaming term $\vec{\Omega} \cdot \nabla \mathbf{I}$. Various ways of truncating the system of equations have been proposed. For the purpose of illustration, the simplest of these ways may be chosen, namely, to assume that moments of the intensity beyond a certain order are negligible. Thus, suppose that $\mathbf{I} = a_0 + \vec{a}_1 \cdot \vec{\Omega}$; in which case

$$\mathbf{E} = \frac{1}{c} \int \mathbf{I} d\Omega = \frac{4\pi a_0}{c} + \frac{\vec{a}_1}{c} \cdot \int \vec{\Omega} d\Omega = \frac{4\pi a_0}{c}$$

and

$$\vec{\mathbf{F}} = \int \vec{\Omega} \mathbf{I} d\Omega = a_0 \int \vec{\Omega} d\Omega + \vec{a}_1 \cdot \int \vec{\Omega} \vec{\Omega} d\Omega = \frac{4\pi \vec{a}_1}{3}$$

That is,

$$\mathbf{I} = \frac{c\mathbf{E} + 3\vec{\mathbf{F}} \cdot \vec{\Omega}}{4\pi} \quad (44)$$

and

$$\begin{aligned}\nabla \cdot \int \vec{\Omega} \vec{\Omega} \mathbf{I} d\Omega &= \nabla \cdot \frac{c\mathbf{E}}{4\pi} \int \vec{\Omega} \vec{\Omega} d\Omega + \frac{3}{4\pi} \nabla \cdot \int \vec{\Omega} \vec{\Omega} \vec{\Omega} d\Omega \cdot \vec{\mathbf{F}} \\ &= \frac{c}{3} \mathbf{E} \nabla\end{aligned}$$

The equations then become

$$\begin{aligned} \frac{\partial E}{\partial t} + \nabla \cdot \vec{F} + c \sigma E &= \int S d\Omega \\ -\frac{1}{c} \frac{\partial \vec{F}}{\partial t} + \frac{c}{3} \nabla E + \sigma \vec{F} &= \int \vec{\Omega} S d\Omega \end{aligned} \quad (45)$$

This approximation, which is sometimes called non-equilibrium diffusion, has been studied in some detail (see Refs. 1 and 2) and is adequate to describe a wide range of interesting configurations. Nevertheless, formula (44) is not a good representation of radiation which is, say, streaming away from a localized source in a thin medium. Theoretically, the approximation can be improved simply by taking account of more moments. The weighting functions most often used for calculating higher moments of functions defined on a sphere are the spherical harmonics, which have the advantage of being orthogonal. However, spherical harmonics are not well adapted to representing the angular dependence of radiant intensity, because the intensity often becomes an almost discontinuous function of angle near abrupt changes in opacity and the expansion of such a function in spherical harmonics converges very slowly. The difficulty cannot, however, be attributed to the use of spherical harmonics. If the intensity were represented as

$$\begin{aligned} I(\vec{\Omega}) &= a_0 + \vec{a}_1 \cdot \vec{\Omega} + (\vec{a}_2 \cdot \vec{\Omega})(\vec{b}_2 \cdot \vec{\Omega}) \\ &+ (\vec{a}_3 \cdot \vec{\Omega})(\vec{b}_3 \cdot \vec{\Omega})(\vec{c}_3 \cdot \vec{\Omega}) + \dots \end{aligned}$$

the rate of convergence would be the same. Yvon (see Ref. 3, p.101) has suggested that the convergence could be improved by expanding I_+ and I_- independently, but it is hard to generalize his idea to two dimensions.

Another disadvantage of the method of moments is that the matrix of the finite difference operator yielded by this method as an approximation

to the differential transport operator $(\vec{\Omega} \cdot \nabla + \sigma)$ is rather difficult to invert, so that a time-consuming iterative procedure is required to calculate the intensity at each time step (see, for example, Ref. 4).

3.3. DISCRETE ORDINATES

Wick (Ref. 5), in studying scattering of light in plane atmospheres, got around the difficulty of representing an intensity whose angular distribution is nearly discontinuous by limiting the determination of $I(\vec{\Omega})$ to a fixed finite set of directions $\vec{\Omega}_i$, $i=1, \dots, n$ which are more or less uniformly distributed. The quantities $I_i = I(\vec{\Omega}_i)$ are the so-called discrete ordinates of the method.

Carlson's S_n method (Ref. 6) is one of the most widely applied numerical versions of the discrete ordinate method. His procedure amounts to replacing the derivatives in the transport equation (43) by finite difference quotients. To do this in finite cylindrical geometry, first set

$$\vec{\Omega} = \mu \vec{k} + (1 - \mu^2)^{1/2} (\cos \phi \vec{i} + \sin \phi \vec{j}) \quad (46)$$

where $\vec{k}$ is a unit vector parallel to the z-axis, $\vec{i}$ is a unit vector perpendicular to $\vec{k}$ and pointing away from the axis of symmetry of the system, and $\vec{j} = \vec{k} \times \vec{i}$. Then $\vec{\Omega} \cdot \nabla$ can be expressed as a sum of partial derivatives, and the transport equation (43) becomes

$$\frac{1}{c} \frac{\partial I}{\partial t} + \mu \frac{\partial I}{\partial z} + (1 - \mu^2)^{1/2} \left(\cos \phi \frac{\partial I}{\partial r} - \frac{\sin \phi}{r} \frac{\partial I}{\partial \phi} \right) + \sigma I = S \quad (47)$$

A discrete system of points in r-z-t space has already been provided by the assumptions concerning the way the hydrodynamics is being computed. It remains only to discretize the angular variables. This is done by selecting a set of μ 's that are evenly distributed between -1 and +1. Then ϕ 's are chosen for each μ in such a way that the resulting directions are more or less evenly distributed over the unit sphere, for example, as shown in Fig.7.

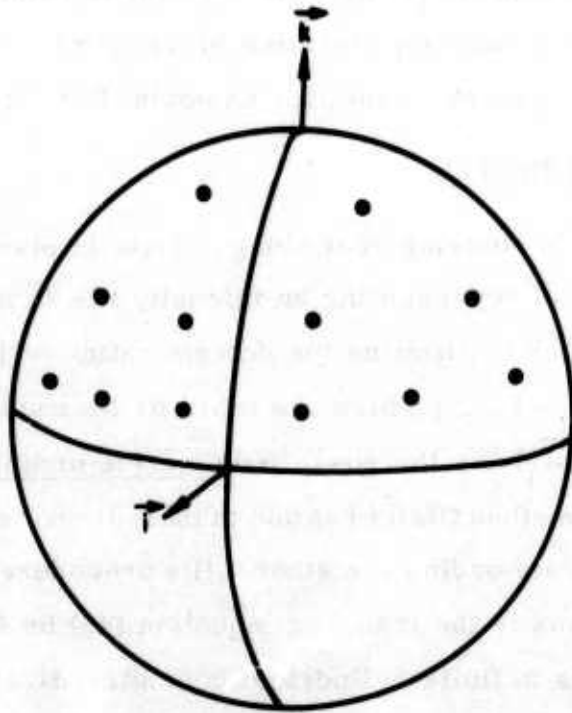


Figure 7. Typical Distribution of Directions.

Having the selected values of ϕ depend on the value of μ causes no difficulty because $\frac{\partial I}{\partial \mu}$ does not occur in the differential equation (47). Let

$$I_{i,j,\bar{m}} = I(r_i, z_{\bar{j}}, \mu, \phi_{\bar{m}}, \nu, t)$$

where

$$z_{\bar{j}} = 1/2(z_j + z_{j-1}), \quad \phi_{\bar{m}} = 1/2(\phi_m + \phi_{m-1})$$

and μ , ν , and t are fixed. Then it is possible to approximate

$$TI = \mu \frac{\partial I}{\partial z} + (1 - \mu^2)^{1/2} \left(\cos \phi \frac{\partial I}{\partial r} - \frac{\sin \phi}{r} \frac{\partial I}{\partial \phi} \right)$$

by

$$\bar{T}I = 2\mu \frac{I_{\bar{i},\bar{j},\bar{m}} - I_{i,j,\bar{m}}}{z_j - z_{j-1}} + (1 - \mu^2)^{1/2} \left[\cos \phi_{\bar{m}} \frac{I_{i,\bar{j},\bar{m}} - I_{i-1,\bar{j},\bar{m}}}{r_i - r_{i-1}} \right.$$

$$\left. + \frac{2\gamma_{\bar{m}}}{r_i} (I_{\bar{i},\bar{j},\bar{m}} - I_{\bar{i},\bar{j},m-1}) \right]$$

where

$$I_{\bar{i},\bar{j},\bar{m}} = \frac{I_{i,\bar{j},\bar{m}} + I_{i-1,\bar{j},\bar{m}}}{2}$$

$$I_{i,j,\bar{m}} = 2I_{\bar{i},\bar{j},\bar{m}} - I_{\bar{i},j-1,\bar{m}}$$

$$I_{\bar{i},\bar{j},m} = 2I_{\bar{i},\bar{j},\bar{m}} - I_{\bar{i},\bar{j},m-1}$$

$$\gamma_m = \gamma_{m-1} - \frac{\cos \phi_{\bar{m}} + \cos \phi_{\bar{m}-1}}{2}$$

and

$$\gamma_1 = -\frac{\cos \phi_1}{2}$$

Here T and $\bar{T}$ denote the differential operator $\vec{\Omega} \cdot \nabla$ and its finite difference approximation, respectively. Then, with the assumption that $I_n = I(r, z, \mu, \phi, \nu, t_n)$, the whole transport equation can be approximated by

$$\frac{1}{c} \frac{I_n - I_{n-1}}{t_n - t_{n-1}} + \frac{\bar{T}I_n + \bar{T}I_{n-1}}{2} + \frac{\sigma_n I_n + \sigma_{n-1} I_{n-1}}{2} = \frac{S_n + S_{n-1}}{2}$$

or

$$\frac{1}{c} \frac{I_n}{t_n - t_{n-1}} + (1/2)(\bar{T}I_n + \sigma_n I_n) \quad (48)$$

$$= \frac{1}{c} \frac{I_{n-1}}{t_n - t_{n-1}} + (1/2)(S_n + S_{n-1} - \bar{T}I_{n-1} - \sigma_{n-1} I_{n-1})$$

The quantities γ_m , which approximate $\sin \phi_m / \Delta \phi$, are chosen as they are so that the difference equations conserve energy exactly.

A difficulty with the method is that the spatial integration, i.e., the solution of Eq. (48) for some particular value of t , tends to become unstable unless

$$r_i - r_{i-1} < \min \frac{(1 - \mu^2)^{1/2} \cos \phi}{\sigma + \frac{1}{c \Delta t}}$$

at all points, a condition which is very likely to be violated in opaque regions unless the mesh is extraordinarily fine. Various remedies are possible. One is to subdivide the mesh in opaque regions so that the optical distance between neighboring mesh points will be below some limit for all zones in the radiation calculation. Another possibility is to make opaque regions external to the transport calculation since they can be adequately treated in a diffusion approximation anyway. The trouble with the first suggestion is that adding subdivisions to opaque regions can increase the amount of computing that must be done by a sizeable factor. The second suggestion has considerable merit if applied in conjunction with the first, but by itself does not help in regions that are thick enough to be unstable in the S_n method but for which the diffusion approximation is poor.

A possibility that abandons the use of linear difference equations to represent the transport operator is one that Richtmyer (see Ref. 7, p.151) attributes to von Neumann. It is variously called the method of direct

integration or the method of characteristics. The basic idea is the observation that solutions of the transport equation must satisfy the equation

$$\begin{aligned}
 I(\vec{x}, \vec{\Omega}, \nu, t) = & I(\vec{x} - s\vec{\Omega}, \vec{\Omega}, \nu, t - \frac{s}{c}) e^{-\int_0^s \sigma(\vec{x} - u\vec{\Omega}, \nu, t - \frac{u}{c}) du} \\
 & + \int_0^s S(\vec{x} - u\vec{\Omega}, \vec{\Omega}, \nu, t - \frac{u}{c}) e^{-\int_0^u \sigma(\vec{x} - v\vec{\Omega}, \nu, t - \frac{v}{c}) dv} du
 \end{aligned} \quad (49)$$

The paths of integration, which are of the form

$$\begin{aligned}
 \vec{x} &= \vec{x}_0 + s\vec{\Omega} \\
 t &= t_0 + \frac{s}{c}
 \end{aligned}$$

where the distance s along the path is a parameter, are paths in space-time. They lie on characteristic cones of the differential operator

$$\frac{1}{c} \frac{\partial}{\partial t} + \vec{\Omega} \cdot \nabla$$

which is the basis for the name "method of characteristics." One can use Eq. (49) to estimate the intensity of radiation at some point $\vec{x}$ with coordinates r_i, z_j at some time t_{n+1} and having some direction $\vec{\Omega}_m$ by finding the smallest value of s for which $\vec{x} - s\vec{\Omega}$ falls on one of the surfaces $r = r_{i\pm 1}$ or $z = z_{j\pm 1}$ or $t = t_n$. Suppose, as shown in Fig. 8, that this point falls on $r = r_{i+1}$ with $z_{j-1} < z < z_j$ and $t_n < t_{n+1} - s/c$. Then, by interpolation, using the points r_{i+1}, z_j and r_{i+1}, z_{j-1} at times t_{n+1} and t_n , one can estimate $I(\vec{x} - s\vec{\Omega}, \vec{\Omega}, \nu, t_{n+1} - \frac{s}{c})$, and then, assuming that one knows σ and S along the path of integration, $I(\vec{x}, \vec{\Omega}, \nu, t_{n+1})$ can be calculated at $\vec{x} = (r_i, z_j)$. Of

course, some of the required information will be missing unless the calculation proceeds in the proper sequence, e.g., r decreasing and z increasing for $\vec{\Omega}$ pointing somewhat upward and toward the axis. Another point that has been glossed over is the fact that the angle ϕ defined by Eq. (46) changes along the path, so an interpolation involving $\vec{\Omega}$ must also be performed. Interpolation in ϕ is particularly bad and is just what the method of discrete ordinates was supposed to avoid. The S_n method, in which $\partial I / \partial \phi$ is approximated by a difference quotient, suffers from the same malady.

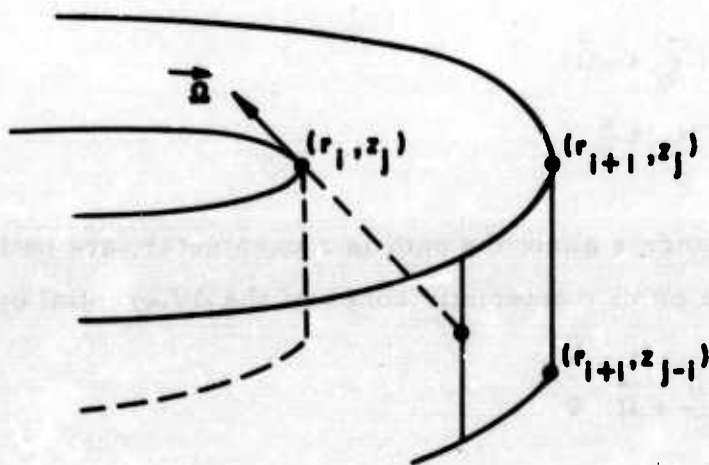


Figure 8. Typical Short Characteristic

The remaining details will not be discussed here; instead the approach will be changed to one avoiding extensive interpolation by integrating Eq. (49) over paths that run straight through the system between pairs of points on the outer boundary. The idea is to ignore the vertices of the mesh and determine the rate of deposition of radiant energy in the zones (which, in the present case, are toroids of rectangular cross section) by suitably averaging the intensities along the paths that they intersect.

