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FIREBALL PHENOMENOLOGY AND CODE DEVELOPMENT

Volume III

SPUTTER Subroutines for Radiation Transport in Spheres

**General Atomic Division of General Dynamics Corporation
Special Nuclear Effects Laboratory**

San Diego, California

Contract AF 29(601)-6492

TECHNICAL REPORT NO. AFWL-TR-65-143, Vol III

July 1966

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

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FOREWORD

This report was prepared by General Atomic Division of General Dynamics Corporation, San Diego, California, under Contract AF 29(601)-6492. The research was performed under Program Element 7.60.06.01.D, Project 5710, Subtask 07.003/005, and was funded by the Defense Atomic Support Agency (DASA).

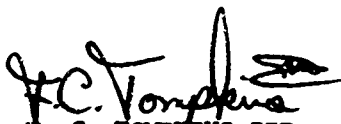
Inclusive dates of research were 1 June 1963 to 13 July 1965. The report was submitted 15 March 1966 by the Air Force Weapons Laboratory Project Officer, 1Lt F. C. Tompkins III (WLRT).

The Contractor's report number is GA-6585.

The report is divided into six volumes as follows: Volume I, Summary and the Fireball Models; Volume II, Early Fireball Phenomena in the TIGHTROPE Event^{*}; Volume III, SPUTTER Subroutines for Radiation Transport in Spheres; Volume IV, SPUTTER Subroutines for Radiation Transport in Planes; Volume V, Material Properties; and Volume VI, Extensions of the Physics and Problem Areas.

The SPUTTER subroutines for radiation transport in spheres described in Volume III were developed by Dr. B. E. Freeman and Dr. C. G. Davis, Jr. The cooperation and contributions of Captains Milton Gillespie, William Whittaker, and George Spillman of the Air Force Weapons Laboratory are gratefully acknowledged.

This technical report has been reviewed and is approved.


F. C. TOMPKINS III
1Lt, USAF
Project Officer


RALPH H. PENNINGTON
Lt Colonel, USAF
Chief, Theoretical Branch


WILLIAM H. STEPHENS
Colonel, USAF
Chief, Research Division

* Volume II has been withdrawn, and will not be published.

ABSTRACT

The radiation transport subroutines of the SPUTTER code for spherical geometry have been revised. The DIFFU subroutine has been eliminated and RADTN, TRANS, and KAPPA have been recoded. The results of this work on the codes are (1) improved logical organization, (2) more efficient and rapid calculation, (3) improved accuracy, (4) more complete documentation, and (5) comparisons with test problems. The much simpler and more accurate diffusion approximation is exploited when a new diffusion criterion is satisfied in shells within the sphere. A more accurate angular integration of the intensity makes use of the y-line integration results more efficiently to give improved fluxes. Reorganization of the calculation, saving of quantities to be used again, and use of a fast exponential routine have resulted in speeding up the routines by approximately a factor of 2. The diffusion and angular integration improvements apparently have resulted in an additional factor of 2 speedup for the same accuracy.

The SPUTTER code subroutines for radiation transport in spheres described herein are as they existed on July 1, 1965. General Atomic has exercised due care in preparation, but does not warrant the merchantability, accuracy, and completeness of these subroutines or of their description contained herein. The complexity of this kind of program precludes any guarantee to that effect. Therefore, any user must make his own determination of the suitability of these subroutines for any specific use and of the validity of the information produced by their use.

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SECTION I

INTRODUCTION

The spherical version of the radiation transport routines for SPUTTER⁽¹⁾ has been completely revised to increase both the speed and the accuracy of the calculation. The new subroutines contain a revised diffusion criterion, the use of Planck means in the transparent, or thin, limit (Rosseland means have always been used in the thick limit), and an improved method of integrating over angles.

The logic in the SRADTN subroutine has been reorganized: first, to select an initial set of y-lines from which the set for each frequency group will be chosen later; second, to merge frequency groups for which the source function is small, even for the highest temperature in the mesh; third, to limit the source calculation to regions of appreciable temperature and thereby reduce the transport calculation; and, finally, to establish diffusion regions and perform the diffusion calculation in SRADTN (formerly this was done in a subroutine called DIFFU). In essence, therefore, the new SRADTN subroutine establishes the limiting set of active zones for sources, y-lines, and frequency groups. The new STRANS subroutine contains the intensity integration along y-lines for the frequency groups selected in SRADTN.

What has been achieved in recoding these subroutines has been the removal from inside the main y-line loop the redundant calculations made previously, and this was principally done by storing the complete set of x-y intersections. The improvement in the angular integration is achieved by storing intensities along the previous y-line and interpolating between y-lines for an improved quadrature summation of fluxes. Both the quadratic and linear forms of interpolation were tested, but since the linear form appears to be more appropriate in most cases, it is used in STRANS.

Appropriate expansions in optical depth for transparent regions as well as diffusion boundary conditions are used in the new subroutines. At present the Rosseland mean is used in the thick limit and the Planck mean in the thin limit. This approach is only temporary, as eventually the more realistic transmission means, which will automatically limit correctly, will be used.

The numerical solution of the radiation transport equation along selected sampling rays through a sphere is discussed in Section II. The improved diffusion approximation is described in Section III, and the frequency integrations needed for the SPUTTER calculations are described in Section IV.

Although most of this report is concerned with the improved SRADTN and STRANS routines, some changes have also been made in certain auxiliary subroutines, e. g., a faster exponential subroutine FREXP, the Planck function subroutine PLNKUT, the absorption coefficient interpolation subroutine KAPPA, etc. These improvements are discussed in Section V, and the listings of the subroutines SRADTN, STRANS, FREXP, KAPPA, and PLNKUT are given in the Appendixes. The preliminary results of the improvements in accuracy and calculation times from comparison with the old subroutines are given in Section VI.

The obvious differences between the new and the old subroutines are in the new angular integration scheme and criteria for diffusion. The y-line integration of intensities is essentially the same. Actually, what has been achieved is a careful re-evaluation of the complete code, which has resulted in many time savings and in some increased accuracy. Additional accuracy can be achieved by going to more complete and therefore more complex integration schemes requiring additional core storage. These schemes will probably need the increased fast-storage capacity of the new generation of computers (e. g., CDC 6600 and IBM 360). Careful comparisons have been made between single cycles of multifrequency transport carried out with the old code and with the new code (as discussed in Section VI). These calculations have pointed up certain limitations in the numerical solution of the radiation transport equations, which are still not completely resolved. Questions as to the treatment of thin (optically) hot zones adjacent to thick cold zones, shock fronts, radiative fronts, the use of Planck emission means or, for that matter, what is the appropriate average, etc., still remain. The frequency-dependent calculations lead to questions regarding the selection of frequency groups and the use of various frequency-group averages. The present subroutines allow for a basic solution of the spherical transport equations, in which many improvements relative to the above questions, as well as additions in respect to such matters as retardation, scattering, etc., can be made.

SECTION II

NUMERICAL SOLUTION OF THE TRANSPORT EQUATION

The radiation routines described herein contain a formulation based on numerical solution of the radiation transport equation along a selection of sampling rays through the sphere. Relevant averages over the angular distribution are obtained by numerical quadrature, as described in Section 2.3, and the numerical solution of the transport equation along the photon ray is presented in Section 2.1. Criteria for selecting the sampling rays are discussed in Section 2.2. All of the derivations of this section apply to photons of a particular frequency; integration over frequency is discussed in Section IV.

The radiation transport equation in spherical geometry that describes the changes in the specific intensity I_ν of photons of frequency ν resulting from pure absorption and emission according to the local thermodynamic equilibrium assumption is

$$\left(\mu \frac{\partial}{\partial r} + \frac{1 - \mu^2}{r} \frac{\partial}{\partial \mu} \right) I_\nu = \sigma'_\nu (B_\nu - I_\nu) ,$$

where

$$B_\nu = \frac{2h}{c} \frac{\nu^3}{e^{h\nu/\theta} - 1} ,$$

$$\sigma'_\nu = \sigma_\nu (1 - e^{-h\nu/\theta}) ,$$

and σ_ν is the pure absorption coefficient. The scattering coefficient is assumed to be negligibly small compared to the absorption coefficient. Additionally, the retardation of the photons is neglected, as is valid when the radiation energy is small and temperatures change slowly. The resulting equation describes the quasi-steady intensity field resulting from the distribution of sources existing at a particular time. This equation is simplified by introducing two new independent variables, x and y , in place of r and μ , where

$$x = r\mu, \quad y = r\sqrt{1 - \mu^2}, \quad r = \sqrt{x^2 + y^2}, \quad \frac{x}{y} = \frac{\mu}{\sqrt{1 - \mu^2}} . \quad (2.1)$$

The distance along the photon ray is measured by x and the distance of closest approach of the undeviated ray is given by y . Since each ray is characterized by a particular y -value, it is also called a y -line. These relations are illustrated in Fig. 2.1, where the geometry of two y -lines is shown in relation to the radius and polar angle (Fig. 2.1a) and these quantities are translated into the corresponding two rays at a typical point on the spherically symmetric surface (Fig. 2.1b). In terms of x and y , the transport equation becomes

$$\frac{\partial I_{\nu}}{\partial x} = \sigma'_{\nu} (B_{\nu} - I_{\nu}) , \quad (2.2)$$

an equation which could equally well be considered the fundamental defining equation for the intensity in that it describes the processes that change the intensity along the ray. Defining the monochromatic optical depth, τ , as

$$\tau = \int_0^x \sigma'_{\nu} dx , \quad (2.3)$$

the differential equation can then be integrated between two points, τ_{i-1} and τ_i , on a ray:

$$I_i = I_{i-1} e^{-(\tau_i - \tau_{i-1})} + \int_{\tau_{i-1}}^{\tau_i} B e^{-(\tau_i - \tau)} d\tau . \quad (2.4)$$

This equation forms the starting point for the numerical solution of the transport equation. For a particular ray having a y -value chosen according to the prescriptions given in Section 2.2, the intensity is evaluated at selected points along the ray, starting from the outside boundary of the sphere with a prescribed boundary value. The immediate problem, then, is to prescribe the method for approximating the quadrature in Eq. (2.4). This prescription and the task of prescribing boundary conditions are discussed next.

2.1. INTEGRATION ALONG Y-LINES

In the finite-zone calculation of the SPUTTER code, the value of the source function, B_{ν} , is known only at a series of radii corresponding to the average positions of zones in the calculation. Intensities are needed, however, at all interfaces between zones in order to determine radiation fluxes. Consequently, it is necessary to construct an interpolation function between known values so that the integration of Eq. (2.4) can be carried out.