The first problem that arises in implementing the method is choosing an appropriate set of paths. The simplest approach is perhaps to choose the paths so that they fill the region of interest more or less uniformly in space and direction. The advantage of this choice is that in calculating rates of deposition of radiant energy from the intensities along the paths, all paths will have about the same weight. To see how lines with the desired uniform distribution can be constructed, define a grid to be a set of parallel lines that intersect a normal plane in a regular pattern of points, e.g., in a square lattice. Next, select a finite set of directions that are more or less uniformly distributed, e.g., the directions from the center of a regular polyhedron to its vertices. Then the set of lines obtained by combining a collection of congruent grids whose directions are those of the selected set will have the desired uniformity. The integration paths are simply obtained as the intersection of the collection of lines with the domain of the hydrodynamical problem, which is a cylinder of finite length.

It is next necessary to consider the problem of calculating intensities and rates of deposition of radiant energy during the time interval $t_n \leq t \leq t_{n+1}$. Suppose that at $t = t_n$ one is given estimates of the intensity at uniformly spaced points along each of the paths. Then, by rewriting (49) as

$$I(\vec{x} + s\vec{\Omega}, \vec{\Omega}, \nu, t + \frac{s}{c}) = I(\vec{x}, \vec{\Omega}, \nu, t) e^{-\int_0^s (\vec{x} + u\vec{\Omega}, \vec{\Omega}, \nu, t + \frac{u}{c}) du} + \int_0^s S(\vec{x} + u\vec{\Omega}, \vec{\Omega}, \nu, t + \frac{u}{c}) e^{-\int_0^u (\vec{x} + v\vec{\Omega}, \vec{\Omega}, \nu, t + \frac{v}{c}) dv} du \quad (50)$$

the intensity can be advanced a distance $c(t_{n+1} - t_n)$ along each path. These pulses of radiation will continually be lost by emerging from the system. They must be replenished by beginning new ones at points where the paths

begin. The initial intensity must be specified as a boundary condition. The energy deposited in a zone during the time interval $t_n \leq t \leq t_{n+1}$ by radiation of frequency ν may then be estimated to be

$$E = V \frac{\sum \int_{s_1}^{s_2} \sigma(\vec{x} + s\vec{\Omega}, \nu, t + \frac{s}{c}) I(\vec{x} + s\vec{\Omega}, \vec{\Omega}, \nu, t + \frac{s}{c}) ds}{\sum (s_2 - s_1)} \quad (51)$$

where the summation is carried out over all paths intersecting the zone, and $s_1 \leq s \leq s_2$ is the segment of the path that the pulse of radiation, which is located at $\vec{x}$ at time t , sweeps out in the zone during the time interval, and V is the volume of the zone.

The version of the method of characteristics just described has two important advantages: (1) It is possible to traverse optically thick segments in one step, and (2) the three-dimensional interpolation of previously described discrete ordinate methods is avoided.

On the other hand, the method has several disadvantages. One of them is the large number of exponentials that must be calculated. However, this is a reasonable price to pay for being able to traverse long segments, because direct methods for evaluating exponentials are more efficient than finite difference methods, and one can say that, in essence, S_n calculates exponentials by a numerical integration. There are other difficulties connected with the absence of interpolation. For example: (1) the summation in Eq. (51) is a rather crude approximation to an integral over x , $\vec{\Omega}$, and t ; (2) if anisotropy of scattering is a significant effect, then the contribution of scattering to the source S in Eq. (50) will be difficult to approximate; (3) in order to get an adequate density of paths near the axis of the system, the density near the boundary must be much higher than necessary; and (4) energy is not conserved in the numerical approximation. Refinements of the method will be left to subsequent reports. It suffices to say that the method can be improved by using some interpolation, but not so much as the earlier versions used.

3.4. THE MONTE CARLO METHOD

The Monte Carlo method discussed below is patterned after one described by Fleck (Ref. 8). As before, the over-all procedure is first to advance the temperature and other material properties from time $t_{n-1/2}$ to time $t_{n+1/2}$ and then to calculate the radiant flux at $t = t_{n+1}$ from that at $t = t_n$, assuming that the average temperature in the time interval $t_n \leq t \leq t_{n+1}$ is its value at $t = t_{n+1/2}$.

The Monte Carlo procedure involves generating a number of pulses of radiation, called photons, from the given temperature distribution and following them until $t = t_{n+1}$ unless they are absorbed or escape first. Those photons that survive until t_{n+1} are noted, and their histories are continued during the next time interval.

The numerical photons, unlike real ones, all have the same energy E_0 . Thus, the number of photons generated in any given zone during the interval $t_n \leq t \leq t_{n+1}$ is the ratio of the radiant energy liberated by the zone during that interval to the energy E_0 of the photons. The fate of a fractional photon is decided by Russian roulette.

The process of following a photon consists first in determining the distance to each of three possible events: (1) penetrating the boundary of a zone, (2) collision, and (3) census. Given the position of a photon and its direction, the distance d_B it has to go before hitting the boundary of the zone it is in can be calculated directly. The distance of the photon from its next collision is

$$d_{col} = -\lambda \log R$$

where λ is the mean distance between collisions, which is a function of the material properties of the zone and the frequency of the photon, and R is a random number drawn from a population distributed uniformly over the real interval $0 \leq R \leq 1$. The distance to census is simply $d_{cen} = (t_{n+1} - t)/c$.

The event which actually occurs next is the one that occurs within the shortest distance. If it is a collision, a new random number R between 0 and 1 is chosen and compared with the absorption probability p . If $R < p$, the collision is declared to have resulted in an absorption and the history of the photon is terminated. Otherwise, a new direction is chosen according to an appropriate scattering law. If the frequency of the photon is so high that the Compton effect is significant, then the change of frequency must also be calculated.

If the next event is a boundary crossing, either the boundary is an external boundary, in which case the photon is lost, or else it is an interface between zones and the history is continued from the new position and time but without change of direction or frequency. Finally, when a photon reaches census, its state is recorded and its history is continued during the next interval of time.

The amount of energy deposited by the photon as it travels between a pair of consecutive events is estimated to be $E_0 \sigma_d s$, where σ_d is the coefficient in Eq. (42), which depends on the frequency of the photon and the state of the zone in which the segment of path lies, and s is the distance between the pair of events. The total amount of radiant energy deposited in each zone during $t_{n-1} \leq t \leq t_n$ is taken to be the sum of such contributions.

3.5. CONCLUSIONS

Among the methods outlined above, Monte Carlo and the method of characteristics appear to be the most promising. The principal advantage of Monte Carlo, in most of its applications, is that it provides a straightforward way to handle the various complications that arise in performing integrations over domains of high dimension. Examples of such complications that occur in problems of radiative transport are retardation, scattering, and, especially in connection with a Lagrangian mesh for describing material properties, geometrical detail. Another advantage of the

Monte Carlo method is that the work can be much reduced if a good estimate of the importance is available. With reference to the present application, this is much the same as saying that the Monte Carlo described above concentrates the numerical work in those regions where the radiant intensity is high because that is where the photons are, whereas the method of characteristics requires about the same amount of calculation in regions of equal size regardless of the intensity.

On the other hand, Monte Carlo methods converge very slowly. Also, while they may provide the best method for obtaining a first estimate of a single multiple integral, they are not generally good for obtaining distributions, which is just what is wanted: the rate of deposition of radiant energy in three dimensions-- r , z , and t .

Further, there are two serious disadvantages of the Monte Carlo procedure described above as applied to the particular present problem. One is that the geometrical calculation has to be repeated every time step, whereas in an Eulerian mesh, nonstochastic methods require that geometrical coefficients be calculated only once. The other is that the method will bog down in any hot opaque zone in which a great number of paths will begin and end.

The conclusion is that the method of moments should be used when the first two moments (of degrees 0 and 1) are adequate, and that the method of characteristics should be used when a better transport approximation is required.

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SECTION IV

NON-EQUILIBRIUM DIFFUSION METHODS FOR HECTIC4.1. INTRODUCTION

The code TDRAD calculates the solution to the two moment equations (45) as the radiation calculation in HECTIC. If we set

$$\int S d\Omega = s \quad \text{and} \quad \int \vec{\Omega} S d\Omega = 0$$

assuming the source to be isotropic, and neglect retardation, the equations become

$$\begin{aligned} \nabla \cdot \vec{F} + c \sigma E &= s \\ \frac{c}{3} \nabla E + \frac{\vec{F}}{\lambda} &= 0 \end{aligned} \tag{52}$$

Here, $\vec{F}/\lambda$ occurs in place of $\sigma \vec{F}$. An improvement in the approximation can be made by allowing $1/\lambda$ to be unequal to σ because the Planck mean opacity is appropriate for estimating emission and absorption coefficients, while the Rosseland mean is the one to use for transmission coefficients.

In cylindrical coordinates, these equations become

$$\begin{aligned} \frac{1}{r} \frac{\partial}{\partial r} (r F_r) + \frac{\partial}{\partial z} F_z + c \sigma E &= s \\ \frac{c}{3} \frac{\partial E}{\partial r} + \frac{1}{\lambda} F_r &= 0 \\ \frac{c}{3} \frac{\partial E}{\partial z} + \frac{1}{\lambda} F_z &= 0 \end{aligned} \tag{53}$$

4.2. THE FINITE DIFFERENCE APPROXIMATION

Let r_i, z_j denote the coordinate pair of the mesh point i, j in HECTIC (see Fig. 9). Let $E_{i+1/2, j+1/2}$ denote the value of E at the center of

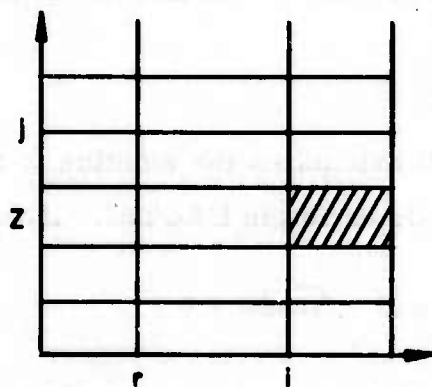


Figure 9. Hydrodynamic Mesh

the zone i, j , i.e., at $r = (r_i + r_{i+1})/2, z = (z_j + z_{j+1})/2$. Let $F_{i+1/2, j}$ denote the value F_z at $z = z_j, r = (r_i + r_{i+1})/2$, and let $G_{i, j+1/2}$ denote the value of $2 r F_r$ at $r = r_i, z = (z_j + z_{j+1})/2$ (see Fig. 10).

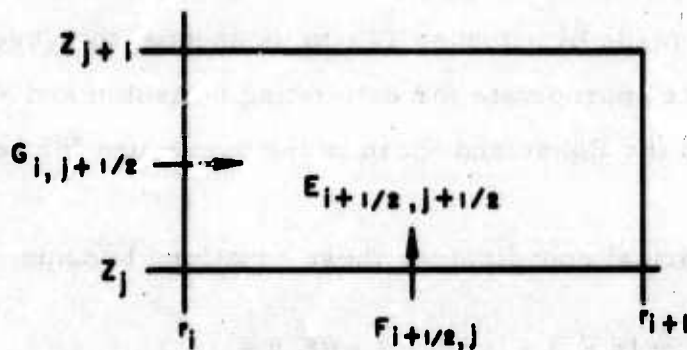


Figure 10. Typical Cell of Mesh

Then a set of difference equations compatible with Eq. (53) is

$$\frac{G_{i+1,j+1/2} - G_{i,j+1/2}}{r_{i+1}^2 - r_i^2} + \frac{F_{i+1/2,j+1} - F_{i+1/2,j}}{z_{j+1} - z_j} + c \sigma_{i+1/2,j+1/2} E_{i+1/2,j+1/2} = s_{i+1/2,j+1/2}$$

$$\frac{2c}{3} \frac{E_{i+1/2,j+1/2} - E_{i+1/2,j-1/2}}{z_{j+1} - z_{j-1}} + \frac{F_{i+1/2,j}}{\lambda_{i+1/2,j}} = 0 \quad (54)$$

$$\frac{4cr_i}{3} \frac{E_{i+1/2,j+1/2} - E_{i-1/2,j+1/2}}{r_{i+1} - r_{i-1}} + \frac{G_{i,j+1/2}}{\lambda_{i,j+1/2}} = 0$$

where

$$\lambda_{i+1/2,j} = \frac{z_{j+1} - z_{j-1}}{\frac{z_{j+1} - z_j}{\lambda_{i+1/2,j+1/2}} + \frac{z_j - z_{j-1}}{\lambda_{i+1/2,j-1/2}}} \quad (55)$$

$$\lambda_{i,j+1/2} = \frac{r_{i+1} - r_{i-1}}{\frac{r_{i+1} - r_i}{\lambda_{i+1/2,j+1/2}} + \frac{r_i - r_{i-1}}{\lambda_{i-1/2,j+1/2}}}$$

Eliminating F and G from Eq. (54) gives

$$A_{ij} E_{i-1/2,j+1/2} + B_{ij} E_{i+1/2,j+1/2} + C_{ij} E_{i+3/2,j+1/2} + \alpha_{ij} E_{i+1/2,j-1/2} + \gamma_{ij} E_{i+1/2,j+3/2} + D_{ij} = 0 \quad (56)$$

where

$$\begin{aligned}
 A_{ij} &= -\frac{4cr_i \lambda_{i,j+1/2}}{3(r_{i+1} - r_{i-1})(r_{i+1}^2 - r_i^2)} \\
 C_{ij} &= -\frac{4cr_{i+1} \lambda_{i+1,j+1/2}}{3(r_{i+2} - r_i)(r_{i+1}^2 - r_i^2)} \\
 \alpha_{ij} &= -\frac{2c \lambda_{i+1/2,j}}{3(z_{j+1} - z_{j-1})(z_{j+1} - z_j)} \\
 \gamma_{ij} &= -\frac{2c \lambda_{i+1/2,j+1}}{3(z_{j+2} - z_j)(z_{j+1} - z_j)} \\
 B_{ij} &= c\sigma_{i+1/2,j+1/2} - A_{ij} - C_{ij} - \alpha_{ij} - \gamma_{ij} \\
 D_{ij} &= -s_{i+1/2,j+1/2}
 \end{aligned} \tag{57}$$

The boundary conditions are described below. The procedure is to solve Eq. (56) for E, then find F and G using Eq. (54). Finally, the rate at which energy is deposited in the zone i, j is determined by

$$\begin{aligned}
 \left(\frac{dE}{dt}\right)_{i+1/2,j+1/2} &= \pi(z_{j+1} - z_j)(G_{i,j+1/2} - G_{i+1,j+1/2}) \\
 &\quad + \pi(r_{i+1}^2 - r_i^2)(F_{i+1/2,j} - F_{i+1/2,j+1})
 \end{aligned} \tag{58}$$

4.3. BOUNDARY CONDITIONS

The axis of the system, which corresponds to $i = 0$, is not a geometrical boundary since $r_0 = 0$ is required. With reference to Eqs. (56) and (57), $i = 0$ is hardly exceptional since $r_0 = 0$ forces $A_{0j} = 0$, which means that $E_{-1/2,j+1/2}$ has a coefficient of 0 and therefore cannot be relevant. Similarly, $G_{0,j+1/2} = 0$, by Eq. (54), which is appropriate for $i = 0$ in Eq. (58).