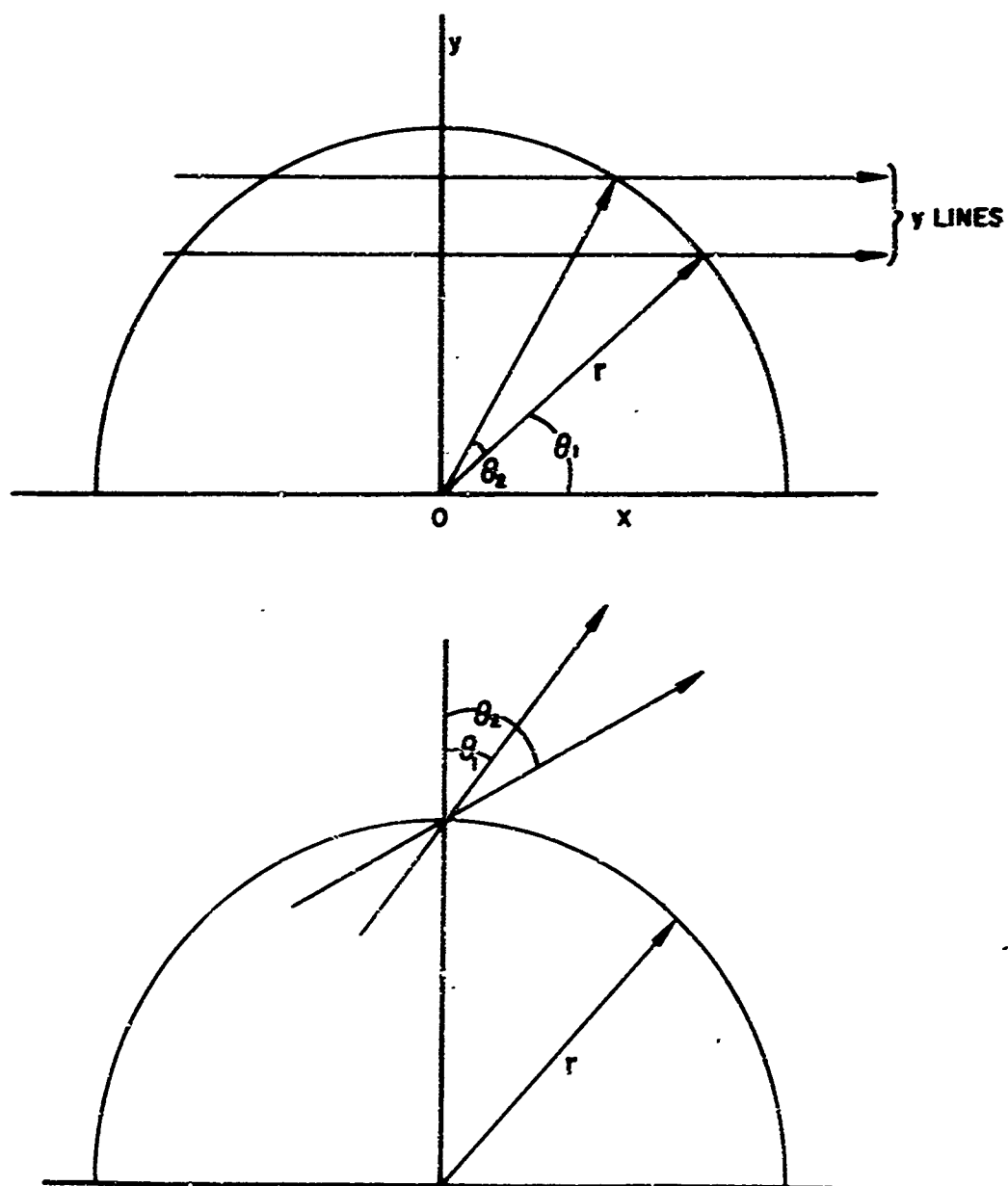


Fig. 2.1--Examples of relationship between y-lines and (r, θ) pairs

Of the many alternatives, a simple scheme is chosen which permits the integration to be performed in closed form.

2.1.1. General Formula

As indicated in Fig. 2.2, the source function is usually assumed to be linear in τ between given values of $B_{i+\frac{1}{2}}$ at the midpoints of zones $\tau_{i+\frac{1}{2}}$. At certain interfaces, however, when the criteria described in Section V are satisfied, the source function is assumed to be constant at the zone value, which is also shown in Fig. 2.2. Values of the source function B_i are first obtained by interpolation at the zone interfaces τ_i .

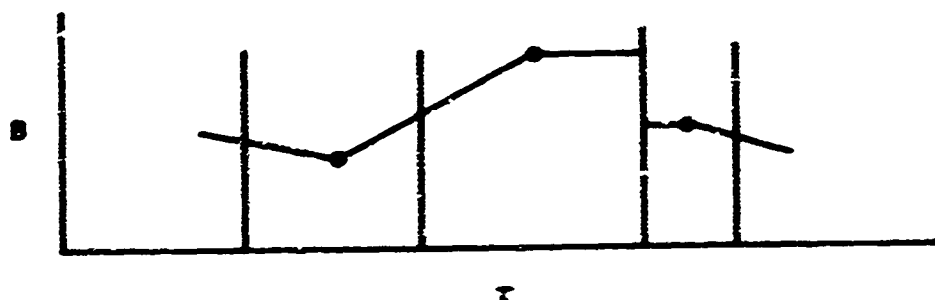


Fig. 2.2--Illustration of discontinuous source function

which, together with the midpoint values, form the termini for the integral of Eq. (2.4). More specifically, in the interval $\tau_{i-1} \leq \tau \leq \tau_i$, the source function takes the values

$$B = a_- + b_- \tau, \quad \tau_{i-1} \leq \tau \leq \tau_{i-\frac{1}{2}},$$

where

$$a_- = \frac{B_{i-1} \tau_{i-\frac{1}{2}} - B_{i-\frac{1}{2}} \tau_{i-1}}{\tau_{i-\frac{1}{2}} - \tau_{i-1}}, \quad b_- = \frac{B_{i-\frac{1}{2}} - B_{i-1}}{\tau_{i-\frac{1}{2}} - \tau_{i-1}} \quad (2.5)$$

and

$$B = a_+ + b_+ \tau, \quad \tau_{i-\frac{1}{2}} \leq \tau \leq \tau_i,$$

where

$$a_+ = \frac{B_{i-\frac{1}{2}} \tau_i - B_i \tau_{i-\frac{1}{2}}}{\tau_i - \tau_{i-\frac{1}{2}}}, \quad b_+ = \frac{B_i - B_{i-\frac{1}{2}}}{\tau_i - \tau_{i-\frac{1}{2}}}.$$

For the case of a constant or step-function source, the source function B takes a value dependent on which interface of the zone is affected. If the left interface ($\tau = \tau_{i-1}$) satisfies the criteria for a constant source,

$$B = B_{i-\frac{1}{2}}, \quad \tau_{i-1} \leq \tau \leq \tau_{i-\frac{1}{2}}.$$

If the right interface ($\tau = \tau_i$) satisfies the criteria,

$$B = B_{i-\frac{1}{2}}, \quad \tau_{i-\frac{1}{2}} \leq \tau \leq \tau_i.$$

The integral of Eq. (2.4) can be evaluated with the interpolation function of Eq. (2.5) to give for the intensity

$$I_i = \alpha_{i-\frac{1}{2}} + [(I_{i-1} + \gamma_{i-\frac{1}{2}})e^{-\Delta/2} + \beta_{i-\frac{1}{2}}]e^{-\Delta/2}, \quad (2.6)$$

where

$$\alpha_{i-\frac{1}{2}} = a_+ + b_+(\tau_i - 1),$$

$$\beta_{i-\frac{1}{2}} = a_- - a_+ + (b_- - b_+)\left(\tau_i - \frac{\Delta}{2} - 1\right),$$

$$\gamma_{i-\frac{1}{2}} = b_- (1 + \Delta - \tau_i) - a_-.$$

In these expressions, $\Delta = \tau_i - \tau_{i-1}$. The coefficients of Eq. (2.6) can be re-expressed by using the definitions of Eq. (2.5):

$$\left. \begin{aligned} \alpha_{i-\frac{1}{2}} &= B_i - \frac{B_i - B_{i-\frac{1}{2}}}{\Delta/2}, \\ \beta_{i-\frac{1}{2}} &= \frac{B_i - B_{i-\frac{1}{2}}}{\Delta/2} - \frac{B_{i-\frac{1}{2}} - B_{i-1}}{\Delta/2}, \\ \gamma_{i-\frac{1}{2}} &= -\left(B_{i-1} - \frac{B_{i-\frac{1}{2}} - B_{i-1}}{\Delta/2}\right) \end{aligned} \right\} \quad (2.7)$$

The terms in Eq. (2.7) may be interpreted as containing combinations of numerical approximations to the values of the source function and the τ derivative of the source function at the boundaries of the interval.

This form of the equation, in fact, can be obtained in another way starting from Eq. (2.4). Two successive integrations by parts transform the expression for I_i into the following equivalent form:

$$I_i = \left(B - \frac{\partial B}{\partial \tau} \right)_i + \left[I_{i-1} - \left(B - \frac{\partial B}{\partial \tau} \right)_{i-1} \right] e^{-\Delta} + \int_{\tau_{i-1}}^{\tau_i} \frac{\partial^2 B}{\partial \tau^2} e^{-(\tau_i - \tau)} d\tau, \quad (2.8)$$

in terms of values of the source function and the first two derivatives of the source function with respect to τ .

In an optically thin interval, the most important contribution arises from the terms I_{i-1} and B , which represent the transmitted intensity and the emission from the zone. The derivative terms cancel in this approximation; this is perhaps more directly indicated by Eq. (2.4). In the optically thick interval, which is the extreme opposite, only the first two terms evaluated at i are usually of significance. The terms from $i-1$ are strongly attenuated and $\partial^2 B / \partial \tau^2$ in the integral is usually small. In the limit, the diffusion approximation results from the term $\partial B / \partial \tau)_i$. Between limits, it is necessary to consider the integral term in Eq. (2.8).

If Δ is not too large, a representative mean value of the exponential in the interval may be taken to give for the integral of Eq. (2.8)

$$\int_{\tau_{i-1}}^{\tau_i} \frac{\partial^2 B}{\partial \tau^2} e^{-(\tau_i - \tau)} d\tau \cong e^{-\Delta/2} \left[\left(\frac{\partial B}{\partial \tau} \right)_i - \left(\frac{\partial B}{\partial \tau} \right)_{i-1} \right],$$

and thus the expression for intensity becomes

$$I_i = \left(B - \frac{\partial B}{\partial \tau} \right)_i + \left\{ \left[I_{i-1} - \left(B - \frac{\partial B}{\partial \tau} \right)_{i-1} \right] e^{-\Delta/2} + \left[\left(\frac{\partial B}{\partial \tau} \right)_i - \left(\frac{\partial B}{\partial \tau} \right)_{i-1} \right] \right\} e^{-\Delta/2}. \quad (2.9)$$

This expression has just the form of Eqs. (2.6) and (2.7) when the difference expressions are identified with the derivatives.

It is clear from the derivation of Eq. (2.6) that the resulting intensity is a positive quantity. With positive values for zone source functions, the linear interpolation expression assures that the integral contribution is always positive. Since the boundary intensity is always a positive quantity, the positivity of all intensities is assured.

In the diffusion approximation limit, however, Eq. (2.9) is to be preferred over Eqs. (2.6) and (2.7), since in this limit only quantities at interface i will survive, and

$$I_i = B_i - \frac{\partial B}{\partial \tau}_i ,$$

which can be evaluated more accurately than the corresponding difference approximation to the derivative of Eq. (2.7). The point is that B depends only on radial position and not on angle, so that an interpolation formula using τ is more artificial than one based on a radial quantity, such as

$$\frac{\partial E}{\partial \tau} = \mu \frac{\partial B}{\partial h} , \quad (2.10)$$

where

$$h = \int_0^r \sigma' dr .$$

The independent variable h depends only on r , so that angular integrations of I_i can be performed explicitly in the diffusion approximation, which takes account of the dependence on angle of Eq. (2.10). A difference approximation can also be based on this expression, assuming that B is linear in h , i. e.,

$$\left(\frac{\partial B}{\partial \tau} \right)_i \cong \frac{B_i - B_{i-\frac{1}{2}}}{h_i - h_{i-\frac{1}{2}}} \mu_i , \quad (2.11)$$

where $\mu_i = x_i/r_i$ is the cosine of the angle of the ray at the interface with radius r_i . The corresponding equation for the intensity is Eq. (2.6), in which

$$\left. \begin{aligned} \alpha_{i-\frac{1}{2}} &= B_i - \mu_i \frac{B_i - B_{i-\frac{1}{2}}}{h_i - h_{i-\frac{1}{2}}} , \\ \beta_{i-\frac{1}{2}} &= \mu_i \frac{B_i - B_{i-\frac{1}{2}}}{h_i - h_{i-\frac{1}{2}}} - \mu_{i-1} \frac{B_{i-\frac{1}{2}} - B_{i-1}}{h_{i-\frac{1}{2}} - h_{i-1}} , \\ \gamma_{i-\frac{1}{2}} &= - \left(B_{i-1} - \mu_{i-1} \frac{B_{i-\frac{1}{2}} - B_{i-1}}{h_{i-\frac{1}{2}} - h_{i-1}} \right) . \end{aligned} \right\} \quad (2.12)$$

In spherical geometry, however, μ varies along the ray, so the difference approximation in Eq. (2.11) is not identical with the linear-in- τ difference approximation. Consequently, Eq. (2.12) is different from Eq. (2.7). Although Eq. (2.12) is superior in the diffusion limit in that the surviving terms give the correct diffusion expression, unfortunately, for the general case, the positivity which applies to Eq. (2.7) is lost; consequently, it is not clear which expression is best. (In slab geometry, where μ does not change along the ray, the difference equation analogue of Eq. (2.10) is exact and the positivity of the equation resulting from the linear-in- h assumption is assured.) The greatest danger of negative intensity comes from regions of small optical depth; however, these are calculated by a limiting form of the equations, as described below. Equations (2.6) and (2.12) are solved in the STRANS subroutine further described in Section V. Should negative intensities result from the calculation, they are replaced by zero.

2.1.2. Special Calculation near $x = 0$

The source function profile shown in Fig. 2.2 fails to take into account all of the information available in the neighborhood of $x = 0$. Since the source function along the y -line displays symmetry about $x = 0$, it is clear that its derivative should be zero there, a condition violated by the preceding interpolation rule. Consequently, a special calculation is performed in the two intervals adjoining $x = 0$, which are formed by the double penetration of the zone by the y -line, as illustrated in Fig. 2.3a. In the half-intervals immediately adjacent to $x = 0$ (see Fig. 2.3b), the source is taken to be quadratic in x , the constants of which are determined by requiring that the derivative be zero at $x = 0$ and that the function take on the known source value at the center of the zone. The source in the remaining intervals is formed from the linear-in- x assumption. Since the interpolation function is contained within a single zone, the function in Fig. 2.3b has exactly the same form as a function of τ as it has as a function of x .

The quantity $x_{\frac{1}{2}}$ is the x -coordinate of the center of the zone having inner radius r_0 and radial thickness Δr (see Fig. 2.3a),

$$x_{\frac{1}{2}} = [\Delta r(r_0 + 0.25 \Delta r)]^{\frac{1}{2}},$$

and corresponds to the value of the source function $B_{\frac{1}{2}}$. Values of the source corresponding to $x = 0$ and $x = x_1$ are B_0 and B_1 .

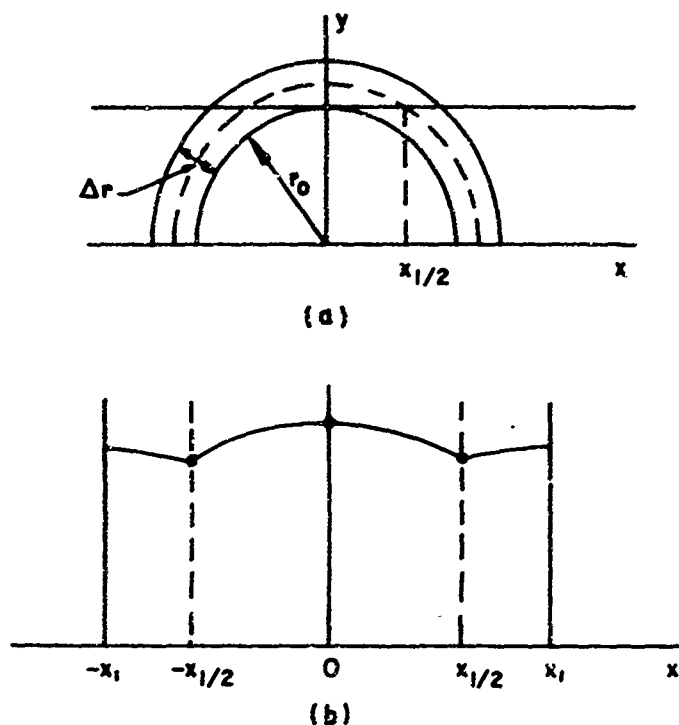


Fig. 2.3--Assumed spatial dependence of source function near $x = 0$

To illustrate the derivation of the intensities $I_0 = I(x = 0)$ and $I_1 = I(x = x_1)$, the following steps in the calculation of the source integral for the interval $-x_1 \leq x \leq 0$ are indicated. In this interval the source function is represented as two parts (see Fig. 2.3b)

$$B = a_- + b_- x, \quad -x_1 \leq x \leq -x_{1/2},$$

where

$$a_- = \frac{x_1 B_{1/2} - x_{1/2} B_1}{x_1 - x_{1/2}}, \quad b_- = \frac{B_{1/2} - B_1}{x_1 - x_{1/2}},$$

and

$$B = a_+ + b_+ x^2, \quad -x_{1/2} \leq x \leq 0,$$

where

$$a_+ = B_0, \quad b_+ = \frac{B_{1/2} - B_0}{x_{1/2}^2}.$$

In terms of these quantities, the integral of Eq. (2.4) is then

$$\int_{-x_1}^0 B e^{\sigma x} \sigma dx = a_- (e^{-\Delta_{\frac{1}{2}}} - e^{-\Delta}) + \frac{b_-}{\sigma} [(\Delta+1)e^{-\Delta} - (\Delta_{\frac{1}{2}}+1)e^{-\Delta_{\frac{1}{2}}}] + a_+ (1 - e^{-\Delta_{\frac{1}{2}}}) + \frac{b_+}{\sigma} [2 - (\Delta_{\frac{1}{2}}^2 + 2\Delta_{\frac{1}{2}} + 2)e^{-\Delta_{\frac{1}{2}}}] ,$$

where $\Delta_{\frac{1}{2}} = \sigma x_{\frac{1}{2}}$ and $\Delta = \sigma x_1$. Substitution and reduction gives the following expression for I_0 :

$$I_0 = B_0 + F + e^{-\Delta_{\frac{1}{2}}} [G - (\Delta_{\frac{1}{2}} + 1)F] + e^{-\Delta} [I(-x_1) - B_1 - G] ,$$

where

$$F = \frac{2(B_{\frac{1}{2}} - B_0)}{\Delta_{\frac{1}{2}}^2} \quad \text{and} \quad G = \frac{B_1 - B_{\frac{1}{2}}}{\Delta - \Delta_{\frac{1}{2}}} . \quad (2.13)$$

In an analogous fashion, I_1 is obtained by integration over the interval $0 \leq x \leq x_1$,

$$I_1 = B_1 - G + e^{-(\Delta - \Delta_{\frac{1}{2}})} [G - (1 - \Delta_{\frac{1}{2}})F] + e^{-\Delta} [I_0 - B_0 - F] . \quad (2.14)$$

Equations (2.13) and (2.14) are evaluated in the "top slice" portions of the code when the y-line integration reaches $x = 0$.

2.1.3. Small-optical-depth Expansion

If the optical depth is very small, the intensity expression in Eq. (2.4) takes a much simpler form,

$$I_i = I_{i-1} + \left[\frac{1}{4} B_i + \frac{1}{4} B_{i-1} + \frac{1}{2} B_{i-\frac{1}{2}} - I_{i-1} \right] \Delta . \quad (2.15)$$

Although this result is the limiting form of Eqs. (2.6) and (2.7), but not of Eqs. (2.6) and (2.12), the terms must cancel through second order in an expansion in Δ before the first surviving term, derived in part from the quadratic terms of the exponentials, is obtained. Consequently, for sufficiently small argument, the finite number of figures used in the exponential will render the result inaccurate. For the exponential from the IBM-7044 system, this restricts the argument to a number greater than $\sim 2 \times 10^{-4}$; but with the lower-accuracy fast exponential (see Section V), the argument must be somewhat larger. Since the relative error approximately equals the argument of the exponential, the criterion for using Eq. (2.15) in the STRANS subroutine is now set at $\Delta \leq 2 \times 10^{-2}$. With this value, the greatest relative error arising from the expansion and cancellation should be on the order of 1 percent.

For the quadratically interpolated intervals near $x = 0$, the small-optical-depth result is different from Eq. (2.15) as follows:

$$\begin{aligned} I_0 &= I(-x_1) + \left[\frac{1}{2} B_1 + \frac{1}{2} B_{\frac{1}{2}} - I(-x_1) \right] \Delta + \left(\frac{2}{3} B_0 - \frac{1}{2} B_1 - \frac{1}{6} B_{\frac{1}{2}} \right) \Delta_{\frac{1}{2}}, \\ I_1 &= I_0 + \left[\frac{1}{2} B_1 + \frac{1}{2} B_{\frac{1}{2}} - I_0 \right] \Delta + \left(\frac{2}{3} B_0 - \frac{1}{2} B_1 - \frac{1}{6} B_{\frac{1}{2}} \right) \Delta_{\frac{1}{2}}. \end{aligned} \quad (2.16)$$

The same criterion for performing the calculation of Eq. (2.16) rather than that of Eqs. (2.13) and (2.14) is used, i.e., $\Delta \leq 2 \times 10^{-2}$.

2.1.4. Y = 0 Ray

The special case of the ray passing through the center of the sphere and having $y = 0$ is required (as described below) in each use of the STRANS subroutine. Equation (2.12) is still appropriate for this case but in a simplified form. For inwardly directed photons, $\mu = -1$; for outwardly directed photons, $\mu = +1$. A separate section of STRANS is used for the $y = 0$ calculation in order to simplify the code and to take into account that the angular integration need not be performed.

2.1.5. Boundary Conditions

Integration of the transport equation to obtain intensities is performed through the thickness of a spherical shell, called a "trans" region. At intersections of y -lines with the inner and outer surfaces of each shell it is necessary to supply the starting value of the intensity I_{i-1} required in Eq. (2.6). Three classes of boundary conditions occur:

1. The trans region outside boundary coincides with outside radius R_{IB+1} of the SPUTTER calculation and a prescribed

function, I_0 , is applied as an outer boundary value:

$$I(R_{IB+1}, \mu) = I_0, \quad \mu \leq 0. \quad (2.17)$$

The trans region inside boundary is at the center of the sphere, $R = 0$.

2. The center of the sphere provides a boundary condition for the $y = 0$ ray at $R = 0$ in the trans region. At $R = 0$, the intensity is isotropic, giving the condition for starting the outward-directed ray calculation:

$$I(R = 0, \mu = +1) = I(R = 0, \mu = -1). \quad (2.18)$$

3. All other trans boundaries are bounded by regions in which the diffusion approximation is valid (see Section III). Consequently, the boundary surface intensities on contiguous trans regions inside or outside of a diffusion region are given by the diffusion approximation intensity derived in Section III:

$$I_{i-1} = B_{i-1} - \mu_{i-1} \left(\frac{\partial B}{\partial h} \right)_{i-1}. \quad (2.19)$$

2.2. Y-LINE POSITIONING REQUIREMENTS

The correct placement of y-lines through regions which are changing rapidly in temperature and/or optical depths is important for an economical and accurate solution of the transport equations using the direct integration method. The advantage of being able to locate y-lines only where they are needed is a decrease in computational time by reducing the number of y-lines calculated.

The decision as to where to place a group of rays depends on the radial position of the region in question. The inner core (or zone) will be the least resolved, but, in general, this is a region of isothermality. For example, in fireball calculations, there is a central diffusion region bounded by a region having rapidly changing conditions due to radiative fronts and hydrodynamic shocks. Under these conditions, there are fewer y-lines placed through the central core, many through the transition regions, and none outside the zones containing sources.

The following description of our placement criteria in SRADTN and STRANS is based on these considerations.

2.2.1. X-storage Limitation and Frequency-independent Criteria in SRADTN

In order to remove the repetitious calculation of x -values at intersections of the y -lines with radii $x = \sqrt{R^2 - Y^2}$, a storage array is set up for the x 's as well as for the quantity y^2 (used in STRANS). The size of this array is limited by available storage; the present limit of 2400 in the x -block allows for approximately 70 y -lines. The principal criterion for selecting a set of y -lines to be used in STRANS is to place y -lines at boundaries where the temperature is changing. For example, if $\log(\theta_{i+1}/\theta_i)$ is greater than CVB (CVB = 0 gives the maximum number of y -lines), a y -line is placed at that boundary, but if the gradient of $\log \theta$ is less than CVB, that zone is skipped. The practical use of this criterion will result in reducing the calculational time for y -lines inside isothermal regions. No y -lines are used in regions outside zones with the temperature less than 0.05 eV (0.025 eV is the temperature for ambient air).

2.2.2. Transport Criteria per Frequency Group in STRANS

In the transport subroutine (STRANS), y -lines from the set established in SRADTN are selected using criteria based on the frequency-dependent-source and optical-depth gradients. If a diffusion region having an outer boundary r_D exists inside the transport region, y -lines are placed as near as possible to $0.5 r_D$, $0.75 r_D$, and r_D penetrating the diffusion region. In addition, if inside of the transport region the gradient inequalities

$$\frac{(b_j \theta^4)_{i+\frac{1}{2}} - (b_j \theta^4)_{i-\frac{1}{2}}}{(b_j \theta^4)_{i+\frac{1}{2}} + (b_j \theta^4)_{i-\frac{1}{2}}} > GL$$

and

$$\frac{\tau_i - \tau_{i-1}}{\tau_i + \tau_{i-1}} > GL$$

are satisfied, where the input number GL is usually around 0.3, a y -line is added at the interface i . Finally, in isothermal source regions outside the diffusion core, every fifth ray is selected. These selection rules could be refined, but at the present time they afford a reasonable representation to be used in the angular integration of the intensities.