The outer surfaces can have either blackbody boundary condition or a reflective boundary condition. For a vacuum boundary condition, a blackbody boundary with $\theta = 0$ is used.

The reflective boundary condition is the condition that $\vec{F} \cdot \vec{N} = 0$, where $\vec{N}$ is the normal to the bounding surface. This is equivalent to

$$\begin{aligned} G_{I,j+1/2} &= C_{I-1,j} = 0 && \text{on the curved boundary} \\ F_{i+1/2,0} &= \alpha_{i,0} = 0 && \text{on the bottom} \\ F_{i+1/2,J} &= \gamma_{i,J-1} = 0 && \text{on the top} \end{aligned} \quad (59)$$

The blackbody boundary condition is analagous to that of ERADTN. (Compare with Eqs. (28) and (29).) Thus,

$$\begin{aligned} G_{I,j+1/2} &= 2r_I \beta \left(-\frac{ac\theta^4}{2} + \frac{c}{2} E_{I-1/2,j+1/2} \right) \\ \frac{1}{\beta} &= 2 - e^{-\alpha(r_I - r_{I-1})/2} \\ \alpha &= \left(\frac{3\mu_{I-1/2,j+1/2}}{\lambda_{I-1/2,j+1/2}} \right)^{1/2} \end{aligned} \quad (60)$$

on the curved boundary $r = r_{I+1}$, $z_j \leq z \leq z_{j+1}$;

$$\begin{aligned} F_{i+1/2,0} &= \beta \left(\frac{ac\theta^4}{2} - \frac{c}{2} E_{i+1/2,1/2} \right) \\ \frac{1}{\beta} &= 2 - e^{-\alpha z_1/2} \\ \alpha &= \left(\frac{3\mu_{i+1/2,1/2}}{\lambda_{i+1/2,1/2}} \right)^{1/2} \end{aligned} \quad (61)$$

on the bottom; and

$$F_{i+1/2, J} = \beta \left(-\frac{ac\theta^4}{2} + \frac{c}{2} E_{i+1/2, J-1/2} \right)$$

$$\frac{1}{\beta} = 2 - e^{-\alpha(z_{J+1} - z_J)/2} \quad (62)$$

$$\alpha = \left(\frac{3\mu_{i+1/2, J-1/2}}{\lambda_{i+1/2, J-1/2}} \right)^{1/2}$$

on the top. Using these formulas in Eq. (54) modifies Eq. (57) at certain points as follows:

on the curved outer surface,

$$C_{I-1, j} = 0$$

$$B_{I-1, j} = c \sigma_{I-1, j} + \frac{cr_I \beta}{r_I^2 - r_{I-1}^2} - A_{I-1, j} - \alpha_{I-1, j} - \gamma_{I-1, j}$$

$$D_{I-1, j} = -s_{I-1, j} - \frac{acr_I \beta \theta^4}{r_I^2 - r_{I-1}^2}$$

on the bottom,

$$\alpha_{io} = 0$$

$$B_{io} = c \sigma_{io} + \frac{\beta c}{2z_1} - A_{io} - C_{io} - \alpha_{io}, \quad (63)$$

$$D_{io} = -s_{io} - \frac{ac\beta\theta^4}{2z_1}$$

on the top,

$$\gamma_{i, J-1} = 0$$

$$B_{i, J-1} = c \sigma_{i, J-1} + \frac{\beta c}{2(z_J - z_{J-1})} - A_{I-1, j} - C_{I-1, j} - \alpha_{I-1, j}$$

$$D_{i, J-1} = -s_{i, J-1} - \frac{ac\beta\theta^4}{2(z_j - z_{J-1})}$$

4. 4. METHODS FOR SOLVING THE SYSTEM

Sets of equations of the type of Eq. (56) occur widely in the application of finite differences to problems of elliptic partial differential equations. In situations where Eddington's so-called diffusion approximation is good, the splitting method used in MOTET can be used to advantage. However, when Δt is large and the state of the radiation field at time t^{n+1} is essentially decoupled from its state at time t^n , the parabolic character of the problem disappears, and it becomes necessary to turn to methods of the sort used to solve elliptic problems. An iterative method due to Oliphant, which is described briefly in Section 4. 5, is used in TDRAD to solve the system (56).

For those problems for which two moments can be expected to provide an adequate description of the field of radiation, Oliphant's method appears to work quite well. When λ becomes large compared with the size of the zones, the method requires an excessive number of iterations to converge. But in these cases, either a full transport approximation is required, or else it is possible to remesh the problem with larger zones.

4. 5. PROCEDURE FOR SOLVING THE SYSTEM

Algebraically, the problem of solving the system of equations (56) is that of finding a column vector e that satisfies

$$be = d$$

(64)

where $b_{k, k-1} = A_{ij}$, $i \neq 0$

$$b_{k, k} = B_{ij}$$

$$b_{k, k+1} = C_{ij}, \quad i \neq I$$

$$b_{k, k-I} = \alpha_{ij}, \quad j \neq 0$$

$$b_{k, k+I} = \gamma_{ij}, \quad j \neq J$$

(65)

$$e_k = E_{i+1/2, j+1/2}$$

$$d_k = -D_{ij}$$

$$k = i + jI + 1$$

The procedure used in TDRAD is due to Oliphant* and is based on the observation that b may be expressed as

$$b = vw + h \tag{66}$$

where $v_{kl} = 0$ unless $k = l, l + 1$, or $l + I$; $w_k = 0$ unless $k = l, l - 1$, or $l - I$; and $h_{kl} = 0$ unless $|k - l| = I - 1$. The product vw is easy to invert because the factors v and w are triangular. It is plausible to suppose that the iteration

$$e^{(n+1)} = w^{-1} v^{-1} (d - h e^{(n)}) \tag{67}$$

will produce a sequence of approximants $e^{(n)}$ that converge to a solution e of Eq. (64) as $n \rightarrow \infty$, and, when b is a matrix arising from a finite difference operator derived from the Laplacian operator, it does, in fact, seem to do so.

Two devices, also recommended by Oliphant, are used to accelerate convergence. The first is to add $(K - 1)u$ to b before performing the

*Oliphant, T. A., "An Extrapolation Procedure for Solving Linear Systems," Quat. Appl. Math. 20, 257 (1962).

factorization (66), u being the part of b above the principal diagonal. To compensate, d is replaced by $d + (K - 1) ue^{(n)}$. The second device is simple extrapolation. Thus,

$$\begin{aligned} e^{(n+1/2)} &= w^{-1} v^{-1} (d + (K - 1) ue^{(n)} - he^{(n)}) \\ e^{(n+1)} &= \omega e^{(n+1/2)} + (1-\omega)e^{(n)} \end{aligned} \quad (68)$$

The pair of values K, ω has to be determined experimentally. Note that if $K = 0$, the method reduces to a sort of Seidel-method-with-extrapolation, because subtracting u from b leaves it lower triangular and so $h = 0$. Setting K and ω both near 1.0 seems to be close to optimal.

4.6. THE SUBPROGRAM TDRAD

The subprogram TDRAD was designed to carry over essentially all the features of the SPUTTER radiation codes (e.g., multifrequency, opacity tables, time-step controls, boundary conditions) to the HECTIC program with minimum disturbance to the latter, while executing the equations given in Section 4.1. Since the radiation calculation would impose a considerable storage burden, a new COMMON statement with dimensions was worked out for IBM-7044 operation. Cell variables (10 in number for regular HECTIC, with 13 added for radiation) were limited to 400 words each; regular HECTIC provides 1200. All cell variables are assigned storage in a statement COMMON/ARRAY/.

In addition, 29 unsubscripted variables are assigned space in the COMMON block named LINDLY. The names of these variables and brief statements of their significance are given in Table IV. The first 21 variables in LINDLY are the input to TDRAD, and the remaining 8 are computed variables. Table V is a glossary of the variables of greatest importance in TDRAD. A list of some variables, pertinent to the radiation calculation and occurring in TDRAD and HECTIC, for which there exist homologous variables in SPUTTER, is given in Table VI.

Table IV
LINDLY COMMON

<u>Name of Variable</u>	<u>Meaning and/or Function</u>	<u>Value for First Test Problem</u>
SLUG	Arbitrary factor used in time step (accuracy) control pertaining to energy change	0.5
RPTAG	If zero, κ Planck used as is; if non-zero, κ Rosseland used instead	0.0
EFRAC	Constant used to determine importance of energy-poor zones in time step calculation	0.001
DTBUGR	Constant used to change time step as finally calculated	1.0
BCLTAG*	Boundary condition indicator on left or inner radial boundary; in-operative now	0.0
BCRTAG*	Boundary condition indicator on right or outer radial boundary	-1.
BCATAG*	Boundary condition indicator on top axial boundary ("above")	0.
BCBTAG*	Boundary condition indicator on bottom axial boundary ("below")	-1.
MERGE (real)	Multifrequency merge criterion; frequency compared with maximum temperature	0.
CMXK	The K used in adjusting the Oliphant iterative matrix inversion	1.4
CMXOM	The ω used in adjusting the Oliphant iterative matrix inversion	1.0
ERRCRT	Convergence error criterion on matrix inversion iteration	0.001
DBGPRT	Nonzero provides debug print	1.0
DIANTP	Logical tape unit on which DIANE tape is to be hung if one is used	0.0

* In all cases, negative = reflection; zero is vacuum; positive is blackbody whose temperature is value of indicator.

Table IV (continued)

<u>Name of Variable</u>	<u>Meaning and/or Function</u>	<u>Value for First Test Problem</u>
DGREY	If nonzero, DIANE tape is used for a grey calculation	0.0
CAPIN	Value of absorption coefficient assumed if no DIANE tape is read	1.0
ODDC	Optical depth difference criterion; average optical depth not calculated if zone depths are too dissimilar	0.333
MFTAG	If nonzero, multifrequency calculation; otherwise, grey calculation	0
IMPTAG	If nonzero, fully implicit calculation is done; inoperative at present	0
ITAG	Indicator of whether or not to iterate on time-centered temperature; nonzero says "do iterate"	0
ITRMAX	Maximum allowed number of iterations in the matrix inversion	30

(Computed Variables, i. e., not input)

SGNL	Material counter for multi-DIANE-tape problems; used in KAPPA and DIANA
IHNU	Frequency index
NHNU	Total number of frequency bands
HNUP	Frequency at upper end of band
NT	DIANE tape unit
DHNU	Width of frequency band
THICK	Not used
NY	Temperature iteration index

Table V
PARTIAL GLOSSARY OF FORTRAN VARIABLES

FORTRAN Variable Name	Designation in Difference Equations	Comments
ALAMH (K)	$\lambda_{i+1/2, j}$	$K = i + j I + 2$
ALAMV (K)	$\lambda_{i, j+1/2}$	
DY (J)	$z_{j+1} - z_j$	
ROSS (K)	$1/\lambda_{i+1/2, j+1/2}$	Rosseland mean opacity, in cm^{-1}
DTAUR	$\frac{r_{i+1} - r_i}{\lambda_{i+1/2, j+1/2}}$	
DTAUL	$\frac{r_i - r_{i-1}}{\lambda_{i-1/2, j+1/2}}$	
DTAUA	$\frac{z_{j+1} - z_j}{\lambda_{i+1/2, j+1/2}}$	
DTAUB	$\frac{z_j - z_{j-1}}{\lambda_{i+1/2, j-1/2}}$	
PUR (I)	$\frac{1}{r_{i+1}^2 - r_i^2}$	defined in the loop DO 150
RUR (I)	$\frac{4}{3} c \frac{\gamma_i}{r_{i+1} - r_{i-1}}$	
PUZ (J)	$\frac{1}{z_{j+1} - z_j}$	defined in the loop DO 160
RUZ (J)	$\frac{2}{3} c \frac{1}{z_{i+1} - z_{j-1}}$	
X(I)	r_{i+1}	Note displacement of index
Y(J)	$j+1$	Note displacement of index

Table V (continued)

FORTTRAN Variable Name	Designation in Difference Equations	Comments
XA(K)	A_{ij}	Defined two lines above statement 531
XC(K)	C_{ij}	Defined at statement 536
XALP(K)	α_{ij}	Defined one line below statement 540
XGAM(K)	γ_{ij}	Defined at statement 546
XD(K)	$-D_{ij}$	
XB(K)	B_{ij}	
PLANCK (K)	$\sigma_{i+1/2, j+1/2}$	Planck mean opacity, in cm^{-1}
B (K)	κ	Source; not explicitly referred to in text
XD (K)	$E_{i+1/2, j+1/2}$	Radiation energy, redefined in matrix inversion
XA (K)	$F_{i+1/2, j}$	Flux; redefined two lines above statement 650
XB (K)	$G_{i, j+1/2}$	Flux; redefined one line below statement 655

Table VI
BERLITZ GUIDE TO TDRAD FOR
THE SPUTTER USER

<u>Name of HECTIC or TDRAD Variable</u>	<u>Name of Sputter Variable</u>
MFTAG	KMAX
RPTAG	SOLID (10)
EFRAC	TELM (37)
IMPTAG	HVB
DTBUGR	TELM (25)
NRM = Z (62)	NTIMES = BOILB
NR	NRAD
DT = Z (3)	DTH2
BCLTAG	GA
BCRTAG	GL
BCBTAG	
BCATAG	
MERGE	CB
ROSS	CAPAR
PLANCK	CAPAC
B	X6
ØDDC	AC (ERADTN only)
DBGPRT	S12
DIANTP	AMASNO(L+17)
DGREY	S15

4.7. OUTLINE OF TDRAD

1. Set up temperature iteration index and turn off divide check light.
2. Call KAPPA and thereby obtain the grey opacities, expressly for the time step calculation.
3. Calculate time step for each zone by two criteria, stability and (energy) accuracy.
4. Find minimum time step and set subcycle quantities if necessary.
5. Test divide check light, calculate geometry factors (saves time but costs storage to do this at this early part of the code), and find the largest temperature. The largest temperature is used only in deciding whether or not to merge frequency groups in a multifrequency calculation. Zero several zone quantities.
6. If doing multifrequency calculation, and if there are frequency groups with too large $u = h\nu/\theta$, merge them together.
7. If doing grey calculation, evaluate source B, set extreme frequency limits, and transfer to (9).
8. If doing a normal multifrequency calculation, update frequency parameters and evaluate source, B.
9. Set blackbody sources if appropriate and test divide check light.
10. Form zone and edge $\kappa\rho$.
11. Form and modify matrix elements.
12. Invert matrix iteratively.
13. Calculate radiation flux and internal energy change.
14. End frequency loop.
15. Iterate on temperature.
16. Reset temperature if necessary and return.

4.8. REVIEW OF THE CODE DEVELOPMENT

In early January 1966 the iterative version was written, and test problems were begun. A rather "thick" problem (one mean free path per cell) was tried, and the results appeared satisfactory after a brief debug phase. Then a run was made to compare directly with ERADTN, with a reflective

outer radial boundary condition chosen to simulate a problem in slab geometry. The interior of this slab comparison was quite thin, and convergence difficulties arose. It was found, after several trials, that a choice of parameters $K = 1.2$, $\omega = 1.0$ (see Section 4.6) was best for this particular problem. Other problems to test the effects of non-squareness of logical mesh (the test problem was 5×50) and thinness were run. It was found that both factors contribute to slow convergence. In February 1966, considerable effort was expended on a different test problem, a thin hot sphere radiating into a thinner, cold medium. The following initial conditions were used:

$$\theta = 5.081 \times 10^{-1} \text{ ev}$$

$$\rho_o = 5.29 \times 10^{-2} \text{ g with ambient density } \rho_A = 1.89 \times 10^{-4}$$

$$\text{HVB} = 4.2 \times 10^{16} \text{ erg}$$

$$\text{HCB} = 1.3 \times 10^{10} \text{ erg}$$

$$\text{CV} = 2.6 \times 10^{10} \text{ erg}$$

$$\text{HCP} = 4. \times 10^9 \text{ erg}$$

$$I = 5.5 \times 10^{10} \text{ erg, of which only } 4.0 \times 10^9 \text{ erg is allowed to go into vapor}$$

$$\gamma = 1.5$$

A perfect gas equation of state was used to describe the vapor expansion. The radiation boundary conditions used are shown in Fig. 11.

A study was made of the convergence of the radiation equation. Various values of K and ω which are used to adjust the iterative matrix inversion were tried. As a result of these tests, the following observations were made:

1. If $E_{i+1/2, j+1/2}$ goes negative for any reason, even if it is subsequently set to zero, the convergence criterion is very hard to meet.

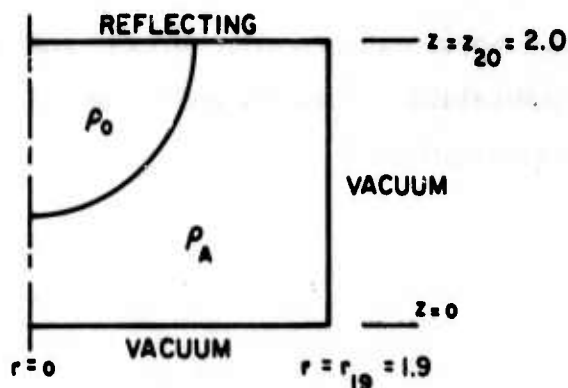


Figure 11. Configuration of Test Problem

2. For $E_{i+1/2, j+1/2}$ always greater than zero, the following seems to be true:
 - a. Initial $E = 137 \theta^4$ seems to converge over the entire mesh faster than $E = 0$.
 - b. $|\Delta E|_i$ for cells with max E is generally only slightly larger than $|\Delta E|_i$ for cell with min E .

In April, a subroutine for completely factoring b was written. Thus,

$$b = vw$$

where $v_{ij} = 0$ unless $j \leq i \leq j+1$ and $w_{ij} = 0$ unless $j-1 \leq i \leq j$. Although this closed method is inferior to the iterative method in all respects — space and time consumed and accuracy — it is a useful diagnostic tool for small test problems because it eliminates the question of convergence. The technique was accommodated by writing all 22 cell arrays on a tape and using the corresponding storage to invert the matrix, limiting l (say, the number of radial columns of cells in a HECTIC mesh) to 22. This version was written and executed, with reasonably satisfactory results. The thin sphere, described above, was tried, and the resulting radiation energy distribution looked about right. However, the radiant flux gradient, which determines actual energy transfer, was quite small and noisy. The

question of limitations on numerical accuracy, and the related question of the range of applicability of the diffusion method to optically thin media, are both under investigation.

4.9. APPENDIX: LISTING OF TDRAD

\$IBFTC TDRAD LIST,DECK,REF

SUBROUTINE TDRAD

COMPILED JANUARY 27, 1966 WBL

C

D I M E N S I O N

C

DIMENSION

1U(400), V(400), AMX(400), AIX(400), P(400),
 2THETA(400), RHO(400), FIOUT(400), CAP(400), KFIT(400),
 3 IW1(50),W2(50),W3(50),TABLM(50),
 4DX(52), X(53), XX(54), DY(100), Y(100), YY(101),
 5TAB(15), AMK(15), PK(15), QK(15), Z(150), IZ(150),
 6TAU(52), PL(200), PR(200), UL(200), UR(200),
 7FLEFT(100),YAMC(100),SIGC(100),GAMC(100),
 8G(50),SOLID(400),TEMP(12)

COMMON Z ,XX ,UR ,PR ,THETA ,YY
 COMMON AID ,AIX ,AM ,AMD ,AMX ,AREA
 COMMON BIG ,BOUNCE ,DDXN ,DDVK ,DVK ,DX
 COMMON UY ,E ,FD ,FS ,FX ,OUT
 COMMON P ,PABOVE ,PBLO ,PIOTS ,PPABOV ,PRR
 COMMON PUL ,QDT ,RC ,REZ ,RHO ,RL
 COMMON RR,SIG,Q000FL,SWITCH ,TABLM,TAU
 COMMON TAUOTS ,TAUDTX ,U ,UK ,URR ,UT
 COMMON UU ,UUU ,UTEF ,UVMAX ,V ,VABOVE
 COMMON VBLO ,VEL ,VK ,VT ,VTEF ,VV
 COMMON VVABOV ,VVBLO ,W2 ,W3 ,WPS ,WS
 COMMON WSA ,WSB ,WSC ,XL ,XLF ,XN
 COMMON XR ,YL ,YLW ,YN ,YU ,ZMAX
 COMMON I ,II ,IN ,IR ,IWS ,IWSA
 COMMON IWSU ,IWSC ,IW1 ,J ,JN ,JP
 COMMON JR ,K ,KN ,KP ,KR ,KRM
 COMMON L ,M ,MA ,MB ,MC ,MD
 COMMON ME ,MZ ,N ,NK ,NKMAX ,NK1
 COMMON NO ,NR ,G ,SOLID ,TEMP
 COMMON FIOUT ,CAP ,KFIT

C

C

C

E Q U I V A L E N C E

0EQUIVALENCE (Z(12),PROB), (Z(2),CYCLE), (Z(3),DT),
 1(Z(4),PRINTS), (Z(5),PRINTL), (Z(6),DUMPT7), (Z(7),CSTOP),
 2(Z(8),PIDY), (Z(9),TMZ), (Z(10),GAM), (Z(11),GAMD),
 3(Z(12),GAMX), (Z(13),ETH), (Z(14),FFA), (Z(15),FFB),
 4(Z(16),TMDZ), (Z(17),TMXZ), (Z(18),XMAX), (Z(19),TXMAX),
 5(Z(20),TYMAX), (Z(21),AMDM), (Z(22),AMXM), (Z(23),DNN),
 6(Z(24),DMIN), (Z(25),FEF), (Z(26),DTNA), (Z(27),CVIS),
 7(Z(28),NPR), (Z(29),NPRI), (Z(30),NC), (Z(31),NPC),
 8(Z(32),NRC), (Z(33),IMAX), (Z(34),IMAXA), (Z(35),JMAX),
 9(Z(36),JMAXA), (Z(37),KMAX), (Z(38),KMAXA), (Z(39),NMAX),
 0EQUIVALENCE (Z(40),ND), (Z(41),KDT), (Z(42),IXMAX),
 1(Z(43),NOD), (Z(44),NOPR), (Z(45),NIMAX), (Z(46),NJMAX),
 2(Z(47),I1), (Z(48),I2), (Z(49),I3), (Z(50),I4),
 3(Z(51),N1), (Z(52),N2), (Z(53),N3), (Z(54),N4),
 4(Z(55),N5), (Z(56),N6), (Z(57),N7), (Z(58),N8),
 5(Z(59),N9), (Z(60),N10), (Z(61),N11), (Z(62),NRM),
 6(Z(63),TRAD), (Z(64),XNRG), (Z(65),SN), (Z(66),DXN),
 7(Z(67),RADER), (Z(68),RADET), (Z(69),RADEB), (Z(70),DTRAD),
 8(Z(71),REZFCT), (Z(72),RSTOP), (Z(73),SHELL), (Z(74),RBOUND),
 9(Z(75),TOZONE), (Z(76),ECK), (Z(77),SBOUND), (Z(78),X1),
 0EQUIVALENCE (Z(79),X2), (Z(80),Y1), (Z(81),Y2),
 1(Z(82),CAULN), (Z(83),VISC), (Z(84),T), (Z(85),GMAX),
 2(Z(86),WSGD), (Z(87),WSGX), (Z(88),GMADR), (Z(89),GMAXR),
 3(Z(90),S1), (Z(91),S2), (Z(92),S3), (Z(93),S4),
 4(Z(94),S5), (Z(95),S6), (Z(96),S7), (Z(97),S8),
 5(Z(98),S9), (Z(99),S10)

C

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0EQUIVALENCE      (Z(100),HVB),      (Z(101),HCB),      (Z(102),CB),
1(Z(103),SV5),    (Z(104),ATOM),    (Z(105),CV),      (Z(106),GV),
2(Z(107),SUMFE),  (Z(108),BETA),    (Z(109),ALCO),    (Z(110),ANN),
3(Z(111),EZERO),  (Z(112),PW),      (Z(113),CAPS),    (Z(114),HNU),
3(Z(115),COE),    (Z(116),SCR),      (Z(117),ISR),      (Z(118),SCDR),
4(Z(119),AHN),    (Z(120),DTH),      (Z(121),IH),      (Z(122),JH),
5(Z(123),UTC),    (Z(124),IC),      (Z(125),JC),      (Z(126),RFT),
X(Z(127),CDUT),   (Z(128),HCP),      (Z(129),HH),      (Z(130),CO),
6(Z(131),J1),     (Z(132),J2),      (Z(133),J3),      (Z(134),J4),
7(Z(135),J5),     (Z(136),J6),
0EQUIVALENCE      (Z(140),VAPE),    (Z(141),RADE),    (Z(142),CNDE),
1(Z(143),SCRE)

```

```

C
0EQUIVALENCE      (XX(2),X(1)),      (UR,UL,FLEFT),    (UR(100),YAMC),
1(PR(100),SIGC),  (PK,PL,GAMC),      (DKE,THETA),      (UR,TAB),
2(UR(16),AMK),    (UR(31),PK),      (UR(46),GK),      (YY(2),Y(1))

```

```

C
COMMON /LINDLY/   SGNL: IHNU, NHNU, HNUP, N., DHNU, THICK, NY,
2 MFTAG, SLUG, RPTAG, EFRAC, IMPTAG, DTBUGR, BCLTAG, BCRTAG, ITAG,
3 BCUTAG, BCATAG, MERGE, CMXK, CMXOM, ERRCRT, ITRMAX, DRGPRT,
4 DIANTP, DGREY, CAPIN, ODDC
COMMON /ARRAY/   ROSS( 400), PLANCK( 400), ER( 400), XCV( 400),
2 XA( 400), XB( 400), XC( 400), XALP( 400), XGAM( 400), B( 400),
3 XD( 400), ALAMH( 400), ALAMV( 400), XG( 400), ERAD( 400),
4 OLDTH( 400)

```

```

C
      C      O      M      M      O      N
DIMENSION PUR(50), PUZ(100), RUR(50), RUZ(100), BETAB(50),
2 BETAA(50), BETAR(100)
REAL MERGE
4 FORMAT (7H1CYCLE F6.0, 7H TIME 1PE13.6, 5H DT 1PE13.6/)
5 FORMAT (      4X1HK, 11X2HXA, 11X2HXB, 11X2HXC, 11X2HXD
2, 9X4HXALP, 9X4HXGAM, 12X1HB, 9X4HROSS, 7X6HPLANCK/)
6 FORMAT (15, 1P9E13.6)
7 FORMAT (1H13X1HK, 7X6HV FLUX, 7X6HH FLUX, 6X7HDELTA E)
8 FORMAT (/10H ITERATION14, 22H MAX. RELATIVE ERROR 1PE9.3,
2 7H ZONE 14, 14H ZONE ENERGY 1PE9.3)
9 FORMAT (3H XG)
10 FORMAT (5H ERAD)
11 FORMAT (1P10E12.5)

```

```

C
NY(IN LINDLEY COMMON) IS TEMPERATURE ITERATION INDEX USED IN KAPPA.
IF (MFTAG.EQ. 0) DHNU = 1.
NVEZ = 1
NY = NVEZ
IF (ITAG.EQ. 0) NVEZ = 2
VEZ = NVEZ
CALL DVCHK (KDMY)

```

DRAD 101
DRAD 104
DRAD 103

```

C
FORM MONOFREQUENCY QUANTITIES AND FIND MIN TIME STEP

```

DRAD 106
DRAD 107
DRAD 108
DRAD 109

```

WSB = 0.0
DO 1076 K = 2, KMAX
1076 WSB = WSB + AIX(K) * AMX(K)
DTR1=1.E10
DTR2=1.E10
IHNU = 0
CALL KAPPA

```

DRAD 112
DRAD 113
DRAD 119

```

C
MUST FORM LOG OF TEMPERATURE AND DENSITY IN KAPPA
1080 DO 1230 I = 1, IMAX
K = I + 1
DO 1229 J = 1, JMAX

```

```

CALL UNCLE IF EITHER KAPPA IS ZERO OR NEGATIVE
IF (AMINI(PLANCK(K), ROSS(K)) .GT. 0.0) GO TO 1120
S1=13.1090
CALL UNCLE

```

DRAD 122
DRAD 124
DRAD 125

```

1120 TEMP(1)=SQRT(PLANCK(K) * ROSS(K))
      TEMP(3) = PLANCK(K)
      IF (HPTAG .EQ. 0.0) GO TO 1125
      TEMP(1) = ROSS(K)
      TEMP(3) = ROSS(K)
1125 IF(0.001 - THETA(K)) 1160,1230,1230
1160 DELTAU = 0.5 * TEMP(1) * RHO(K)
      TEMP(1) = 1.E10
      TEMP(2) = 1.E10
      IF (ER(K).EQ.0.) GO TO 1170
      WSBH = AIX(K) * AMX(K)
      IF (EFRAC .EQ. 0.0) GO TO 1170
      IF (WSBH - EFRAC * WSB) 1170, 1165, 1165
C     ACCURACY CRITERION -- DONE UNCONDITIONALLY
1165 TEMP(1) = SLUG * AMX(K) / ABS(ER(K)) * AIX(K)
1170 IF (MFTAG .EQ. 0 .AND. IMPTAG .NE. 0 ) CONTINUE
C     GO TO 1172 REPLACED BY CONTINUE UNTIL FULLY IMPLICIT CODING IS PUT IN
C     STABILITY CRITERION -- BYPASSED IN FULLY IMPLICIT CASE
      DENOM = 4.1132E12 * TEMP(3) * THETA(K)**4 / AIX(K)
      TEMP(2) = (0.5 + 1.5 * (DELTAU * AMIN1(DX(I), DY(J)))**2) / DENOM
1172 TEMP(2) = AMIN1(TEMP(1), TEMP(2))
      TEMP(2)=TEMP(2)*DTBUGR
C*****
C     FIND MINIMUM TIME STEP
C
C     IF (TEMP(2)) 1230,1230,1190
1190 IF (TEMP(2)-DTR1) 1200,1210,1210
1200 DTR2=DTR1
      KMN2=KMN1
      DTR1=TEMP(2)
      KMN1=K
      GO TO 1230
1210 IF (TEMP(2)-DTR2) 1220,1230,1230
1220 DTR2=TEMP(2)
      KMN2=K
1229 K = K + IMAX
1230 CONTINUE
      DTRMIN=DTR1
C
C     PRINT MINIMUM TIME STEPS BETWEEN EDITS
C     DELETED UNTIL WE KNOW THE OIL PRINT ROUTINE
C
C     DETERMINE IF RADIATION OR HYDRO WILL SUBCYCLE
C     NO HYDRO SUBCYCLE IN THIS VERSION
C     FOR INITIAL START, DT AND TRAD NEED TO BE PROVIDED AS INPUT.
CAVEAT. OIL PROBABLY DOES THINGS DIFFERENTLY.
      IF (DTRMIN - TRAD) 1280, 125, 125
C*****
C     REDUCE TIME STEP
C
1280 NR = DT / DTRMIN + 1.0
      TRAD = DT / FLOAT(NR)
      IF (NR .LE. NRM ) GO TO 125
1290 S1=13.1290
      CALL UNCLE
125 THTAMX=.025
      CALL DVCHK(KDMY)
      GO TO (127, 130), KDMY
127 S1 = 13.0127
      CALL UNCLE
C     CALCULATE GEOMETRY FACTORS AND FIND HIGHEST TEMPERATURE

```

AFWL-TR-66-108, Vol I

```

130 DO 150 I = 1, IMAX  

    PUR(I) = PIDY / TAU(I)  

150 RUR(I+1) = 4.0E10 * X(I) / (X(I+1) - X(I-1))  

    DO 160 J = 1, JMAX  

    PUZ(J) = 1. / DY(J)  

160 RUZ(J+1) = 2.0E10 / (Y(J+1) - Y(J-1))  

    DO 180 K = 2, KMAX  

    IF (THETA(K) .LE. THTAMX) GO TO 180  

    THTAMX=THETA(K)  

180 CONTINUE  

    THTAMX = AMAX1(THTAMX, BCLTAG, BCRTAG, BCBTAG, UCATAG)  

    REENTRY POINT FOR SECOND TEMPERATURE ITERATION  

200 DO 210 K = 2, KMAX  

    XA(K) = 0.  