2.3. ANGULAR INTEGRATIONS

Intensities calculated in the integrations along y-lines are used in several ways in the SPUTTER calculation. In addition to displaying the intensities in a special edit (see Section 5.5), integrals over angle of the intensity are used in the calculation of the evolution of the system in time. Additional integral quantities are of interest in evaluating the progress of the problem and in preparing thermal environment data for subsequent calculations. The desired integral quantities are formulated in Section 2.3.1.

To calculate the desired integral quantities from the intensities obtained in the integrations along a discrete sampling of y-lines, as described in Section 2.1, it is necessary to perform numerical quadratures. At a given interface radius no regular interval in the angle variable (either μ , x , or y) is available. Consequently, the numerical quadrature is based on an interpolation expression, described in Section 2.3.2, in which no regularity can be assumed. Finally, in Section 2.3.3, the numerical quadrature formulas are given.

2.3.1. Integral Formulations of Flux, Energy, and Pressure

One of the most important of the angular integrals of intensity is the radiative flux, the divergence of which gives the radiative contribution to the rate of change of the material energy. The net flux is a vector quantity, the component of which in the direction of the unit vector $\vec{r}_1$, $\phi(\vec{r}_1)$ (in ergs/cm²-sec), is given by the expression

$$\phi(\vec{r}_1) = c \int I \cos \Theta \, d\Omega \quad , \quad (2.20)$$

which also depends on the spatial position $\vec{r}$.

In Eq. (2.20) the intensity is a function of position $\vec{r}$ and direction, denoted by the unit vector $\vec{\hat{r}}$, the Cartesian components of which can be expressed in terms of the polar angle θ between $\vec{\hat{r}}$ and the radial direction $\vec{k}$ and the azimuthal angle ϕ measured between the meridian planes of $\vec{\hat{r}}$ and an arbitrary direction $\vec{j}$ normal to $\vec{k}$, and hence

$$\vec{\hat{r}} = \cos \theta \vec{k} + \sin \theta (\sin \phi \vec{i} + \cos \phi \vec{j}) \quad .$$

The angle between $\vec{\hat{r}}$ and $\vec{r}_1$ is Θ , so that $\cos \Theta = \vec{\hat{r}} \cdot \vec{r}_1$, and the element of solid angle is $d\Omega = d\phi \sin \theta \, d\theta$. The net flux in the $\vec{r}_1$ direction is given

by the integration of $d\Omega$ over the entire sphere. The forward and backward currents, ϕ^+ and ϕ^- , however, are obtained by integration over the hemispheres H^+ and H^- about $\vec{r}_1$ and about $-\vec{r}_1$, respectively; i. e.,

$$\phi^+(\vec{r}_1) = c \int_{H^+} I \cos \Theta \, d\Omega \quad , \quad (2.21)$$

$$\phi^-(\vec{r}_1) = -c \int_{H^-} I \cos \Theta \, d\Omega \quad .$$

In terms of these quantities, the net flux is

$$\phi(\vec{r}_1) = \phi^+(\vec{r}_1) - \phi^-(\vec{r}_1) \quad . \quad (2.22)$$

In spherical geometry, in which I depends on θ but not on ϕ , the integration over azimuthal angle can be performed, and the result depends only on the radial distance r and the component direction $\vec{r}_1$. In order to evaluate the progress of the calculation and to provide relevant thermal environment data for subsequent calculations, three representative currents are formed--the forward and backward currents in the radial direction and the current in the direction normal to the radius vector. Only one such lateral current is needed since the currents in all lateral directions are the same for spheres. For the forward current, ϕ^+ , the quantities in Eq. (2.21) are $\vec{r}_1 = \vec{k}$, $\cos \Theta = \cos \theta = \mu$, and the integral is over $0 \leq \theta \leq \pi/2$ and $0 \leq \phi \leq 2\pi$; thus

$$\phi^+ = 2\pi c \int_0^1 I \mu \, d\mu \quad . \quad (2.23)$$

For the backward current, ϕ^- , the quantities are $\vec{r}_1 = -\vec{k}$, $\cos \Theta = \mu$, and the integral is over $\pi/2 \leq \theta \leq \pi$, $0 \leq \phi \leq 2\pi$; thus

$$\phi^- = -2\pi c \int_{-1}^0 I \mu \, d\mu \quad . \quad (2.24)$$

For the lateral current, ϕ^0 , the forward-current expression of Eq. (2.21) may be evaluated by taking $r_1 = \bar{r}$, $\cos \Theta = \sqrt{1 - \mu^2} \sin \phi$, and $0 \leq \Theta \leq \pi$, $0 \leq \phi \leq \pi$, so that

$$\phi^0 = 2c \int_{-1}^1 I \sqrt{1 - \mu^2} d\mu . \quad (2.25)$$

In spherical geometry the term entering the energy equation, $\nabla \cdot \vec{\phi}$, in which $\vec{\phi}$ is the radiative net flux vector, takes the form

$$\frac{1}{r} \frac{\partial}{\partial r} (r^2 \phi_r) ,$$

in which ϕ_r is the net flux component in the radial direction $\hat{k}$. Two of the above quantities are related to ϕ_r in that

$$\phi_r = \phi^+ - \phi^- . \quad (2.26)$$

Consequently, of the three quantities, ϕ_r , ϕ^+ , and ϕ^- , only two, ϕ_r and ϕ^+ , are formed.

Two additional angular integrals of the intensity are useful in evaluating the progress of the transport calculation and, in addition, they are used in more accurate formulations of the radiation transport equation. The first of these quantities, the radiation energy density, E_R (in ergs/cm³), gives a quantitative measure of the energy stored in the radiation field for comparison with the material energy. If E_R is not negligible (as assumed to be the case in this formulation), it should be taken into account in the radiation transport equation in which retardation is included (see Section 2.1 of Volume VI). The same angular integral also plays a role in the Thomson scattering integral of the Compton scattering by free electrons, as discussed in Section 3.1 of Volume VII (the effect of which is also neglected in this formulation).

The radiation energy is given by

$$E_R = \int I d\Omega ,$$

which, for spherical geometry, in which the azimuthal integration can be

performed, reduces to

$$E_R = 2\pi \int_{-1}^1 I d\mu . \quad (2.27)$$

The second quantity is the radiation pressure, $P_R(\vec{r}_1)$ (in ergs/cm⁻³), which is defined as the net rate of transfer of the radiant momentum component in the $\vec{r}_1$ direction across the unit surface whose normal is also in the $\vec{r}_1$ direction. In terms of $\cos \theta = \vec{r}_1 \cdot \vec{r}$, the cosine of the angle which the photon beam makes with the surface normal, the pressure exerted across $\vec{r}_1$ by the radiation field is

$$P_R(\vec{r}_1) = \int I \cos^2 \theta d\Omega ,$$

in which the integral over solid angle extends over the complete sphere.

The pressure $P_R(\vec{r}_1)$ is also obtained from the radiation pressure tensor $\tilde{P}$ by the operations $\vec{r}_1 \cdot \tilde{P} \cdot \vec{r}_1$. For spherical geometry in which the azimuthal angle integration can be performed, all of the off-diagonal elements of the pressure tensor vanish, whereas all of the diagonal elements can be expressed in terms of the diagonal element in the radial direction,

$$P_R(\vec{k}) = 2\pi \int_{-1}^1 I \mu^2 d\mu \equiv P_R , \quad (2.28)$$

and the radiation energy integral of Eq. (2.27). Furthermore, the integral of Eq. (2.28) is also contained in the expression for the Thomson limit of the Compton scattering into the beam in both plane and spherical geometries.

In summary, the radiation integrals are calculated in the radiation subroutine STRANS in terms of the following quantities: ϕ^+ , Eq. (2.23); ϕ^0 , Eq. (2.25); ϕ_r , Eq. (2.26); E_R , Eq. (2.27); and P_R , Eq. (2.28).

2.3.2. Angular Interpolation of Intensities

To form numerical approximations to the angular integrals derived above, it is necessary to select a quadrature formula. Equivalently, the rule must be specified for the angular interpolation of intensities at a given radius between values calculated at different values of x (or μ) in the integrations along y -lines. Unfortunately, from the point of view of the

angular integration, as a result of the application of the y-line selection criteria, the values of x are not regularly spaced so no simple high-order rule is easily applicable. In the current version, the interpolation is performed within the interval between adjacent x values by making use of the two values of intensity at the end points of the interval only.

An accurate integration will result if the interpolation formula conforms to the actual angular dependence of the intensity. To illustrate the range of possible dependencies which may occur in a fireball calculation, Figs. 2.4 through 2.7 show a selection of curves of angular dependence of intensity corresponding to selected radii and photon frequencies. It is clear from these curves that no simple dependence will be universally successful. In fact, these curves point up the desirability, in a more advanced code, of having an interpolation formula in which information from several angular positions is used.

In the preparation of the current version of the STRANS subroutine, two interpolation rules were investigated: linear-in- μ^2 and linear-in- μ dependence. Although the μ^2 interpolation is suitable for some cases, such as that of Fig. 2.6, the linear-in- μ dependence approximates the behavior of most of the cases illustrated. Furthermore, both the diffusion approximation and the transparent isothermal regime have this dependence as a limiting value. Consequently, the linear-in- μ interpolation formula has been incorporated into the STRANS routine.

2.3.3. Numerical Quadrature Formulas

The contribution of the angular interval (μ_i, μ_{i+1}) to these integrals at position r is derived in the linear-in- μ approximation. The intensity in this approximation is

$$I = a + b\mu, \quad \mu_i \leq \mu \leq \mu_{i+1},$$

where

$$a = \frac{\mu_{i+1} I_i - \mu_i I_{i+1}}{\mu_{i+1} - \mu_i} = \frac{x_{i+1} I_i - x_i I_{i+1}}{x_{i+1} - x_i},$$

$$b = \frac{I_{i+1} - I_i}{\mu_{i+1} - \mu_i} = r \frac{I_{i+1} - I_i}{x_{i+1} - x_i};$$