    XB(K) = 0.  

    XC(K) = 0.  

    XALP(K) = 0.  

    ER(K) = 0.0  

210 XGAM(K) = 0.  

C  

C *****  

C  

C BEGIN FREQUENCY LOOP  

C *****  

C  

C SET UP MAX FREQ BOUNDARY  

C  

    HNUP=1.0E6  

    HNUP4=1.0E24  

    IF (MFTAG .EQ. 0) GO TO 280  

220 IHNU = IHNU + 1  

    CALL KAPPA  

    HNUP4=HNUP**4  

    DHNU = HNUP - HNU  

C  

C MERGE GROUPS WITH HNU MORE THAN (MERGE) TIMES LARGEST THETA  

C  

    IF (MERGE .GT. 0.0) GO TO 225  

    SI = 13.0225  

    CALL UNCLE  

225 IF (THTAMX - HNU / MERGE) 240, 230, 230  

230 IF (IHNU - 1) 235, 370, 260  

235 SI = 13.0235  

    CALL UNCLE  

C  

C REJECT TAPE IF MORE THAN HALF OF GROUPS MERGE  

C  

240 IF (IHNU+IHNU-DHNU) 260,250,250  

250 IF (AMOD(MERGE,1.) .EQ. 0.5) GO TO 260  

    S1=13.0250  

    CALL UNCLE  

260 DO 270 K = 2, KMAX  

    T4 = THETA(K)**4  

    UETA=HNU/THETA(K)  

    BETAP=HNUP/THETA(K)  

    DFB=PLNKUT(BETA,UETAP)  

    IF (DFB.EQ.0.) GO TO 270  

    TEMP(1) = DFB * T4  

    EMB1=EXP(-BETA)  

    EMB2=EXP(-BETAP)  

    TEMP(2)=DFB*0.0384974 / T4 *(IHNU4/(1.0-EMB1)  

    1*EMB1-HNUP4/(1.0-EMB2)*EMB2)  


```

C	FORM NUMERATORS AND DENOMINATORS OF MERGED KAPPAS	DRAD 289
C		DRAD 290
	XA(K)=XA(K)+TEMP(1)	
	XB(K)=XB(K)+TEMP(2)	
	XC(K) = XC(K) + PLANCK(K) * TEMP(1)	
	XALP(K) = XALP(K) + TEMP(2) / ROSS(K)	
270	CONTINUE	DRAD 295
	HNUP=HNU	DRAD 296
	HNUP4=HNUP	DRAD 298
	IF (THITAMX- HNU/ MERGE) 220,310,310	
C		DRAD 300
C	FORM MERGED KAPPAS	DRAD 301
C		DRAD 302
310	DO 350 K = 2, KMAX	
	IF (XA(K)) 320,350,330	
320	S1=13.0320	DRAD 305
	CALL UNCLE	DRAD 306
330	ROSS(K) = XB(K) / XALP(K)	
	PLANCK(K) = XC(K) / XA(K)	
350	CONTINUE	DRAD 309
	HNUP=1.0E6	
	HNUP4=1.0E24	
	CHNU = HNUP - HNU	DRAD 312
	GO TO 480	
C		DRAD 315
C	MONOFREQUENCY CALCULATION	DRAD 316
C		DRAD 317
280	HNNU=1	DRAD 318
	IHNU = 1	
	DO 290 K = 2, KMAX	
290	B(K) = THETA(K)**4	
	HNU = .001	DRAD 326
	GO TO 480	DRAD 327
C		DRAD 328
C	TYPICAL GROUP CALCULATION OF SOURCES	DRAD 329
C		DRAD 330
360	IHNU = IHNU +1	
	CALL KAPPA	DRAD 332
	HNNU=HNUP-HNU	DRAD 333
	HNUP4=HNUP**4	
370	DO 392 K = 2, KMAX	
	DFB = PLNKUT(HNU / THETA(K), HNUP / THETA(K))	
392	B(K) = DFB * THETA(K)**4	DRAD 363
C		
C	SET BLACKBODY CONDITIONS	DRAD 365
C		
C	INNER CYLINDRICAL RADIUS NOT ASSUMED ZERO	
480	BBL = 0.	
	IF (BCLTAG .LE. 0.0) GO TO 490	
	DFB = PLNKUT(HNU / BCLTAG, HNUP / BCLTAG)	
	BBL = BCLTAG**4 * DFB	
490	BBR = 0.	
	IF (BCRTAG .LE. 0.0) GO TO 500	
	DFB = PLNKUT(HNU / BCRTAG, HNUP / BCRTAG)	
	BBR = BCRTAG**4 * DFB	
500	BBB = 0.0	
	IF (BCBTAG .LE. 0.0) GO TO 510	
	DFB = PLNKUT(HNU / BCBTAG, HNUP / BCBTAG)	
	BBB = BCBTAG**4 * DFB	
510	BBA = 0.0	
	IF (BCATAG .LE. 0.0) GO TO 520	
	DFB = PLNKUT(HNU / BCATAG, HNUP / BCATAG)	
	BBA = BCATAG**4 * DFB	
520	CALL DVCHK(KDMY)	
	GO TO (522, 521), KUMY	

```

522 S1 = 13.0522
    CALL UNCLE
C
C          FORM RUSSELAND AND PLANCK OPTICAL DEPTHS
C
C          DOUBLE ON STORAGE FOR ABSORPTION COEFFICIENTS, MU, AND LAMBDA
521 DO 530 I = 1, IMAX
    K = I + 1
    M = K - IMAX
    DO 530 J = 1, JMAX
        FACTOR = 1.
        IF (RPTAG .NE. 0.0) FACTOR = ROSS(K) / PLANCK(K)
        ROSS(K) = AMAX1(ROSS(K) * RHO(K), 1.E-20)
        PLANCK(K) = AMAX1(PLANCK(K) * RHO(K) * FACTOR, 1.E-20)
C          FORM LAMBDA, MEAN FREE PATH AT CELL EDGES
        IF (I .EQ. 1) GO TO 525
C          MAY BE ABLE TO SAVE STORAGE BY EQUIVALENCING ALAMH WITH ROSS.
CAVEAT. LOGIC WOULD BE MORE COMPLEX AND ONE 1-D ARRAY WOULD BE NEEDED.
        DTAUR = ROSS(K) * DX(I)
        DTAUL = ROSS(K-1) * DX(I-1)
        IF (ABS(DTAUR - DTAUL) / (DTAUR + DTAUL) .LE. 0.0001) GO TO 523
        ALAMV(K) = AMAX1(1. / ROSS(K), 1. / ROSS(K-1))
        GO TO 525
523 ALAMV(K) = (DX(I) + DX(I-1)) / (DTAUR + DTAUL)
525 IF (J .EQ. 1) GO TO 529
        DTAUA = ROSS(K) * DY(J)
        DTAUB = ROSS(M) * DY(J-1)
        IF (ABS(DTAUA - DTAUB) / (DTAUA + DTAUB) .LE. 0.0001) GO TO 527
        ALAMH(K) = AMAX1(1. / ROSS(K), 1. / ROSS(M))
        GO TO 529
527 ALAMH(K) = (DY(J) + DY(J-1)) / (DTAUA + DTAUB)
529 M = M + IMAX
    K = K + IMAX
530 CONTINUE
C*****DRAD 412
C          BEGIN NONEQUILIBRIUM DIFFUSION TREATMENT
C          DRAD 413
C          FORM MATRIX ELEMENTS XA, XB, XC, XD, XALP, XGAM
C          THIS SECTION ALSO EXECUTES EQS. 45 AND 46 OF OLIPHANT
C          BOUNDARY CONDITION MODIFIES XB AND XD.
C          THIS CODING ASSUMES DX(I) = X(I+1) - X(I), SAME FOR Y.
    DO 560 I = 1, IMAX
        K = I + 1
        N = K + IMAX
        DO 560 J = 1, JMAX
            XB(K) = 0.
            XD(K) = 0.
            IF (I .EQ. 1) GO TO 531
            XA(K) = -PUR(I) * RUR(I) * ALAMV(K)
            GO TO 535
531 XA(K) = 0.0
C          INNER CYLINDRICAL RADIUS ASSUMED ZERO
535 IF (I .EQ. IMAX) GO TO 538
536 XC(K) = -PUR(I) * RUR(I+1) * ALAMV(K+1)
            GO TO 540
538 XC(K) = 0.0
            IF (BCRTAG .LT. 0.0) GO TO 540
            BETAR(J) = 1.0 / (2. - EXP(-DX(I)) * SQRT(0.75 * ROSS(K)
            2 * PLANCK(K)))
            XB(K) = XB(K) + PUR(I) * 3.E10 * X(I) * BETAR(J)
            XD(K) = XD(K) - 4.104E12 * PUR(I) * X(I+1) * RBR
540 IF (J .EQ. 1) GO TO 543
            XALP(K) = -PUZ(J) * RUZ(J) * ALAMH(K)
            GO TO 545
543 XALP(K) = 0.0

```

```

      IF (BCBTAG .LT. 0.0) GO TO 545
      BETAB(I) = 1.0 / (2. - EXP(-DY(I) * SQRT(0.75 * ROSS(K)
2 * PLANCK(K))))
      XB(K) = XB(K) + PUZ(I) * 1.5E10 * BETAB(I)
      XD(K) = XD(K) - PUZ(I) * 2.052E12 * BHA
545 IF (J .EQ. JMAX) GO TO 548
546 XGAM(K) = -PUZ(J) * RUZ(J+1) * ALAMH(N)
      GO TO 549
548 XGAM(K) = 0.0
      IF (BCATAG .LT. 0.0) GO TO 549
      BETAA(I) = 1.0 / (2. - EXP(-DY(J) * SQRT(0.75 * ROSS(K)
2 * PLANCK(K))))
      XB(K) = XB(K) + PUZ(J) * 1.5E10 * BETAA(I)
      XD(K) = XD(K) - PUZ(J) * 2.052E12 * BHA
549 XB(K) = XB(K) + 3.E10*PLANCK(K) - XA(K) - XC(K) - XALP(K) -XGAM(K)
      XD(K) = XD(K) - 4.104E12 * PLANCK(K) * B(K)
C * * * * *
C INITIAL ERAD(K)=0. FOR LOW FLUX AND B(K)*137. FOR HIGH FLUX
      ERAD(K) = B(K) * 137.
C * * * * *
      IF (IMPTAG .EQ. 0 .OR. MFTAG .NE. 0) GO TO 559
C FULLY IMPLICIT ADJUSTMENT OF XB AND XD
C VDOT, DE(M)/DT, G, PHIN, AND SO FORTH NOT YET AVAILABLE.
      S1 = 13.0559
      CALL UNCLE
      XB(K) = XB(K)
      XD(K) = XD(K)
559 K = K + IMAX
      N = N + IMAX
560 CONTINUE
C FIRST PASS -- P. 16, EQS. 47-49 OF OLIPHANT
      DO 570 K = 2, KMAX
      M = K - IMAX
      XB(K) = XB(K) - XALP(K) * XGAM(M) - XA(K) * XC(K-1)
      XGAM(K) = XGAM(K) * CMXK / XB(K)
      XC(K) = XC(K) * CMXK / XB(K)
570 CONTINUE
      CALL DVCHK(KDMY)
      GO TO (572, 573), KDMY
572 S1 = 13.0572
      CALL UNCLE
573 IF (AMOD(CYCLE,PRINTL). NE. 0.) GO TO 580
      WRITE(6,4) CYCLE, T, DT
      WRITE (6,5)
      DO 575 K = 2, KMAX
575 WRITE (6,6) K, XA(K), XB(K), XC(K), XD(K), XALP(K), XGAM(K), R(K),
2 ROSS(K), PLANCK(K)
580 ITER = 1
C SECOND PASS -- EQS. 50, 51 OF OLIPHANT
590 DO 600 K = 2, KMAX
      M = K - IMAX
      N = K + IMAX
      XH = -XD(K) + XALP(K) * XC(M) * ERAD(M+1) + XA(K) * XGAM(K-1) *
2 ERAD(N-1) + (CMXK - 1.) * XD(K) / CMXK * (XGAM(K) * ERAD(N) +
3 XC(K) * ERAD(K+1))
      XG(K) = (XH - XALP(K) * XG(M) - XA(K) * XG(K-1)) / XB(K)
600 CONTINUE
C BACKWARD PASS -- EQ. 52 OF OLIPHANT
      ERROR = 0.
      EMIN = 1.E20
      DO 620 L = 2, KMAX
      K = KMAX + 1 - L
      N = K + IMAX
      ENEW = CMXOM * (XG(K) - XGAM(K) * ERAD(N) - XC(K) * ERAD(K+1)) +
2 (1. - CMXOM) * ERAD(K)

```

```

C   MAY BE TOO SEVERE FOR CELLS WITH VERY LITTLE OF THE TOTAL ENERGY
    EMIN = AMIN1(EMIN, ENEW)
    ERRT = ABS((ENEW - ERAD(K)) / ENEW)
    IF (ERRT .LE. ERROR) GO TO 619
    ERROR = ERRT
    KME = K
    EME = ENEW
619 ERAD(K) = ENEW
620 CONTINUE
    IF (AMOD(CYCLE, PRINTS).EQ.0.)
1WRITE (6,8) ITER, EKHOR, KME, EME
    IF (AMOD(CYCLE, PRINTL).NE.0.) GO TO 635
    IF (DBGPRT .EQ. 0.0) GO TO 635
    WRITE (6,9)
    WRITE (6,11) (XG(K), K=2,KMAX)
    WRITE (6,10)
    WRITE (6,11) (ERAD(K), K=2,KMAX)
635 GO TO 640
    S1 = 13.0635
    CALL UNCLE
640 CALL DVCHK(KDMY)
    GO TO (641, 645), KDMY
641 S1 = 13.0641
    CALL UNCLE
645 ITER = ITER + 1
    IF (ITER .LE. ITHMAX) GO TO 648
    S1 = 13.0648
    CALL UNCLE
648 IF (ERROR .GT. EKHCHT) GO TO 590
CALCULATE FLUXES, USING XA AND XB FOR STORAGE
DO 680 I = 1, IMAX
    K = I + 1
    M = K - IMAX
    DO 680 J = 1, JMAX
    IF (J .EQ. 1) GO TO 650
    XA(K) = RUZ(J) * ALAMH(K) * (ERAD(M) - ERAD(K))
    GO TO 655
650 IF (BCBTAG) 651, 652, 652
651 XA(K) = 0.0
    GO TO 655
652 XA(K) = 2.052E12 * BBD - 1.5E10 * ERAD(K) * BETAB(I)
655 IF (I .EQ. 1) GO TO 660
    XB(K) = HUR(I) * ALAMV(K) * (ERAD(K-1) - ERAD(K))
    GO TO 665
660 XB(K) = 0.0
665 K = K + IMAX
    M = M + IMAX
680 CONTINUE
    DO 690 I = 1, IMAX
    K = I + 1
    N = K + IMAX
    DO 690 J = 1, JMAX
    FABV = XA(N)
    IF (J .NE. JMAX) GO TO 683
    IF (BCATAG) 681, 682, 682
681 FABV = 0.0
    GO TO 683
682 FABV = -2.052E12 * BBA + 1.5E10 * ERAD(K) * BETAA(I)
683 FRT = XB(K+1)
    IF (I .NE. IMAX) GO TO 686
    IF (BCRTAG) 684, 685, 685
684 FRT = 0.0
    GO TO 686
685 FRT = -2.052E12 * BBL + 3.0E10 * ERAD(K) * X(IMAX) * BETAR(J)
686 ER(K) = ER(K) + (XA(K)-FABV) * TAU(I) + (XB(K)-FRT) * PIDY * DY(J)