I_i is the value of the intensity at μ_i . According to the y-line integration

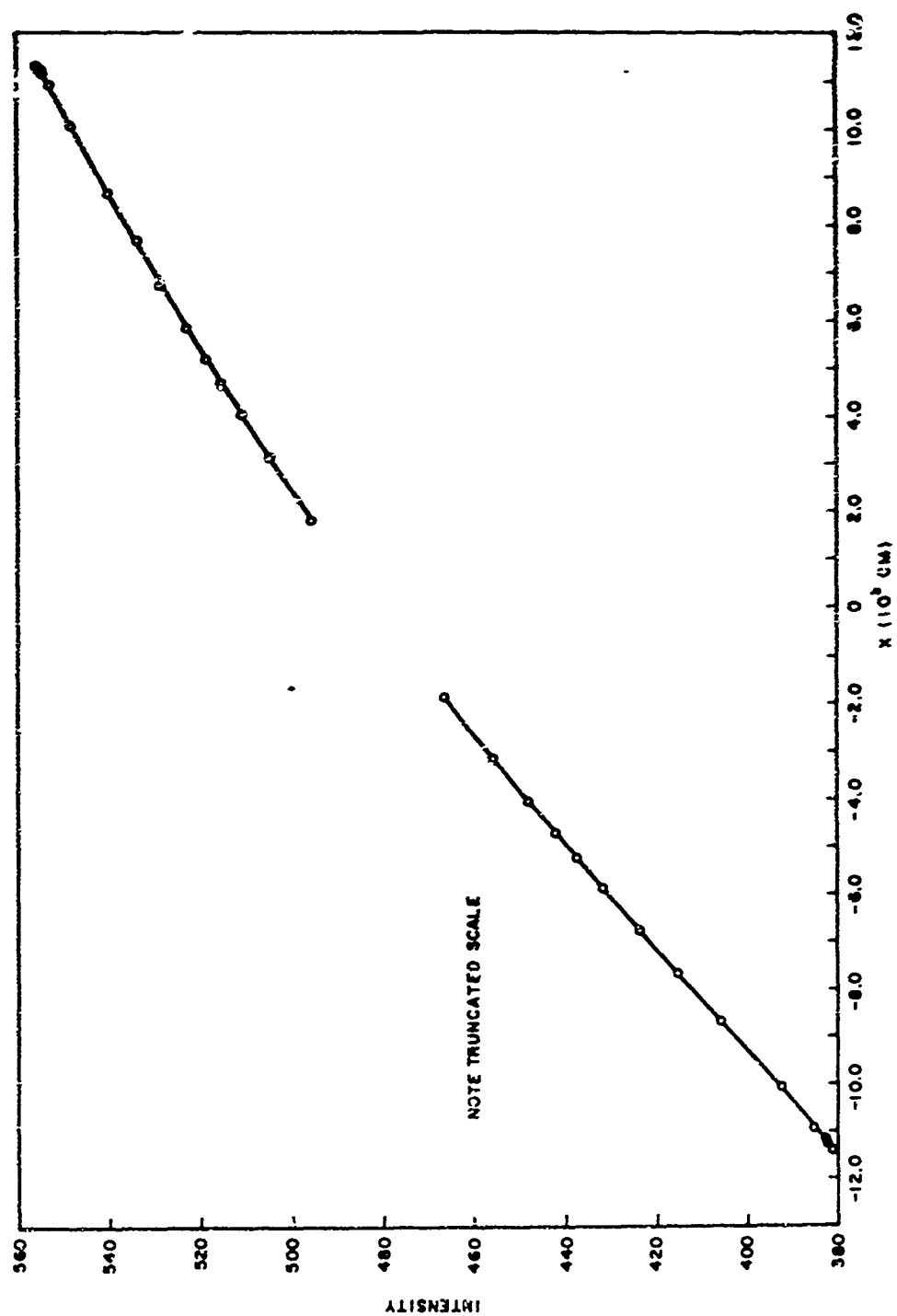


Fig. 2.4--Example of angular dependence of intensity

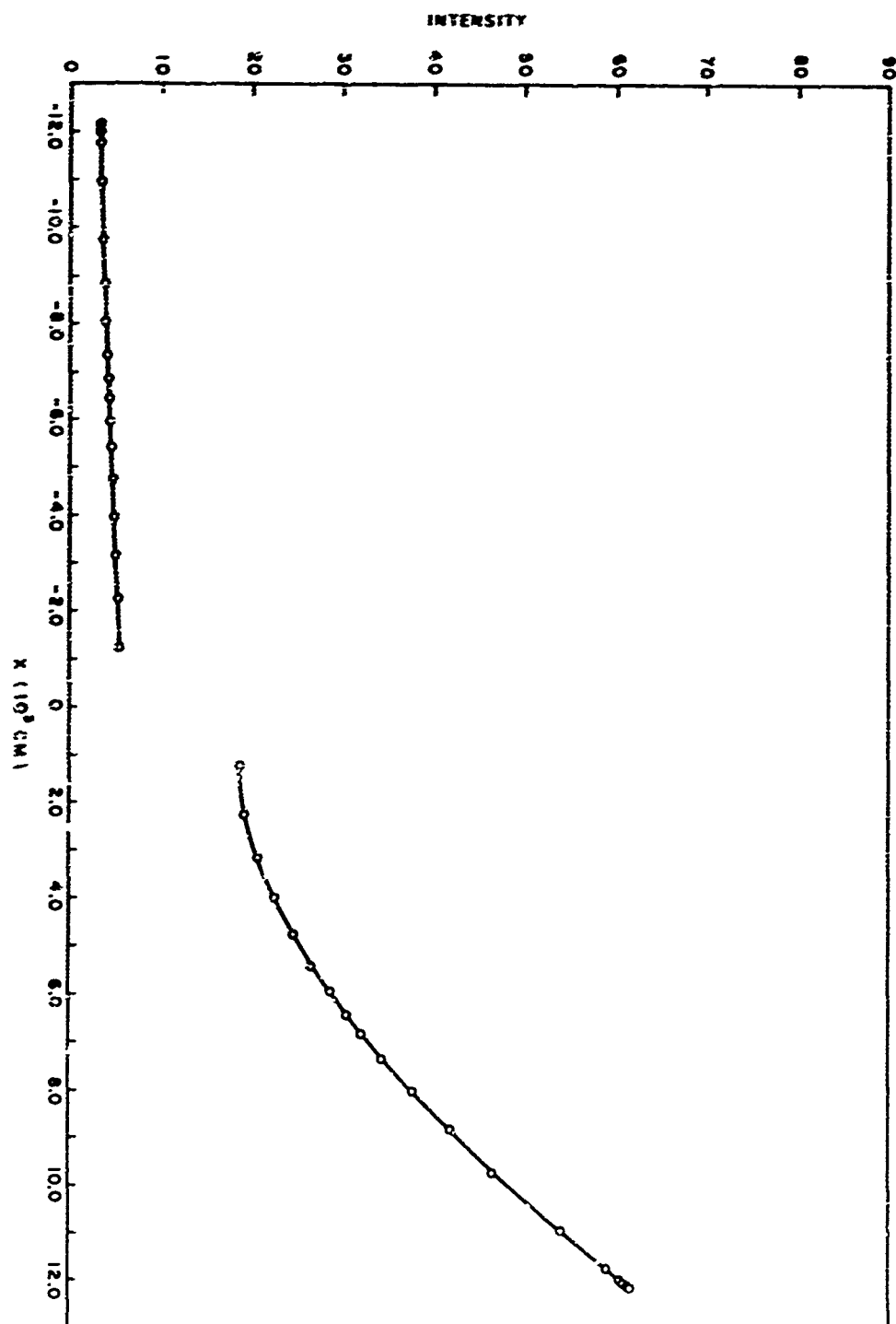


Fig. 2.5--Example of angular dependence of intensity

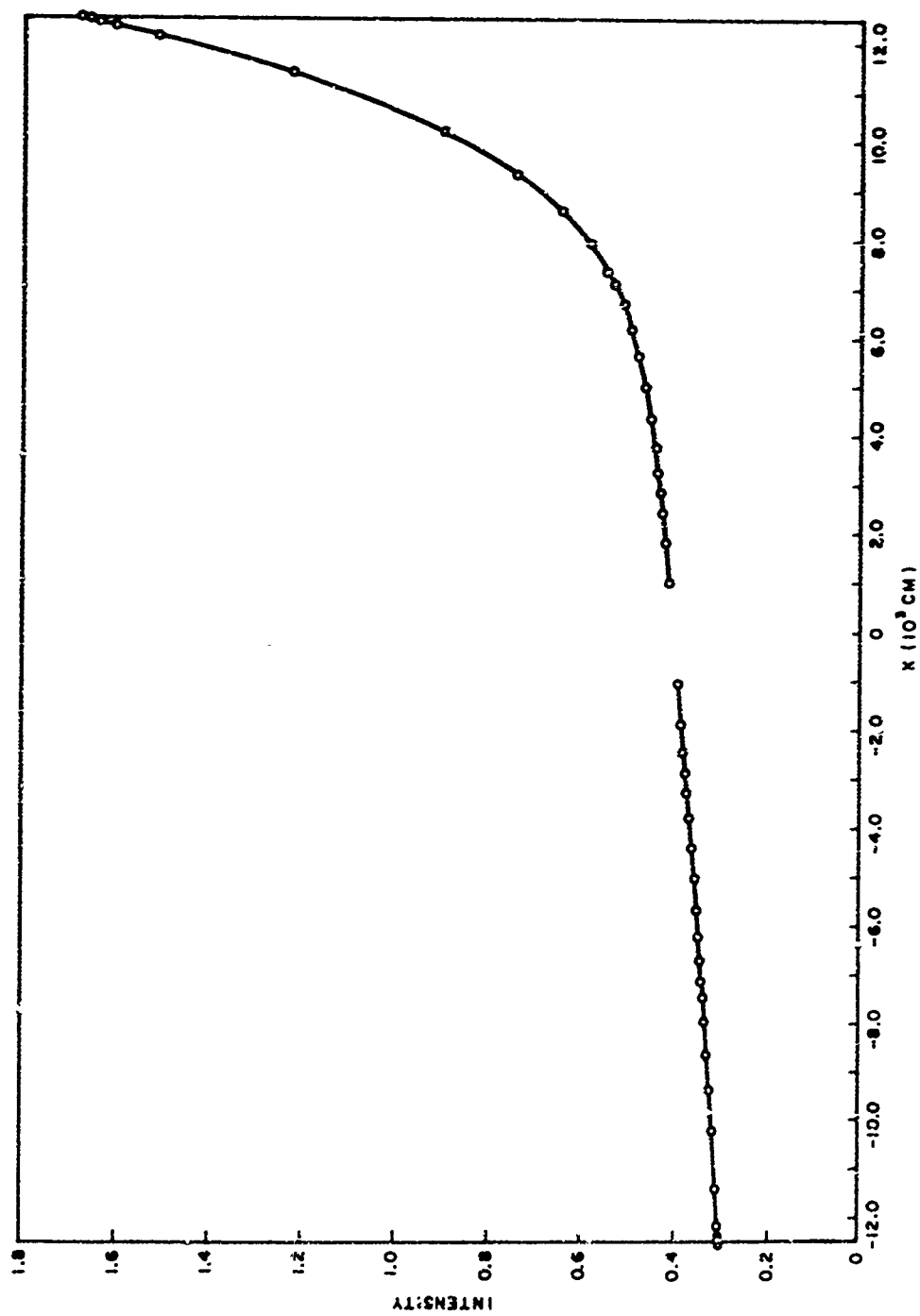


Fig. 2.6--Example of angular dependence of intensity

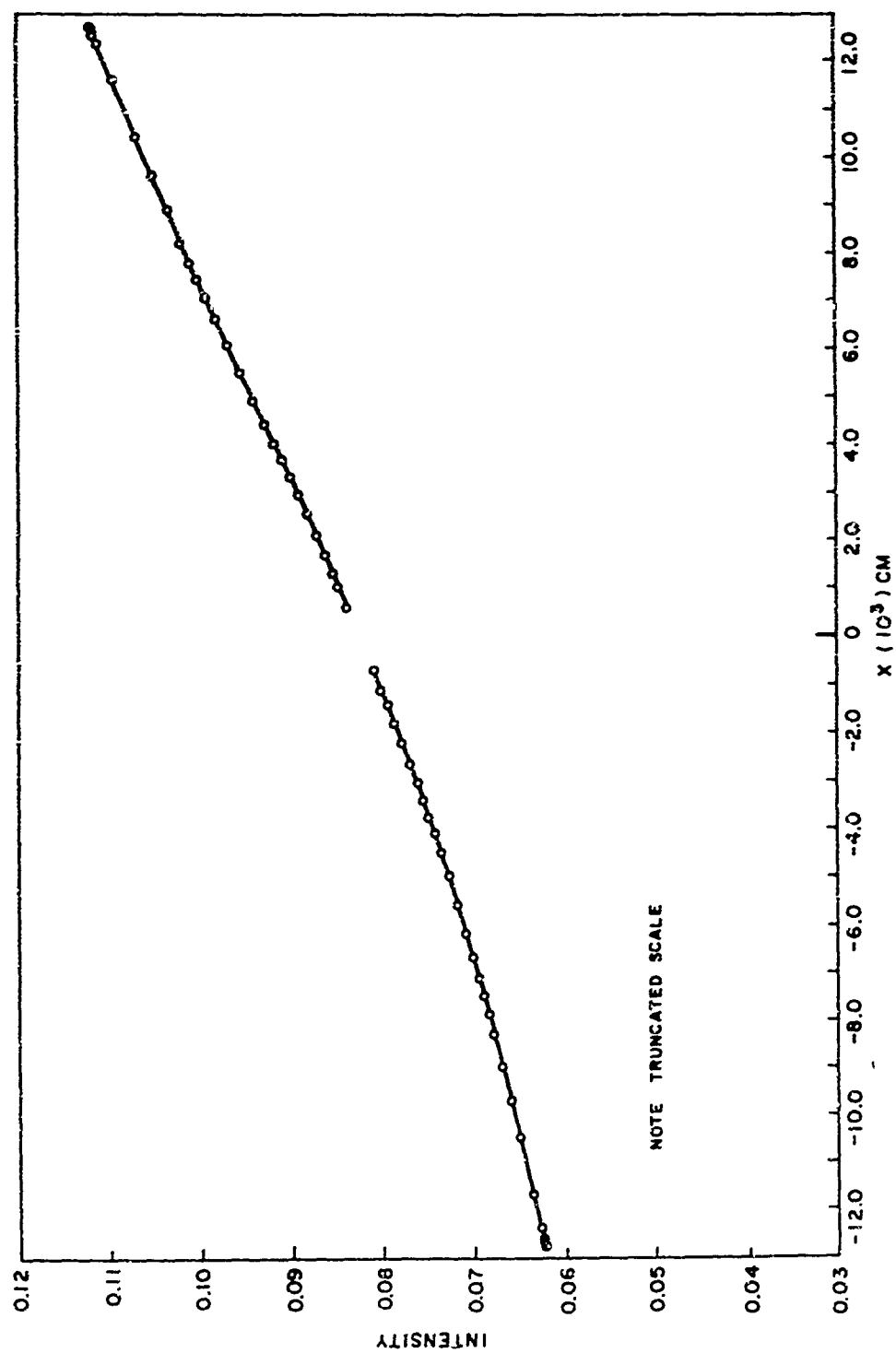


Fig. 2.7--Example of angular dependence of intensity

scheme, μ_i and μ_{i+1} correspond to the angles formed at the intersections of two adjacent y-lines with the interface radius, at which point the integrals are to be formed. Two intervals are symmetrically located about $\mu = 0$ by a pair of y-lines, as shown in Fig. 2.8. It is clear from the figure that