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AFWL-TR-66-108, Vol I

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      K = K + IMAK
      N = N + IMAK
690 CONTINUE
C
C      OPTIONAL EDIT OF FLUX AND ENERGY CHANGE
C
      IF (AMOD(CYCLE,PRINTL).NE.0.) GO TO 1020
      IF (DBGPRT.EQ. 0.0) GO TO 1020
      WRITE (6,7)
      DO 1010 K = 2, KMAX
1010 WRITE (6,6) K, XA(K), XB(K), ER(K)
C
C      ADVANCE FREQ, STORE EMERGENT FLUX, TEST FOR COMPLETION OF GROUPS
C
1020 CALL DVCHK (KMY)
      GO TO (1050,1040), KMY
1040 HNUP=HNUP+1
      HNUP4=HNUP/4
      IF (IHNU-NHNU)360,1060,1050
C*****
C      END FREQUENCY LOOP
C*****
1050 S1 = 13.1050
      CALL UNCLE
C      ITERATE ON TEMPERATURE
1060 GO TO (1061, 1065), NVEZ
1061 NVEZ = 2
      VEZ = NVEZ
      NY = NVEZ
      IHNU = 0
      DO 1062 K = 2, KMAX
C      WORK, SOURCE TERMS OMITTED
      BNTH = THETA(K) + ER(K) * TRAD / (AMX(K) * XCV(K))
      OLDTH(K) = THETA(K)
      THETA(K) = 0.5 * (OLDTH(K) + BNTH)
1062 CONTINUE
      IF (MFTAG.EQ. 0) CALL KAPPA
      GO TO 200
1065 IF (ITAG.EQ. 0) GO TO 1067
      DO 1066 K = 2, KMAX
1066 THETA(K) = OLDTH(K)
1067 RETURN
      END

```

DRAD 555

DRAD 557

DRAD 576

DRAD 577

DRAD 578

DRAD 583

DRAD 586

*DRAD 587

*DRAD 588

*DRAD 589

*DRAD 590

DRAD 591

DRAD 592

DRAD 593

DRAD 594

DRAD 595

DRAD 596

DRAD 597

DRAD 605

SECTION V

THE METHOD OF CHARACTERISTICS IN CYLINDRICAL GEOMETRY

5.1. INTRODUCTION

As a first step in the development of a true two-dimensional transport code, a subprogram called TRAN2 has been written to treat the case in which retardation and scattering can be ignored. TRAN2 is designed to operate in HECTIC, which is a code that calculates hydrodynamical problems having axial symmetry, and which normally uses the diffusion approximation for computing the rate of flow of radiation.

Consider a cylindrical region of outer radius R and altitude Z . Assume that the axis of the cylinder is an axis of symmetry for all the properties of the material contained in the cylinder so that all quantities of interest can be expressed as functions of two cylindrical coordinates, the distance r from the axis and the altitude z above the bottom.

In TRAN2, the transport equation is integrated along a system of characteristic lines, called rays, which are distributed throughout the system in a more or less uniform manner.

5.2. THE LOCAL COORDINATE SYSTEM

Given any point P in the system, let there be three associated unit vectors: $\vec{k}$, a vector which is parallel to the axis of the system and which points in the same direction, called "upward," for all points P ; $\vec{j}$, a unit vector parallel to the radial direction at P ; and $\vec{i} = \vec{j} \times \vec{k}$.

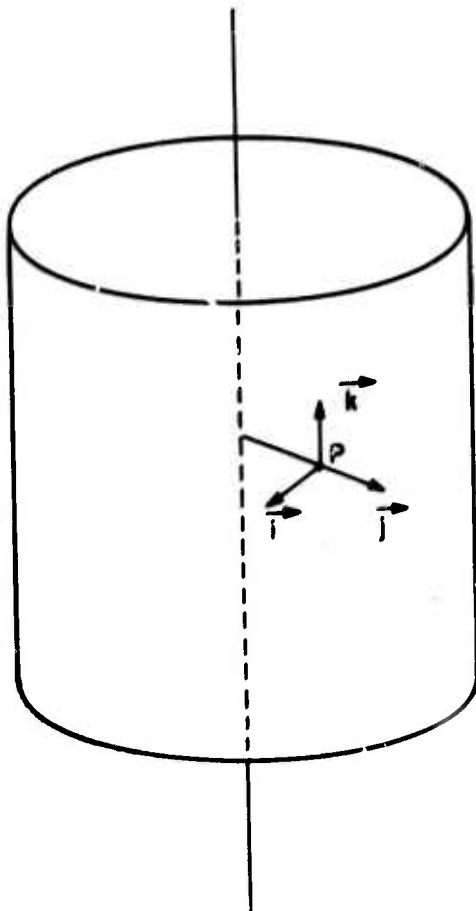


Figure 12. Coordinate Vectors

5.3. DISTRIBUTION OF RAYS

A ray is a directed line segment

$$L: \vec{r}(s) = s\vec{\Omega} + \vec{p} \quad \text{for} \quad -S \leq s \leq S$$

where $\vec{\Omega}$ is a unit vector called the direction of L and $\vec{p}$ is the midpoint of L . There are groups, called combs, of rays lying in the same vertical plane and having the same length $2S$ and direction $\vec{\Omega}$. The midpoints of the rays of a comb lie in a vertical line at altitudes $z = 0, \Delta z, 2\Delta z, \dots$, where $\Delta z = Z/m$, m being an integer, is the same for all combs. If a comb is thought of as going to infinity in both directions, then the reflection of a comb is the same in both ends of the system and is another comb

with the same midpoints and the same $\vec{\Omega} \times \vec{k}$. Thus, if a ray strikes the end of the system, its reflection is a ray in the reflected comb.

It will be convenient to consider groups of rays of another type, called grids (see Section 3.3). A different definition is given there but they turn out to be equivalent. A grid consists of all rays for which $\vec{\Omega} \cdot \vec{k}$ has a given value μ . In view of the symmetry of the system, it can be assumed that the midpoints of all rays of a grid lie in the same vertical half-plane and that their directions all have positive projections on the same normal of the half-plane, in which case they will be parallel to each other. The rays of a comb, being parallel, all lie in the same grid and are separated by a distance of $\Delta z(1 - \mu^2)^{1/2}$, where $\mu = \vec{\Omega} \cdot \vec{k}$. The combs that make up the grid are to have a constant separation $d(\Omega)$ which will generally differ from $\Delta z(1 - \mu^2)^{1/2}$, so that the lattice of points in which the rays of a grid intersect a mutually perpendicular plane will be rectangular.

By considering all rays together, it ought to be possible to infer the essential features of the distribution of the directions they assume at some particular radial distance r from the axis of the system, when the angles at which rays penetrate a cylindrical strip of radius r and altitude $\Delta z = Z/m$ are given. The reasons are clear. First, this set of angles is the same for all such strips because the distribution of rays is periodic with period $\Delta z \vec{k}$. Consequently, it suffices to specify them for one arbitrarily chosen strip. Second, because of the axial symmetry of the system, rotation of the ray about the axis leaves the ray in essentially the same position. Third, it is assumed that Δz is so small that moving a ray up or down through such a distance will not have a significant effect on the accuracy of the results.

In terms of the local coordinate vectors $\vec{i}$, $\vec{j}$, $\vec{k}$ associated with some particular point on a ray, the direction $\vec{\Omega}$ of the ray can be expressed as $\vec{\Omega} = \mu \vec{k} + (1 - \mu^2)^{1/2}(\vec{i} \sin \phi + \vec{j} \cos \phi) = \mu \vec{k} + \lambda \vec{i} + \eta \vec{j}$, where $\mu^2 + \lambda^2 + \eta^2 = 1$, and, because of symmetry, $0 \leq \phi \leq \pi$ and $0 \leq \lambda \leq 1$.

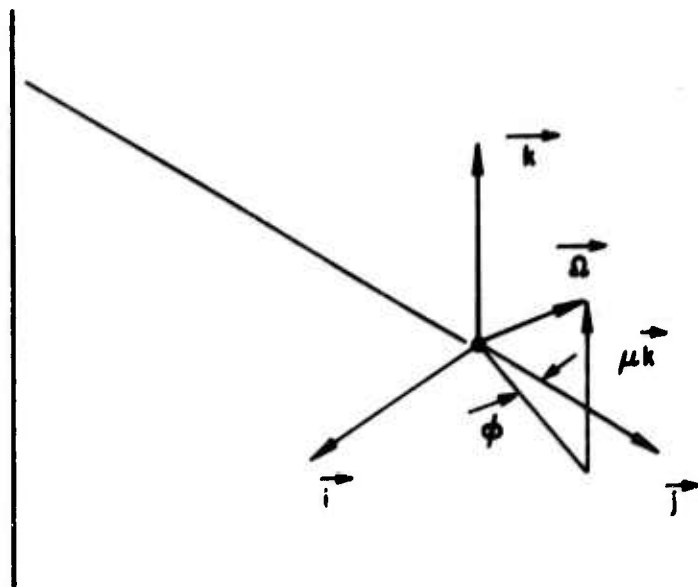


Figure 13. Components of Ω

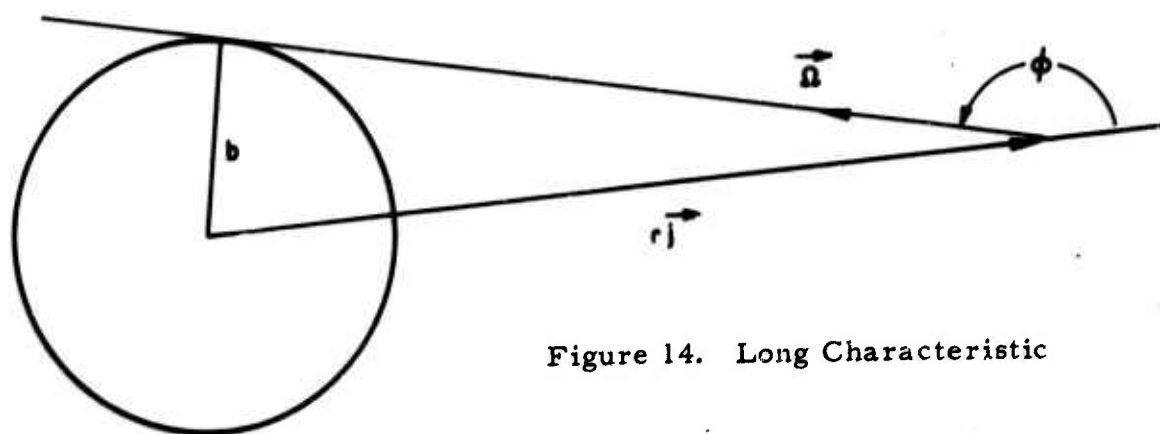


Figure 14. Long Characteristic

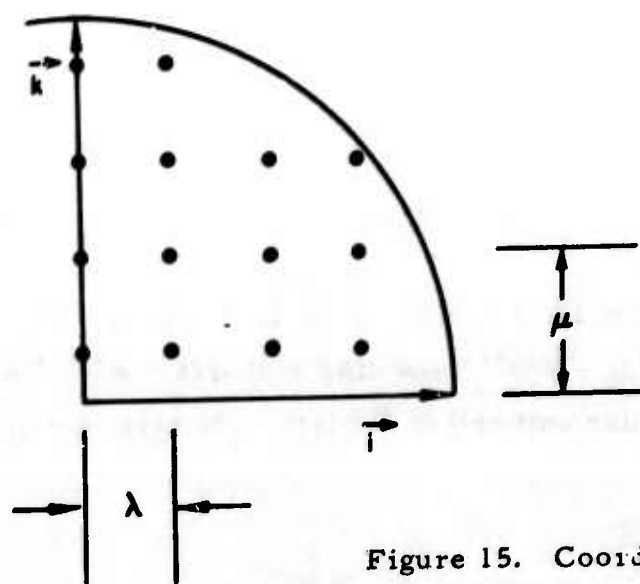


Figure 15. Coordinates μ and λ

As the point moves along the ray in the direction $\vec{\Omega}$, μ is fixed, but unless $\mu^2 = 1$, ϕ decreases. It can be seen that $\sin \phi = b/r$, where b is the distance between the ray and the axis. (See Figs. 13 and 14.)

The projection of the direction $\vec{\Omega}$ of a ray in the i - k plane is $\vec{\Omega} - \vec{\Omega} \cdot \vec{j} \vec{j} = \mu \vec{k} + \lambda \vec{i} = \mu \vec{k} + (1 - \mu^2)^{1/2} \sin \phi \vec{i}$. The distribution of directions of rays that intersect a given strip of radius r and altitude z will be isotropic if the distribution of their projections is uniform over the unit disk in the i - k plane. (See Fig. 15.) In such a λ, μ plot, the rays of one grid will lie in a horizontal line $\mu = \vec{\Omega} \cdot \vec{k} = \text{const}$. As r changes, μ remains fixed, and since $\lambda = (1 - \mu^2)^{1/2} (b/r)$, λr remains fixed also. Given two radii, r_1 and r_2 with $r_1 < r_2$, a ray with $\lambda = \lambda_2$ at $r = r_2$ will have $\lambda = \lambda_2 r_2 / r_1$ at $r = r_1$ (assuming that the distance b from the ray to the axis of the system is no greater than r_1), so that on a plot of projections like Fig. 15, moving from r_2 to r_1 will cause a dilation of the pattern of projections by a factor of r_2 / r_1 . Those projections for which $\lambda_2^2 > 1 - \mu^2$ correspond to points that fall outside the unit circle, but they are associated with the rays for which $r_1 < b \leq r_2$. At any rate, the dilation is constant for all directions, so a distribution that is uniform at r_2 will, of course, remain uniform at r_1 . Unfortunately, the density of directions is much reduced at smaller radii, which is a basic difficulty with the method.

The method that is used in TRAN2 to obtain a uniform distribution of projections on the unit disk is to choose N equally spaced values of μ ,

$$\mu = \frac{2n - 1}{2N}, \quad n = 1, 2, \dots, N$$

and for each μ to let $\lambda = Cj$, $j = 0, 1, 2, \dots, j < (1 - \mu^2)^{1/2} / C$, at $r = R$. Then $b = RCj / (1 - \mu^2)^{1/2}$ and $d(\mu) = RC / (1 - \mu^2)^{1/2}$ are the dimensions of the rectangular unit cell in the lattice of rays in a grid.

5.4. CALCULATION OF INTENSITIES

Let V_i denote the volume of zone i of the mesh imposed on the hydrodynamical calculation by HECTIC; let L_i denote the sum of the lengths of segments of rays intersected by zone i ; and set $A_i = 4\pi V_i / L_i$. Then A_i should not vary much from zone to zone. Radical variations in A_i indicate that the density of rays in the grid is too low.

The quantity A_i has the dimensions of area and is, in a way, taken to be a measure of the cross section of a beam associated with the ray. The quantity that is calculated at each point along a ray is the rate of flow of energy through the beam that the ray represents. In zone i this is

$$J(s) = J(0) e^{-\sigma_i s} + A_i S_i s \frac{1 - e^{-\sigma_i s}}{\sigma_i s}$$

assuming that the source S_i and volume coefficient of absorption σ_i are constants. The rate of energy deposition in zone i is then

$$\frac{dE_i}{dt} = \sigma_i \sum \int_0^l J(s) ds = J_{i0} \sum (1 - e^{-\sigma_i l}) + A_i S_i \sum l \left(1 - \frac{1 - e^{-\sigma_i l}}{\sigma_i l} \right)$$

where the summations range over rays that intersect zone i . The rate of emission is, of course, $A_i S_i L_i = 4\pi S_i V_i$.

The rate at which radiation passes through a surface is just the sum of the J 's over all points at which rays intersect the surface.

It remains to discuss the calculation of J at the point at which a ray enters the system. At the curved outer surface, it is easy to see what to do. The boundary condition must specify for each strip of altitude ΔZ on the outer surface what the incident radiant intensity is as a function of direction. By using μ and λ as coordinates, the direction of each incoming ray may be projected as a point on the unit disk, as was done in Fig. 15. The area of the disk is then subdivided so that in each subdivision

there is one point more or less in the center. The initial energy J carried by a given ray is then

$$J = 2\pi R \Delta z I^*$$

where I^* is the integral of the intensity over the solid angle of directions that are projected on the subdivision of the unit disk associated with the given ray.

In TRAN2, only isotropic boundary radiation is presently handled, so $J = (4\pi^2 R \Delta z I)/N_0$, where I is the mean intensity on the strip through which the ray enters and N_0 is the number of grids, or, in other words, the number of rays entering through a strip of altitude Δz .

The situation at the ends of the cylindrical system could be quite difficult to treat by a method analogous to the one just described for the curved surface. TRAN2 treats two cases: (1) no incident radiation, and (2) perfect reflection. But the way to treat a boundary condition like that corresponding to an incident laser beam is to introduce an entirely new set of rays which have no role in the calculation of radiative transfer of energy within the system but simply provide channels for the deposition of external radiation.

5.5. THICK ZONES

Experience (with SPUTTER* for example) has shown that the method of characteristics must be applied with care when the distance between zone boundaries becomes more than a few times the length of a mean free path. In some cases, it might be impossible to determine the distribution of radiation within a thick zone because of loss of information due to mixing, and a reduction of the mesh spacing would be necessary. Frequently, the diffusion approximation will give satisfactory results without

*Freeman, B.E., and C.G. Davis, "Fireball Phenomenology and Code Development. Vol. III, "SPUTTER Subroutines for Radiation Transport in Spheres," Air Force Weapons Laboratory Report AFWL-TR-65-143, General Atomic Division, General Dynamics Corporation, August, 1965.

refinement of the spatial mesh when the transport approximation used in TRAN2, which assumes constant source strengths throughout individual zones, does not. For this reason, it will be necessary to treat thick zones by a special method. An application of the diffusion approximation to thick zones is being developed as follows. When the number of mean free paths between the boundaries of a zone is above a critical value specified by input, that zone is classified as thick. When two thick zones have a common boundary surface, the rays intersecting that surface are ignored and the diffusion approximation is applied to calculate the rate of transfer of radiant energy between them. When a thick zone has a boundary in common with an ordinary one, the energy that it radiates through that surface is calculated and divided uniformly among the rays that pass through it. Similarly, the energy coming in along these rays from the ordinary zone is all dumped into the thick zone, all transmission factors being neglected.

SECTION VI

FREQUENCY-AVERAGED TRANSMISSION FUNCTIONS6.1 INTRODUCTION

In this section a technique is proposed for the implementation of the treatment of the characteristic equation of radiative transport theory suggested by B. E. Freeman (Ref. 1). A review of the formulation is presented first, both to establish notation and to describe certain modifications made in the originally proposed formulation.

The characteristic equation for the intensity $I(\underline{\Omega}, \tau, \nu)$ of radiation of frequency ν in a direction $\underline{\Omega}$ at optical depth τ is

$$\frac{d}{d\tau} I(\underline{\Omega}, \tau, \nu) + I(\underline{\Omega}, \tau, \nu) = B(\underline{\Omega}, \theta, \nu) \quad (69)$$

where $B(\underline{\Omega}, \theta, \nu)$ is the blackbody source intensity for temperature θ :

$$B(\underline{\Omega}, \theta, \nu) d\nu = \frac{2h\nu^3}{c^2} (e^{h\nu/\theta} - 1)^{-1} d\nu \quad (70)$$

It is necessary to evaluate the integral of $I(\underline{\Omega}, \tau, \nu)$ over prescribed intervals of $\underline{\Omega}$, τ , and ν . In systems with plane or spherical symmetry, the intensity as well as the source is independent of azimuth, so that the integration over this part of $\underline{\Omega}$ may be performed at once. Integration over μ , the cosine of the angle between the ray and the normal direction $\underline{r}$, is carried out after integration along the ray, and is not discussed in this report. For the sake of brevity, the argument μ for the intensity and source functions will be suppressed. The element of optical depth is defined by

$$d\tau = \sigma(\theta, \rho, \nu) ds \quad (71)$$

where the cross section

$$\sigma(\theta, \rho, \nu) = \rho \kappa'(\theta, \rho, \nu) = \rho \kappa(\theta, \rho, \nu)(1 - e^{-h\nu/\theta}) \quad (72)$$

includes the usual correction for induced emission, and the element of length along the ray is defined by

$$ds = \frac{dr}{\mu} \quad (73)$$

in plane geometry, while in spherical geometry with

$$x = r\mu, \quad y = r\sqrt{1 - \mu^2} \quad (74)$$

$$ds = dx \quad (75)$$

Equation (69) therefore becomes

$$\frac{d}{d\tau} I(\tau, \nu) + I(\tau, \nu) = B(\theta, \nu) \quad (76)$$

with

$$B(\theta, \nu)d\nu = \frac{4\pi h\nu^3}{c^2} (e^{h\nu/\theta} - 1)^{-1} d\nu \quad (77)$$

If the variable $u = h\nu/\theta$ is introduced, then Eq. (77) is equivalent to

$$B(\theta, u)du = \frac{4\pi\theta^4}{h^3 c^2} \frac{u^3}{e^u - 1} du \quad (78)$$

In terms of the normalized Planck function,

$$W_1(u) = \frac{15}{\pi^4} \frac{u^3}{e^u - 1} \quad (79)$$

$$B(\theta, u)du = \frac{ac}{2} \theta^4 W_1(u)du \quad (80)$$

where

$$\frac{ac}{2} = 2\sigma = \frac{4\pi^5}{15h^3 c^2} \quad (81)$$

is twice the Stefan-Boltzmann constant; if θ is in ev units, $a = 137.20$.

For later reference, the functions

$$f(u) = \int_u^\infty W_1(u') du' \quad (82)$$

$$g(u) = \frac{u}{4} W_1(u) \quad (83)$$

and

$$W_2(u) = \left(\frac{df}{du} + \frac{dg}{du} \right) = \frac{15}{4\pi^4} \frac{u^4 e^u}{(e^u - 1)^2} \quad (83a)$$

are needed. For example,

$$\int_{u_1}^{u_2} B(\theta, u) du = \frac{ac}{2} \theta^4 [f(u_1) - f(u_2)] \quad (84)$$

$$\begin{aligned} \int_{u_1}^{u_2} \frac{dB}{d\theta} du &= 2 ac \theta^3 \int_{u_1}^{u_2} W_2(u) du = 2 ac \theta^3 [f(u_1) - f(u_2) \\ &\quad + g(u_1) - g(u_2)] \end{aligned} \quad (85)$$

It is customary to absorb a factor $1/c$ in the definitions of B and I , in which case the factor c does not appear in Eqs. (80), (84), and (85).

Since the temperature varies with position, and therefore with optical depth, the notation $B(\tau, \nu)$ may be introduced in place of $B(\theta(\tau), \nu)$. The integral with respect to τ of Eq. (76) over an interval $\tau_0 < \tau < \tau_1$ is then

$$I(\tau_1, \nu) = I(\tau_0, \nu) e^{-(\tau_1 - \tau_0)} + \int_{\tau_0}^{\tau_1} B(\tau, \nu) e^{-(\tau_1 - \tau)} d\tau \quad (86)$$

Assume that $B(\tau, \nu)$ is linear in τ over this interval with slope $\partial B / \partial \tau$; then

$$I(\tau_1, \nu) = B(\tau_1, \nu) - \frac{\partial B}{\partial \tau} + \left[I(\tau_0, \nu) - B(\tau_0, \nu) + \frac{\partial B}{\partial \tau} \right] e^{-(\tau_1 - \tau_0)} \quad (87)$$

The first two terms on the right side of Eq. (87) represent the diffusive intensity. The quantity in brackets represents the streaming (nondiffusive) part of the intensity at τ_0 , which is attenuated by an exponential "transmission function" on the way to τ_1 .