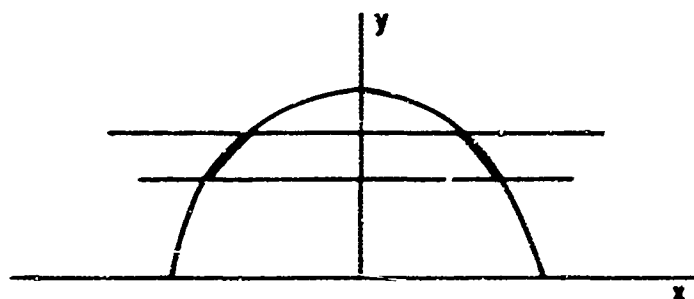


Fig. 2.8--Angular intervals between adjacent y-lines

these two intervals can be treated together in the integrations over the interval $-1 \leq \mu \leq 1$. Denoting intensities with positive μ by I^+ and those with negative μ with I^- , the integrals can be grouped according to whether the integrand is even or odd. For even integrands,

$$\int_{-1}^1 I f(\mu) d\mu = \int_0^1 (I^+ + I^-) f(\mu) d\mu, \quad (2.29)$$

where $f(-|\mu|) = f(|\mu|)$, and for odd integrands,

$$\int_{-1}^1 I f(\mu) d\mu = \int_0^1 (I^+ - I^-) f(\mu) d\mu, \quad (2.30)$$

where $f(-|\mu|) = -f(|\mu|)$, $I(|\mu|) \equiv I^+(\mu)$ and $I(-|\mu|) \equiv I^-(\mu)$ in which $0 \leq \mu \leq 1$.

For a given radius r , the quantities μ , x , and y associated with the interval $(|\mu_i|, |\mu_{i+1}|)$ satisfy the following inequalities:

$$|\mu_{i+1}| > |\mu_i|, \quad x_{i+1} > x_i, \quad y_i > y_{i+1},$$

where $x_i = |\mu_i| r$ and $y_i = \sqrt{r^2 - x_i^2}$.

In terms of the above quantities, the contributions to the integrals of the interval $(|\mu_i|, |\mu_{i+1}|)$ in the linear-in- μ approximation are obtained as follows:

Forward Flux, ϕ^+ (Eq. (2.23)):

$$\begin{aligned} \int_{\mu_i}^{\mu_{i+1}} I^+ \mu d\mu &= \frac{a^+}{2} (\mu_{i+1}^2 - \mu_i^2) + \frac{b^+}{3} (\mu_{i+1}^3 - \mu_i^3) \\ &= \frac{(x_{i+1} - x_i)}{6r^2} [(x_{i+1} + 2x_i) I_i^+ + (2x_{i+1} + x_i) I_{i+1}^+] \end{aligned} \quad (2.31)$$

Net Flux, ϕ_r (Eq. (2.26)):

$$\begin{aligned} \int_{\mu_i}^{\mu_{i+1}} (I^+ - I^-) \mu d\mu &= \frac{(a^+ - a^-)}{2} (\mu_{i+1}^2 - \mu_i^2) + \frac{(b^+ - b^-)}{3} (\mu_{i+1}^3 - \mu_i^3) \\ &= \frac{(x_{i+1} - x_i)}{6r^2} [(x_{i+1} + 2x_i)(I_i^+ - I_i^-) \\ &\quad + (2x_{i+1} + x_i)(I_{i+1}^+ - I_{i+1}^-)] \end{aligned} \quad (2.32)$$

Lateral Flux, ϕ^0 (Eq. (2.25)):

$$\begin{aligned} \int (I^+ + I^-) \sqrt{1 - \mu^2} d\mu &= \frac{(a^+ + a^-)}{2r^2} \left[x_{i+1} y_{i+1} - x_i y_i \right. \\ &\quad \left. + r^2 \left(\sin^{-1} \frac{x_{i+1}}{r} - \sin^{-1} \frac{x_i}{r} \right) \right] \\ &\quad + \frac{(b^+ + b^-)}{3r^3} (y_i^3 - y_{i+1}^3) \end{aligned} \quad (2.33)$$

Radiation Energy, E_R (Eq. (2.27)):

$$\int_{\mu_i}^{\mu_{i+1}} (I^+ + I^-) d\mu = (a^+ + a^-)(\mu_{i+1} - \mu_i) + \frac{(b^+ + b^-)}{2} (\mu_{i+1}^2 - \mu_i^2)$$

$$= \frac{(x_{i+1} - x_i)}{2r} (I_i^+ + I_i^- + I_{i+1}^+ + I_{i+1}^-) \quad (2.34)$$

Radiation Pressure, P_R (Eq. (2.28)):

$$\int_{\mu_i}^{\mu_{i+1}} (I^+ + I^-) \mu^2 d\mu = \frac{(a^+ + a^-)}{3} (\mu_{i+1}^3 - \mu_i^3) + \frac{(b^+ + b^-)}{4} (\mu_{i+1}^4 - \mu_i^4)$$

$$= \frac{1}{12r^3} [(I_i^+ + I_i^-)(\gamma - 4x_i^3) + (I_{i+1}^+ + I_{i+1}^-)(4x_{i+1} - \gamma)] \quad (2.35)$$

where $\gamma = (2r^2 - y_i^2 - y_{i+1}^2)(x_i + x_{i+1})$.

SECTION III

THE DIFFUSION APPROXIMATION

The radiation transport equation in the limiting case of an optically thick medium admits of the diffusion approximation in which the expression for the radiation intensity is greatly simplified; only the local properties affect the radiation intensity at the point in question. An expansion of the radiation source function B_ν about the point r permits the intensity $I_\nu(\mu)$ of the radiation field in the direction making an angle, whose cosine is μ , with the radial direction to be formed.

3.1. DIFFERENTIAL FORM OF THE DIFFUSION FLUX

The general solution of the transport equation forms the starting point of the derivation. The integral expression for the intensity applicable to all geometries is

$$I(\tau) = \int_{-\infty}^{\tau} B(\tau') e^{-(\tau-\tau')} d\tau' ,$$

where $\tau = \int_0^r \kappa_\nu \rho ds$, in which κ_ν is the monochromatic absorption coefficient (in cm^2/g) at frequency ν . By expanding $B(\tau')$ in series about the point τ , i. e.,

$$B(\tau') = B(\tau) + \frac{\partial B}{\partial \tau} (\tau' - \tau) + \frac{1}{2} \frac{\partial^2 B}{\partial \tau^2} (\tau' - \tau)^2 + \dots ,$$

the intensity becomes

$$I = B - \frac{\partial B}{\partial \tau} + \frac{1}{2} \frac{\partial^2 B}{\partial \tau^2} - \dots$$

or

$$I = B - \frac{\mu}{\kappa \rho} \frac{\partial B}{\partial r} + \frac{\mu^2}{\kappa \rho} \frac{\partial}{\partial r} \left(\frac{1}{\kappa \rho} \frac{\partial B}{\partial r} \right) - \dots$$

for spherically symmetric geometry.

The diffusion approximation results from retention of only the first two terms, so that the diffusion intensity is

$$I = B - \frac{\mu}{\kappa \rho} \frac{\partial B}{\partial r} \quad (3.1)$$

and the monochromatic diffusion flux ϕ_r and radiation energy E_R are

$$\phi_r = 2\pi c \int_{-1}^1 I \mu \, d\mu = -\frac{4\pi c}{3} \frac{1}{\kappa \rho} \frac{\partial B}{\partial r} \quad (3.2)$$

$$E_R = 2\pi \int_{-1}^1 I \, d\mu = 4\pi B$$

3.2. CRITERIA FOR THE SELECTION OF DIFFUSION REGIONS

The criteria for the validity of the diffusion approximation can be obtained by examination of the above derivation--namely, that the expansion of the source function be justified and that the expansion converge rapidly so that the neglect of all but the leading terms is valid. If the source function is linear in τ' at the point in question and is also linear for a distance of the order of one mean free path on either side of the point, the criteria are satisfied. These criteria are difficult to quantify since they refer to a finite region containing the point in question. If all of the terms (or a large number of them) were checked for rapid convergence, this would imply (making a smoothness assumption) that the diffusion criterion is met. It is not possible with finite differences, however, to form the higher-order local derivative approximations.

In the SPUTTER subroutine SRADTN, criteria designed to give an indication of both the local and nonlocal behavior have been employed. First, at the zone interface at which the intensity and flux are to be evaluated, the inequality

$$\left| \frac{\partial B}{\partial h} \right| \ll B \quad (3.3)$$

is required. In this expression $h = \int \kappa \rho \, dr$ is the radial optical depth; the derivative is approximated by the centered first difference of B between adjacent zones. The resulting expression, of course, contains some non-local aspects resulting from the finite difference approximation, which ensures that when neighboring zones are optically thick, no nonlocal source perturbation is close enough to invalidate the diffusion approximation.

However, to provide for the cases when a source perturbation is located a fraction of an optical depth from an interface meeting the condition of Eq. (3.3), the diffusion region is constricted. Starting from the closest interfaces outside the diffusion region (where Eq. (3.3) is not satisfied), all of those interfaces lying within a prescribed number of mean free paths are removed from the diffusion region.

The criteria used in SPUTTER are controlled by input numbers. The criterion of Eq. (3.3) uses the input number HCB:

$$|TG| < HCB \times Y2, \quad (3.4)$$

where TG is the difference approximation to the gradient and Y2 is the source function evaluated at the interface by interpolation. The second criterion uses the input number HVB (in mean free paths). If

$$|Q3(I) - Q3(J)| > HVB, \quad (3.5)$$

then the interface with index J which satisfies Eq. (3.4) is removed from the diffusion region. In Eq. (3.5), Q3 is the radial optical depth and I is the index of the nondiffusion interface adjoining the diffusion region.

Although the diffusion calculation is considerably faster than the transport, the establishment of two transport regions separated by the single zone requires still more calculation to set up y-lines and perform bookkeeping operations. To avoid the duplicate setup calculations required for an additional transport region, a test is made to eliminate a diffusion region consisting of a single zone.

3.3. DIFFERENCE FORM OF THE DIFFUSION FLUX

The diffusion intensity derived above is

$$I = B - \frac{\mu}{\kappa \rho} \frac{\partial B}{\partial r}.$$

In the group frequency approximation of SPUTTER, the intensity integrated over a frequency interval (ν_j, ν_{j+1}) is required:

$$\int_{\nu_j}^{\nu_{j+1}} I \, d\nu = \int_{\nu_j}^{\nu_{j+1}} B \, d\nu - \frac{\mu}{\rho} \frac{\partial \theta^4}{\partial r} \int_{\nu_j}^{\nu_{j+1}} \frac{\partial B}{\partial \theta^4} \frac{d\nu}{\kappa_\nu}.$$

In terms of the partial Rosseland mean absorption coefficient

$$\kappa_j = \frac{\int_{\nu_j}^{\nu_{j+1}} \frac{\partial B}{\partial \theta^4} d\nu}{\int_{\nu_j}^{\nu_{j+1}} \frac{\partial B}{\partial \theta^4} \frac{d\nu}{\kappa_\nu}},$$

the frequency group intensity becomes

$$I_j = \int_{\nu_j}^{\nu_{j+1}} I d\nu = \int_{\nu_j}^{\nu_{j+1}} B d\nu - \frac{\mu}{\rho} \frac{\partial \theta^4}{\partial r} \frac{\int_{\nu_j}^{\nu_{j+1}} \frac{\partial B}{\partial \theta^4} d\nu}{\kappa_j} \quad (3.6)$$

It is desired to evaluate this quantity at each zonal interface in the mesh. Since the known quantities are the zone temperatures and densities, the absorption coefficients κ_j and the integrated source functions $X_6 = \int B d\nu$ are first evaluated not at the interfaces but at positions representative of each zone.