6.2 FREQUENCY AVERAGING FOR THE TRANSPORT EQUATION

The problem to be discussed is the way in which the integration of Eq. (87) over the frequency ν should be carried out. The simplest approach is just to substitute frequency-averaged optical depths for the variable τ in Eq. (87). The appropriate average for $\partial B/\partial \tau$ is $\partial B/\partial \tau^R$, where τ^R is the Rosseland mean optical depth (see Eq. (93) below). However, the Rosseland mean is frequently inappropriate for use in the exponential transmission function. The Planck mean defined by Eq. (94) below is valid in the limit of an extremely thin region ($\tau^P \ll 1$), while the Rosseland mean is preferable in the thick limit, where the transmission function is relatively small anyway. Other means can be constructed from the Planck and Rosseland means, such as the geometric mean $\sqrt{\tau^P \tau^R}$ or the mean proposed by Sampson (Ref. 2):

$$\bar{\tau} = \left(\frac{b + \tau^R}{b + \tau^P} \right) \tau^P$$

where b is an adjustable parameter of order unity. Without doubt, such means, particularly the last-mentioned, are useful expedients in many cases, but experience has shown that they must be used with some caution. In this report, Eq. (87) is treated in a more systematic manner, as in Ref. 1.

The medium is divided for computational purposes into zones by interfaces whose coordinates are denoted by r_i . A subscript $i-1$, i , $i+1$, etc., on a quantity implies that the quantity is to be evaluated on an interface, while a subscript such as $i-1/2$ or $i+1/2$ implies evaluation either for the zone as a whole or for an interior point in the zone. This point will be assumed to be the midpoint of the ray, so that

$$s_i - s_{i-1/2} = s_{i-1/2} - s_{i-1} = \delta_{i-1/2} \quad (88)$$

is the half-width of zone $i-1/2$, measured along the ray. In particular, the density $\rho_{i-1/2}$ and temperature $\theta_{i-1/2}$ are given quantities associated with each zone or zone midpoint, and it is desired to calculate intensities $I_i(\nu)$ at the interfaces. It is therefore natural to carry out the integration of Eq. (86) in half-zone steps, within each of which $B(\tau, \nu)$ can be assumed linear in τ . Thus,

$$I(\tau_i, \nu) = B(\tau_i, \nu) - \left(\frac{\partial B}{\partial \tau}\right)_i + \left[I(\tau_{i-1/2}, \nu) - B(\tau_{i-1/2}, \nu) + \left(\frac{\partial B}{\partial \tau}\right)_i \right] e^{-(\tau_i - \tau_{i-1/2})} \quad (89)$$

$$I(\tau_{i-1/2}, \nu) = B(\tau_{i-1/2}, \nu) - \left(\frac{\partial B}{\partial \tau}\right)_{i-1} + \left[I(\tau_{i-1}, \nu) - B(\tau_{i-1}, \nu) + \left(\frac{\partial B}{\partial \tau}\right)_{i-1} \right] e^{-(\tau_{i-1/2} - \tau_{i-1})} \quad (90)$$

In order to carry out the integration of Eqs. (89) and (90) over frequency, three further assumptions are required. First, it will be assumed that cross sections have a piecewise-constant dependence upon position. This is done for simplicity, since it provides for a piecewise-linear relationship between position and optical depth which is more convenient than a quadratic or other type relationship and is no less consistent with the available information. Second, the cross sections will be evaluated at, or at least associated with, zone boundaries rather than zone midpoints (using, for example, an interpolated density and temperature at each boundary). This choice is made primarily for experimental reasons, but is guided also by the physical consideration that the opacity is ultimately needed for the calculation of radiative flux across zone boundaries, and is in this sense most naturally defined as a boundary-centered, rather than a zonal, quantity. There is probably no single best method for evaluating opacity at

zone interfaces; in some cases it might suffice to use the lesser of the adjacent zone opacities. If interpolation is to be done, however, it is simpler and probably less dangerous to interpolate temperatures and densities than to interpolate zonal opacities directly. The formulation adopted is in any case quite general. The most economical method would prescribe the cross section as constant from one midpoint to the next, but allowance can also be made for possible interface discontinuity.

The third assumption is made purely for convenience. It will be assumed that $I(\tau, \nu)$ has a frequency dependence within each group proportional to that of $B(\tau, \nu)$. The validity of this assumption depends on the variation of opacity within the group, and cannot be taken for granted in a few-group calculation.

The following definitions are needed:

$$B_{ij} = \int_{\nu_j}^{\nu_{j+1}} B(\theta_i, \nu) d\nu, \text{ the group source} \quad (91)$$

$$I_{ij} = \int_{\nu_j}^{\nu_{j+1}} I(\tau_i, \nu) d\nu, \text{ the group intensity} \quad (92)$$

$$\sigma_{ij}^R = \frac{dB_{ij}/d\theta}{\int_{\nu_j}^{\nu_{j+1}} \frac{1}{\sigma(\theta_i, \rho_i, \nu)} \left(\frac{dB}{d\theta}\right)_{\theta_i} d\nu}, \text{ the group Rosseland mean cross section} \quad (93)$$

$$\sigma_{ij}^P = \int_{\nu_j}^{\nu_{j+1}} B(\theta_i, \nu) \sigma(\theta_i, \rho_i, \nu) d\nu / B_{ij}, \text{ the group Planck mean} \quad (94)$$

$$S_{ij}(\delta) = \int_{\nu_j}^{\nu_{j+1}} B(\theta_i, \nu) e^{-\sigma(\theta_i, \rho_i, \nu)\delta} d\nu / B_{ij}, \text{ the Planck transmission function} \quad (95)$$

and

$$T_{ij}(\delta) = \int_{\nu_j}^{\nu_{j+1}} \frac{1}{\sigma(\theta_i, \rho_i, \nu)} \left(\frac{dB}{d\theta} \right)_{\theta_i} e^{-\sigma(\theta_i, \rho_i, \nu) \delta} d\nu / \left(\frac{1}{R} \frac{dB_{ij}}{d\theta} \right)_{\sigma_{ij}} \quad (96)$$

the Rosseland transmission function.

Equations (89) and (90) then may be integrated over the j^{th} frequency group; notation is further specified as follows:

$$I_{ij} = \bar{B}_{ij} - \left(\frac{dB}{d\tau} \right)_{ij} + (I_{i-1/2,j} - \bar{B}_{i-1/2,j}) S_{ij}^-(\delta_{i-1/2}) + \left(\frac{dB}{d\tau} \right)_{ij} T_{ij}^-(\delta_{i-1/2}) \quad (97)$$

$$I_{i-1/2,j} = \bar{B}_{i-1/2,j} - \left(\frac{dB}{d\tau} \right)_{i-1,j} + (I_{i-1,j} - \bar{B}_{i-1,j}) S_{i-1,j}^+(\delta_{i-1/2}) + \left(\frac{dB}{d\tau} \right)_{i-1,j} T_{i-1,j}^+(\delta_{i-1/2}) \quad (98)$$

Since I is needed only on interfaces, $I_{i-1/2,j}$ may be eliminated from Eqs. (97) and (98):

$$I_{ij} = \bar{B}_{ij} + \left\{ (I_{i-1,j} - \bar{B}_{i-1,j}) S_{i-1,j}^+(\delta_{i-1/2}) - \left(\frac{dB}{d\tau} \right)_{i-1,j} \left[1 - T_{i-1,j}^+(\delta_{i-1/2}) \right] \right\} S_{ij}^-(\delta_{i-1/2}) - \left(\frac{dB}{d\tau} \right)_{ij} \left[1 - T_{ij}^-(\delta_{i-1/2}) \right] \quad (99)$$

It remains to discuss the definitions of the quantities θ_i , ρ_i , $\bar{B}_{ij}$, and $(dB/d\tau^R)_{ij}$. The interface temperature may be defined by some mean value such as

$$\theta_i = \left(\frac{\theta_{i-1/2}^4 + \theta_{i+1/2}^4}{2} \right)^{1/4} \quad (100)$$

$$T_{ij}(\delta) = \int_{\nu_j}^{\nu_{j+1}} \frac{1}{\sigma(\theta_i, \rho_i, \nu)} \left(\frac{dB}{d\theta} \right)_{\theta_i} e^{-\sigma(\theta_i, \rho_i, \nu) \delta} d\nu / \left(\frac{1}{R} \frac{dB_{ij}}{d\theta} \right)_{\sigma_{ij}} \quad (96)$$

the Rosseland transmission function.

Equations (89) and (90) then may be integrated over the j^{th} frequency group; notation is further specified as follows:

$$I_{ij} = \bar{B}_{ij} - \left(\frac{dB}{d\tau} \right)_{ij} + (I_{i-1/2,j} - \bar{B}_{i-1/2,j}) \bar{S}_{ij}^-(\delta_{i-1/2}) + \left(\frac{dB}{d\tau} \right)_{ij} T_{ij}^-(\delta_{i-1/2}) \quad (97)$$

$$I_{i-1/2,j} = \bar{B}_{i-1/2,j} - \left(\frac{dB}{d\tau} \right)_{i-1,j} + (I_{i-1,j} - \bar{B}_{i-1,j}) S_{i-1,j}^+(\delta_{i-1/2}) + \left(\frac{dB}{d\tau} \right)_{i-1,j} T_{i-1,j}^+(\delta_{i-1/2}) \quad (98)$$

Since I is needed only on interfaces, $I_{i-1/2,j}$ may be eliminated from Eqs. (97) and (98):

$$I_{ij} = \bar{B}_{ij} + \left[(I_{i-1,j} - \bar{B}_{i-1,j}) S_{i-1,j}^+(\delta_{i-1/2}) - \left(\frac{dB}{d\tau} \right)_{i-1,j} \left[1 - T_{i-1,j}^+(\delta_{i-1/2}) \right] \right] \bar{S}_{ij}^-(\delta_{i-1/2}) - \left(\frac{dB}{d\tau} \right)_{ij} \left[1 - T_{ij}^-(\delta_{i-1/2}) \right] \quad (99)$$

It remains to discuss the definitions of the quantities θ_i , ρ_i , $\bar{B}_{ij}$, and $(dB/d\tau^R)_{ij}$. The interface temperature may be defined by some mean value such as

$$\theta_i = \left(\frac{\theta_{i-1/2}^4 + \theta_{i+1/2}^4}{2} \right)^{1/4} \quad (100)$$

which is used in MOTET. Again, no single prescription can be expected to represent all cases equally well. Provision should be made for alternative methods in special cases; one such method would be use of the zone temperatures on each side of the interface. The + and - superscripts on σ^R , S , and T indicate possible use of such a discontinuous interface treatment (for temperature, density, or both).

The interface density may be evaluated either by position interpolation or by use of a mean value such as the ratio of the combined masses of the two zones to their combined volume. Again, provision for a discontinuity at the interface is desirable.

Simple and consistent definitions of $\bar{B}_{ij}$ and $(dB/d\tau^R)_{ij}$ are obtained by use of source functions evaluated at zone temperatures with Rosseland optical depth interpolation:

$$\left(\frac{dB}{d\tau^R}\right)_{ij} = \frac{B_{i+1/2,j} - B_{i-1/2,j}}{\sigma_{ij}^{R+} \delta_{i+1/2} + \sigma_{ij}^{R-} \delta_{i-1/2}} \quad (101)$$

$$\bar{B}_{ij} = B_{i-1/2,j} + \left(\frac{dB}{d\tau^R}\right)_{ij} \sigma_{ij}^{R-} \delta_{i-1/2} = B_{i+1/2,j} - \left(\frac{dB}{d\tau^R}\right)_{ij} \sigma_{ij}^{R+} \delta_{i+1/2} \quad (102)$$

It should be noted that both $\bar{B}_{ij}$ and $(dB/d\tau^R)_{ij}$ are single-valued, regardless of whether or not σ_{ij}^R is, and further that $\bar{B}_{ij}$ must be evaluated by means of Eq. (102), and not evaluated at the interface temperature θ_i . The latter procedure would yield B_{ij} as defined in Eq. (91), and would be inconsistent with Eq. (101), which is based upon an assumption that B is continuous.

The present formulation closely resembles that of Ref. 1, differing chiefly in that opacities are evaluated at interfaces rather than at zone midpoints. This variation is intended to facilitate a more versatile treatment of radiation front propagation with little or no accompanying increase in computation.

The cross section σ , considered as a function of ν , or of $u = h\nu/\theta$, has too detailed a structure to permit approximation in one stage to be a practical procedure. Subintervals Δu_k are therefore defined which are sufficiently small so that within them the variations of the Planck and Rosseland spectrum functions, $W_1(u)$ and $W_2(u)$, are negligible. The opacity within these subintervals may or may not show considerable variation. In any case, it can be at least partially described by the direct and inverse means (Ref. 3)

$$\sigma_k^d = \int_{\Delta u_k} \sigma(u) du / \Delta u_k \quad (103)$$

$$\sigma_k^i = \Delta u_k / \int_{\Delta u_k} du / \sigma(u) \quad (104)$$

which are in effect microscopic Planck and Rosseland means, respectively.

The number of these subintervals is, typically, of order 10^2 to 10^4 . The number of groups employed in transport calculations, however, is of order 1 to 10^2 . It is not generally possible to neglect the variation of $W_1(u)$ and $W_2(u)$ within these groups. Thus, for the subintervals Δu_k contained within a group $u_j \leq u < u_{j+1}$, one defines normalized Planck and Rosseland weights:

$$P_k = \frac{f(u_k) - f(u_k + \Delta u_k)}{f(u_j) - f(u_{j+1})} \quad (105)$$

$$R_k = \frac{[f(u_k) - f(u_k + \Delta u_k) + g(u_k) - g(u_k + \Delta u_k)] / \sigma_k^i}{\sum_l [f(u_l) - f(u_l + \Delta u_l) + g(u_l) - g(u_l + \Delta u_l)] / \sigma_l^i} \quad (106)$$

The group Planck and Rosseland cross sections and transmission functions are thus, respectively,

$$\sigma_{ij}^P = \sum_k P_k \sigma_k^d \quad (107)$$

$$\sigma_{ij}^R = \sum_k R_k \sigma_k^i \quad (108)$$

$$S_{ij}(x) = \sum_k P_k e^{-\sigma_k^d x} \quad (109)$$

$$T_{ij}(x) = \sum_k R_k e^{-\sigma_k^i x} \quad (110)$$

These are the discrete analogs of Eqs. (93) through (96). Although Eqs. (107) and (108) are essentially exact, Eqs. (109) and (110) are already approximations which are accurate only to first order in x . Even so, they are still far too cumbersome for use by the transport routines, which require representations $\tilde{S}_{ij}(x)$ and $\tilde{T}_{ij}(x)$ of $S_{ij}(x)$ and $T_{ij}(x)$ involving at most five or six parameters each, with the use of exponential or similar functions kept to a minimum. On the other hand, the optical thickness of zones employed in transport calculations is unrestricted, so that the parameterization must not fail in a gross manner for any nonnegative x .

6.3 PARAMETRIC REPRESENTATION OF TRANSMISSION FUNCTIONS

The method to be described employs piecewise-linear, and linear rational approximations to the logarithm of the transmission function. Both functions (109) and (110) are of the form

$$F(x) = \sum_k Q_k e^{-\sigma_k x} \quad (111)$$

with

$$F(0) = \sum_k Q_k = 1 \quad (112)$$

In accordance with Eq. (107) or (108), define

$$-F'(0) = \sum_k Q_k \sigma_k = \bar{\sigma} \quad (113)$$

The (Planck or Rosseland) optical depth variable is then

$$\tau = \bar{\sigma} x \quad (114)$$

Let

$$\overline{\sigma^2} = \sum_k Q_k \sigma_k^2 \quad (115)$$

Then the expansion of (111) in powers of τ is

$$F(x) = F(\tau) = 1 - \tau + 1/2 \frac{\overline{\sigma^2}}{\bar{\sigma}^2} \tau^2 - \dots \quad (116)$$

The approximation

$$\bar{F}(\tau) = e^{-\tau \bar{H}(\tau)} \quad (117)$$

with

$$\bar{H}(\tau) = 1 - \frac{\overline{\sigma^2} - \bar{\sigma}^2}{2\bar{\sigma}^2} \tau, \quad 0 \leq \tau < \tau_1 \quad (118)$$

agrees with Eq. (116) to second order in τ . For τ not small compared with unity, this approximation can be very poor. The general linear fit is therefore used:

$$\bar{H}(\tau) = \bar{H}(\tau_2) + \frac{H(\tau_3) - H(\tau_2)}{\tau_3 - \tau_2} (\tau - \tau_2), \quad \tau_1 \leq \tau < \tau_3 \quad (119)$$

where τ_1 is the abscissa of the intersection of the two lines (118) and (119), τ_2 and τ_3 are prescribed values such as

$$\tau_2 = \bar{\sigma}/\sigma^P, \quad \tau_3 = \bar{\sigma}/\sigma^R \quad (120)$$

and

$$H(\tau_2) = -\ln F(\tau_2)/\tau_2, \quad H(\tau_3) = -\ln F(\tau_3)/\tau_3 \quad (121)$$

(It is assumed that $\sigma^P > \sigma^R$ so that $\tau_3 > \tau_2$. If scattering is included in σ^R but not in σ^P , this condition may not be satisfied and a different prescription of τ_2 and τ_3 should be used). Finally, for $\tau \rightarrow \infty$ the approximation used is the linear rational function

$$\bar{H}(\tau) = \frac{b_1 + b_2 \tau}{b_3 + b_4 \tau} \quad \tau_3 \leq \tau < \infty \quad (122)$$

where $b_1 = H(\tau_3)H(\tau_4)\tau_4(\tau_4 - \tau_3) + H(\tau_4)\tau_3 - H(\tau_3)\tau_4$

$$b_2 = H(\tau_3) - H(\tau_4)$$

$$b_3 = \tau_3 + \tau_4 [H(\tau_4)\tau_4 - H(\tau_3)\tau_3 - 1]$$

$$b_4 = \tau_4 b_2$$

$$\tau_4 = \frac{\bar{\sigma}}{\min(\sigma_k)}$$

$$H(\tau_4) = -\ln F(\tau_4)/\tau_4$$

This function has the properties

$$\bar{H}(\tau_3) = H(\tau_3)$$

$$\bar{H}(\tau_4) = H(\tau_4)$$

and $\lim_{\tau \rightarrow \infty} \bar{\sigma} \bar{H}(\tau) = \lim_{\tau \rightarrow \infty} \bar{\sigma} H(\tau) = \min(\sigma_k)$, where $\min(\sigma_k)$ is the smallest of all the σ_k^d or σ_k^i in the group.

The parameterization described requires storage of 12 parameters on a "DIANE"-type data file for use by the radiation transport routines; for example; $\sigma^P, \sigma^R, \min(\sigma_k^d), \min(\sigma_k^i), \tau_1^P, \tau_1^R, H^P(\tau_1), H^R(\tau_1), H^P(\tau_3), H^R(\tau_3), H^P(\tau_4),$ and $H^R(\tau_4)$. The accuracy of fit attainable with these parameters has been investigated for a few artificial examples. The poorest fit generally occurs in the S function for cases in which $\sigma^P \gg \sigma^R$, for widths $\delta = x$ such that

$$\frac{1}{\sigma^P} \ll x \ll \frac{1}{\sigma^R}$$

In extreme cases of this type the fit is still usually within a factor of two. If σ^P and σ^R are within one or two orders of magnitude, the worst fit is of the order of 10%. For depths small compared with a mean free path, the fit is generally excellent, although in the worst cases the T function may be in error by 10% or so near $\sigma^R = 0.5$. Since the difference between $\min(\sigma_k^d)$ and $\min(\sigma_k^i)$ is not significant except at very large depths, it would be possible to use a single value for both, reducing the required number of parameters to 11. Still fewer parameters could be used if the resulting loss of accuracy is considered acceptable.

A number of other parameterizations were explored, including fitting by sums of exponentials and various techniques using orthogonal polynomials and higher order rational approximants to the logarithm of the transmission function. Of those investigated, only the fit by a sum of exponentials appeared at all satisfactory, and the technique described above offers comparable results with much less computational time involved. Undoubtedly, the present parameterization can be further improved, but it is believed that this type of approach offers acceptable accuracy along with reasonable economy in the handling of data better than most others.

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