The question remains as to how best to approximate the derivatives and interpolate for the coefficients in Eq. (3.6) at the interfaces from the quantities available at zone positions. The answer depends on the temperature and density profile across the interface from which these terms could be calculated directly. Since the profile is not known, we must select a reasonable approximation which will permit the calculation to be carried out. In fact, the appropriate profile depends on the events which have taken place in the calculation and on the energy transport mechanisms of greatest importance in it. As extreme examples, a problem dominated by hydrodynamics might have quantities determined by passage of a strong shock and subsequent linearization in mass coordinates of the pressure behind the shock, whereas a radiation-dominated diffusion problem is characterized by linearity of the radiation potential, which, in turn, depends on the Rosseland opacity. Of course, such detailed information about the progress of a problem is generally unavailable, so, at best, an approximation based on over-all accuracy is needed.

Since the terms under consideration are the radiation diffusion equations, the interpolation is performed in a way to give greatest accuracy when the diffusion terms are most important--namely, when the profile

is being determined entirely by radiation diffusion. It is also desirable to reduce the number of coefficients requiring interpolation. This can be done by noting the identity

$$\frac{\partial}{\partial r} \int_{\nu_j}^{\nu_{j+1}} B \, d\nu = \frac{\partial \theta^4}{\partial r} \int_{\nu_j}^{\nu_{j+1}} \frac{\partial B}{\partial \theta^4} \, d\nu$$

and by forming the variable $\tau = \int \rho \kappa_j \, dr$. In terms of these quantities, the intensity can be written as

$$I_j = \int_{\nu_j}^{\nu_{j+1}} B \, d\nu - \mu \frac{\partial \int_{\nu_j}^{\nu_{j+1}} B \, d\nu}{\partial \tau}.$$

SECTION IV

FREQUENCY INTEGRATION

Equations derived in Sections II and III which are applicable to a particular frequency of the radiation field are of limited usefulness in the SPUTTER calculations. Although in principle a calculation at a particular frequency might be valuable for comparison with high-resolution spectroscopy, in practice no such data have been available. Of much more use are intensities averaged over a wide frequency band. These quantities can be compared with data from wide-band measurements and, most important of all, can be summed for use in the energy integration in the SPUTTER code. The quantities to be summed are the frequency-integrated radial flux component, the radiation energy density, and the radiation pressure. For performing interaction calculations, it is also valuable to form other components of the radiation flux.

Basically, the quantity which is required for each of the above applications is the frequency-group intensity I_{ij} ,

$$I_{ij} = \int_{\nu_j}^{\nu_{j+1}} I_i d\nu . \quad (4.1)$$

Then, for example, this quantity can be integrated over angles to form ϕ_{rij} , the contribution to the radial flux at position i of frequency group j :

$$\phi_{rij} = \int_{-1}^1 (I_{ij}^+ - I_{ij}^-) \mu d\mu ,$$

and thus the total radiant flux at position i is

$$\phi_{ri} = \sum_j \phi_{rij} .$$

Equation (2.9) gives the expression for the frequency-dependent intensity to be used in Eq. (4.1). The frequency integration of Eq. (2.9) is discussed in Section VII of Volume V, but the current SPUTTER code does not include the transmission functions. The first two terms of Eq. (2.9) which form the diffusion limit can be integrated, as in Section 3.3, to give

$$I_{ij} = B_{ij} - \frac{\mu}{\sigma_{Rj}} \frac{\partial B_{ij}}{\partial r} \quad (\text{diffusion limit}) , \quad (4.2)$$

in which the first term

$$B_{ij} = \int_{\nu_j}^{\nu_{j+1}} B_i(\nu) d\nu$$

is the frequency-group Planck function and the second term contains the frequency-group Rosseland mean absorption coefficient $\sigma_{Rj} = \rho \kappa_j$. In this form, Eq. (4.2) correctly gives the frequency-group intensity for the optically thick limiting case. The remaining B_i and $\partial B / \partial \tau_i$ terms of Eq. (2.9) are formed in the same way. Thus,

$$I_{ij} = B_{ij} - \left(\frac{\mu}{\sigma_R} \frac{\partial B}{\partial r} \right)_{ij} + \left[\left(\frac{\mu}{\sigma_R} \frac{\partial B}{\partial r} \right)_{ij} - \left(\frac{\mu}{\sigma_R} \frac{\partial B}{\partial r} \right)_{i-1,j} \right] \overline{e^{-\Delta/2}} + \left[I_{i-1,j} - B_{i-1,j} + \left(\frac{\mu}{\sigma_R} \frac{\partial B}{\partial r} \right)_{i-1,j} \right] \overline{e^{-\Delta}} . \quad (4.3)$$

In Eq. (4.3), mean values of the exponentials have been extracted from the frequency integrals and the outstanding problem is to specify their values. Two options are available; they differ in the absorption coefficient used to calculate the optical depth. The first is

$$\overline{e^{-\Delta}} = e^{-\sigma_R \delta} \quad (4.4)$$

and the second is

$$\overline{e^{-\Delta}} = e^{-\sigma_P \delta} ,$$

where

$$\sigma_P = \frac{\int_{\nu_j}^{\nu_{j+1}} \sigma_{\nu} B_{\nu} d\nu}{B_{ij}}$$

and

$$\delta = x_i - x_{i-1}.$$

For small optical depth, the correct result makes use of the Planck mean absorption coefficient. From Eq. (2.15) the frequency integration then gives

$$I_{ij} = I_{i-1,j} + \left[\frac{1}{4} B_{ij} + \frac{1}{4} B_{i-1,j} + \frac{1}{2} B_{i-\frac{1}{2},j} - I_{i-1,j} \right] \sigma_P \delta. \quad (4.5)$$

The above prescriptions for frequency-group means are far from satisfying and call for further work. Considerable economies can be made through reductions in the number of frequency groups if a more accurate means of averaging within groups can be found. Presently used choices of frequency groups appear to give a reasonably accurate result, however, as indicated by comparisons between calculations with the nominal number of frequency groups and calculations with a very large number of frequency groups. (It is expected that a unique correct result will be obtained as the number of frequency groups is increased, irrespective of the choice of the weighting function in the frequency-group-average absorption coefficient.) Consequently, a very few frequency groups should be adequate if a suitable averaging procedure were developed.

Even with a crude averaging scheme, considerable improvement in accuracy results from choice of frequency-group boundaries so as to reduce the variation of the absorption coefficient within the group.

Work on the absorption coefficient for air indicates that approximately 20 groups, carefully selected as to their locations, afford quite adequate resolution. Enough information is known about air to make this selection appear quite reasonable. Air absorption coefficient tapes (DIANE)* have been prepared for 18, 20, and 90 groups. The 90-group tape is used to check on the frequency integrations at selected times. The proper averages to use are difficult to decide on at this time. There are provisions for reading into storage from the DIANE tapes both the Rosseland and Planck averages, which are used at present in the thick or thin limits, respectively.

* See Section VI of Volume V.

SECTION V

SUBROUTINE ORGANIZATION AND ECONOMICS

The present spherical transport subroutines were written with the idea of removing unnecessary calculations from inside the frequency loop and characteristic ray (y-line) integrations while improving the accuracy in the angular integrations by using an interpolation between y-lines. These improvements required an increase in storage for the subroutines to attain a decrease in calculational time and an increase in accuracy. It is now practical to use fewer y-lines and thus a factor of approximately 4 in savings on calculational times over the old routines may be achieved. The reorganized subroutines will be discussed in two sections, corresponding to the two major subroutines: (1) the radiation subroutine (SRADTN) in which most of the preliminary setup and the diffusion calculation is completed and (2) the transport subroutine (STRANS) in which the intensity calculation and angular integrations are performed. The subroutines which execute the opacity interpolations (KAPPA), Planck function (PLNKUT⁽²⁾), and fast exponential (FREXP) will be discussed in Section 5.3. The input numbers and the output edits will be presented in Sections 5.4 and 5.5.

5.1. THE SRADTN SUBROUTINE

In SRADTN, the main y-line array is set up, high-frequency groups are merged, a source region is established, boundary sources and derivatives are calculated, regions for transport and diffusion are formed, diffusion fluxes are calculated, frequency integration is performed, and the radiation time-step control is evaluated. Each of these activities in SRADTN will be discussed in subsequent paragraphs.

5.1.1. Set Initial Y-line Array

The number of y-lines is limited by the storage allocated for the x-block. A test is made, and if this storage is to be exceeded by the placing of a y-line at each radius, the y-array is reconstructed by using every other radius for the y-line placement. However, an additional y-line is added at each zone interface where the temperature gradient is large (refer to Section 2.2.1).

5.1.2. Merge Frequency Groups

Frequency groups that are too far out on the Planck tail for a "maximum" temperature in the mesh are merged. The criterion used is as follows: If the lower frequency boundary $h\nu_1$ of the group in question ($h\nu_1, h\nu_2$) is greater than ten times the maximum temperature (THMAX) in the mesh, this group will be merged with the next lower group. Merging will continue until over half the groups have been merged; at this point, either the calculation is terminated or a second DIANE tape is called. On merging, Rosseland and Planck averages are formed by using the following equations for $dB/d\theta^4$ and the appropriate sums:

$$\frac{dB_\nu}{d\theta^4} \cong \frac{0.0384974}{\theta^4} \left[\left(\frac{h\nu_2^4}{1 - e^{-h\nu_2/\theta}} \right) e^{-h\nu_2/\theta} - \left(\frac{h\nu_1^4}{1 - e^{-h\nu_1/\theta}} \right) e^{-h\nu_1/\theta} \right],$$

$$\sum b_j \theta^4, \quad \sum \frac{dB_\nu}{d\theta^4}, \quad \sum b_j \theta^4 \kappa_P, \quad \text{and} \quad \sum \frac{dB_\nu}{d\theta^4 \kappa_R}. \quad (5.1)$$

The Planck weighting functions (b_j) are obtained from PLNKUT, as described later. On completing the merging, the merged opacities are formed:

$$\overline{\kappa_R} = \sum dB_\nu / d\theta^4 / \sum dB_\nu / (d\theta^4 \times \kappa_R) \quad (\text{CAPAR}) ,$$

$$\overline{\kappa_P} = \sum b_j \theta^4 \kappa_P / \sum b_j \theta^4 \quad (\text{CAPAC}) .$$

(5.2)

5.1.3. Set Up Sources and Derivatives

The frequency-dependent sources must be established at the interfaces from the zonal quantities $b_j \theta_{i+\frac{1}{2}}^4$ (X6(i)) and $\tau_{i+\frac{1}{2}}$ (H3(i)). The difference equations used were given in Section 2.1. Before the calculation of the Planck function (b_j) is made, i. e., before calling PLNKUT, a test is made to see if u_1 (i. e., the reduced frequency $h\nu_1/\theta$) ≥ 19 ; if so, $b_j = 0$ (i. e., the source X6(i) = 0.0). If $u_1 < 19.0$ and $u_2 \leq 0.01$, then $b_j = 0$ also, assuming that for $\theta^4 < 10^5$, the small b_j ($b_j \sim 10^{-5}$) will produce a negligibly small source contribution. An index (ICX) is set equal to the last zone that contains a source. This source index is used to limit the transport calculation to the region containing sources. While setting up the sources and derivatives, tests are made on their discontinuous nature to use either a linear or constant form in the intensity integrations. The initial check is on the minimum optical

depth of adjacent zones to ensure that both are transparent (less than 0.3). If this condition holds and if both the sources and optical depths are changing rapidly in r (change greater than a factor of two), the derivative at that interface ($TG(i)$) is set equal to zero. The zero source derivative is used in STRANS, as a test, to set up the constant source terms. For the intensity integration, special boundary sources and derivatives are also established at the edge of the source region ($I = ICX$) and at the outside of the mesh ($I = IM$) (see Section 2.1.4).

5.1.4. Determine Diffusion Region

The principal criterion for defining a diffusion region is that the first derivative of the source function (TG) be small compared to the source ($Y2$) (see Section 3.2). When the zone is found to be diffusion, the boundary is tagged by setting ($X3 = -1.$). Before incorporating this interface into a diffusion region, the possible influence from sources on either side is considered and a further test is made. From the last diffusion boundary, a test is made for an optical depth in succeeding zones to the left. If more than HVB optical depths appear in the next zone, then this zone is calculated by transport and removed from the diffusion region (set $X4(i) = -1.0$). HVB is an input number, which is usually around 5. When $r = 0$ is reached after testing each zone, zones out to the right of the present transport region are tested in the same manner. The above test buffers the transport region with an (HVB) mean-free-path-thick diffusion boundary. If the zone boundary stays diffusion, i. e., $X3(i) = -1.0$ and $X4(i) = 0.0$, a diffusion flux is calculated from the source gradients, as described in Section 3.1. The regions where $X3(i) = 0.$ or $X3(i) = -1.$ and $X4(i) = -1.$ have been established as transport regions because they did not meet the diffusion criteria or they reverted to transport regions by the optical-depth test described above. This transport region is then identified by setting the left boundary to IAX and the right boundary to IBX. More than one trans region may be set up in SRADTN, and if so, an STRANS calculation will be made for each region. No one-zone diffusion region is allowed and the region outside the sources ($I > ICX$) is always considered a transport region.

5.1.5. Time-step Control and Monofrequency Calculation

These two aspects of the new code are related since the "grey" absorption coefficients from the DIANE tape are used to estimate a radiation time step as well as to form the monofrequency time-dependent calculation. In the multifrequency calculation, after all groups have been processed, an additional call for KAPPA is made to read in the grey absorption coefficients. These averages were obtained by integrating the frequency-dependent absorption coefficients for both Planck ($\overline{\kappa_P}$) and Rosseland ($\overline{\kappa_R}$) in the DIANE code. The actual time step for radiation transfer is then obtained from the formula

$$\Delta t_R = (0.5 + 1.5 H3(i)^2) / (ac \kappa_R \theta^3) \times CV(i) , \quad (5.3)$$

where $CV(i)$ is the specific heat and $ac = 4.12 \times 10^{12}$. The mass point in question is also checked to ensure that it will not gain or lose more than half its original energy:

$$\Delta t_R = 0.5 \times CV(i) \times \theta(i) \times G(i) / |ER(i)| , \quad (5.4)$$

where $ER(i)$ is the divergence of the flux and $G(i)$ is the mass in the zone. The minimum of these values is compared to the hydro time step (Courant) and if smaller,

$$NRAD = \text{FIX}(DTH2/DTRMIN) \quad \text{and} \quad DTR = DTH2/NRAD \quad (5.5)$$

is set to cycle $NRAD$ times through the radiation routine.

The monofrequency calculation also uses the grey absorption coefficients from the DIANE tape. If $KMAX = 0.0$ and $S15 = 1.0$, the frequency-averaged opacities are bypassed on the tape and only the grey absorption coefficients are read into storage. For succeeding cycles, $S15$ is set equal to zero and the interpolations for κ_R and κ_P are performed in KAPPA using the stored opacities originally read into KAPPA's common storage. When the problem is restarted it is therefore necessary to reload $S15$ equal to one. If the DIANE tape is not designated (the tape unit assigned must be stored in $AMASNO(J+17)$, where J is the material number), then the KAP routine is called (KAP8 for air) and used for the monofrequency calculation.

5.2. THE STRANS SUBROUTINE

The subroutine STRANS is called by SRADTN to carry out the intensity integration between IAX and IBX, saving various quantities on the inward pass that will be used on the outward pass as well as the angular integration of the flux between y-lines ($\int_{-1}^1 I_\mu d\mu$). The logic is to calculate first the intensities along the central ray ($y = 0$), storing these values and the exponentials ($e^{-\Delta\tau}$) for use on the outward pass. The outward pass is then calculated using the above exponentials and the new intensities are saved separately. After the intensity transport along a typical ray ($y \neq 0$) is done, the flux calculation is done while the right side of the calculation is being completed. The angular integration is based on a linear interpolation of the intensities between y-lines. The logic in STRANS is described in detail in the following sections.

5.2.1. Y-line Placement

In SRADTN, a complete set of y-lines was established, based on storage limitation and temperature gradients. In STRANS, y-lines in each frequency group are selected more judiciously, based on a number of conditions. First, if a diffusion core exists ($IAX > 1$), three rays that will penetrate the core are selected. As each ray is selected, the intensity calculation and angular integration is completed. In the transport region, a test is made for steep gradients between pairs of zones, as indicated in Section 2.2.2. If changes greater than approximately 15 percent occur, a y-line is selected; if not, every fifth y-line is used.

5.2.2. Intensity Integration Along Y-lines

As indicated in Section II, the central $y = 0$ integration is carried out first and the intensities at each intersection are stored in working arrays. The integration using Eq. (2.9) starts from the outside IBXPl and works inward, storing the exponentials $e^{-\Delta\tau}$ in $H4(i)$ and the intensities I_i in $SUMX3(i)$ to zone IAX. For the outward pass, these exponentials are used in Eq. (2.9), but now the sign of the derivatives is changed to $dB/d\tau \rightarrow -dB/d\tau$. After the selection of a y-line, the intensity calculation is performed. Now, not only the exponential is stored, but also $\mu(\partial B/\partial h)_{i+\frac{1}{2}}$ in $X8(i)$ on the inward pass for use on the outward pass. During the outward pass, the angular integration is accomplished and stored in $X2(i)$ using the intensities calculated on both y-lines, as described in Section 5.3. The special condition where a y-line intersects a zone near $x = 0$ is treated differently (see Section 2.1).

The regions where constant sources, and therefore zero boundary derivatives, should be used in the intensity integrations were established in SRADTN by setting $TG(i)$ equal to zero. In the integration along a particular y-line, a test is made on $TG(i)$ at each interface; if zero, the source terms $Y2(i-1)$ and $Y2(i)$ are set equal to $X6(i + \frac{1}{2})$ (see Fig. 2.2).

As was discussed in Section 2.1.1, the accuracy of the exponential term and the effect of truncation errors mean that the general formula will not reduce in the limit of small optical depths to the transparent case. To correct this situation, a test is made on τ_i (the one-half optical depth stored in $H3(i)$ as calculated) and if it is less than 10^{-2} , a switch is made to the limiting form of the transport equation (Eq. (2.15)) developed in Section II.

5.2.3. Angular Integration

This section of STRANS uses the intensity information stored on adjacent y-lines to give a more accurate angular integration. The linear interpolation of the intensities is used in the quadrature formulation of the fluxes (Eq. (2.32))

in Section 2.3). While the intensity integration is being completed on the right-hand side (RHS), use is made of stored intensities on the left-hand side (LHS) for adjacent y-lines to calculate the fluxes across radial boundaries $X2(i)$. The stored quantities used are: $SUMX3(i)$ for the LHS intensity on the present y-line, $FM(i)$ for the LHS intensity on the previous y-line, and $SUMX4(i)$ for the RHS intensity from the previous y-line pass. $F2$ is the current intensity being calculated along the y-line in question. The special condition to complete the flux integrations where no y-lines exist uses a "top-slice" approximation, as discussed in Section 5.2.5.

5.2.4. Boundary Conditions

The usual assumption of zero intensity at the surface of the sphere is used; i. e., $I_{i-1} = 0$ to start the intensity calculation. If the indication is that a diffusion region bounds the transport region ($IBX < IM$), a diffusion boundary condition for the intensity is applied (see Section 2.1.5). At the center, the outward intensity is set equal to the inward intensity.

5.2.5. "Top Slices" and Finish Up

The term "top slice" is used to describe the integration of the flux for zones which do not have y-lines. For instance, outside the sources there is no need for y-lines, and therefore it is assumed that the intensity drops to zero at the outside. If there exist zones with sources (the normal case) between y-lines, then a linear interpolation from y_1 to y_2 is used to establish intensities for integration at those zones. The interpolation formula used is given in Section III. If a diffusion region bounds the transport region, a diffusion intensity for the interpolation is calculated (see Section III).

5.3. AUXILIARY SUBROUTINES

In addition to the two new basic subroutines SRADTN and STRANS, some changes have been made in the auxiliary subroutines EXP, PLNKUT, and KAPPA. These changes include (1) a fast exponential (FREXP), (2) a two-argument Planck function, and (3) the use of the average opacities from KAPPA (θ and ρ interpolation) for the monofrequency calculation as well as for the Planck opacities.

The new fast exponential routine uses table lookup and interpolation rather than the normal expansion methods. The routine is written in machine language but uses the library routine $EXP(X)$ for positive X or $X > -10$. An over-all gain in speed of a few percent was achieved in one comparison SPUTTER calculation.

The PLNKUT routine, with its associated tables PLNKTT, has been corrected and made more efficient by using a two-argument call which now calculates from either the analytic form or from the tables the difference in

$$b(u_1, u_2) = \frac{1}{B} \int_{\nu_1}^{\nu_2} \frac{h\nu^3}{c^2} \frac{1}{e^{-h\nu/kT} - 1} d\nu = b_j \quad (5.6)$$

The accuracy is improved since now not only differences of nearly equal numbers are subtracted.

The subroutine KAPPA, which calls in the group-averaged absorption coefficients from the DIANE tape and performs a bilinear log interpolation in temperature and density, has been modified to obtain the grey absorption coefficients as well as the Planck averages. At present the format of the DIANE (absorption coefficient) tape includes a BCD record for tape identification, the Rosseland and Planck averages for a selected set of temperatures and densities from 0.25 ev to 50 ev and from 10 normal to 10^{-6} normal, and the actual integration, $\int \kappa_\nu d\nu$, for the grey case. The grey or frequency-integrated averages are also used for an estimate of the time step in SRADTN. KAPPA reads in first the tape name, the number of frequency groups, and the size of the records. If the sentinel for multi-frequency is set to KMAX = 1, then the first frequency group, $h\nu_1$, and its absorption coefficients are read into storage. The interpolations in $\log \theta_i$ and $\log \rho_i$ are performed and a return to SRADTN is made. If KMAX = 0, then KAPPA skips over the frequency-dependent absorption coefficients and reads into storage the grey averages. A signal, S15 = 0, is subsequently set, and for further cycles the interpolations are made on the stored quantities; the tape is not called again.

5.4. INPUT NUMBERS

The input quantities used in the radiation transport subroutines and their functions are listed below by card number. Included is a set of values for the input quantities selected for solving typical problems.

Card No.	Quantity	Value	Purpose
44	KMAX	1.	Signal to do multifrequency
77	CVB	0	Select all y-lines
81	HVB	5.	Buffer of trans region in number of optical depths
83	HCB	0.1	Diffusion criteria (see Section 5.4)

<u>Card No.</u>	<u>Quantity</u>	<u>Value</u>	<u>Purpose</u>
87	CB	0	Brightness print on cycles
88	GA	0.33	Gradients in optical depths and sources for applying TG criteria (see Section 5.3)
90	GL	0.3	Gradients in source and MFP for selecting y-lines
121	CMIN	0.3	Minimum depth of adjacent zones for applying TG criteria (see Section 5.3)
127	AC03T4	0.1	One-half optical depth for Planck-Rosseland transition
147	S12	10.	Cycles between multifrequency prints
150	S15	1.	Restart on grey calculation
8478	TELM(37)	0.005	Fraction of total energy in zone for time-step criteria
8725	AMASNO(25)	9.	To select B5, in this case for air tape
8858	SOLID(10)	10.	Signal to use Planck mean free paths
8466	TELM(25)	1.	Constant multiplying radiation time step

5.5. EDITS

The editing of such frequency-dependent quantities as H3, the optical depth (Rosseland), X6, the source (b_0^4), X2, the flux (in $\text{ergs}/4/3 \pi \text{ sec}$), ER, the radiation energy (in ergs/cm^3), PR, the radiation pressure (in dynes/cm^2), PHO, the sidewise flux (in $\text{ergs}/\text{cm}^2\text{-sec}$), PH1, the forward flux ($\text{ergs}/\text{cm}^2\text{-sec}$), and PH2, the backward flux (in $\text{ergs}/\text{cm}^2\text{-sec}$) versus radius is accomplished by setting S12 to the desired number of cycles between prints. These multifrequency edits have been used to evaluate the criteria for the subroutines as well as for diagnostics during the calculations. For example, one quantity found to be most useful for fireball diagnostics has been the flux out in various frequency groups. Because of this, the flux out is edited out in the standard SPUTTER output, X7.

A list of sample editing for a particular frequency group is given on page 45. The HNU is in electron volts.

To obtain a limited set of intensities for purposes of debugging the code, a "debug print" option can be added. The FORTRAN statements and input cards necessary for debugging are listed on page 46. The quantities

found useful to display for each frequency group and for a central y-line and a selected y-line are listed on pages 47 and 48.

SAMPLE MULTIFREQUENCY EDIT FOR STRANS

45

Table 5.2
INPUT CARDS FOR DEBUG OPTION

*	*	*	LOCATION OF VARIABLE IN SPUTTER COMMON NUMBER OF INPUT WORDS THIS CARD INPUT WORD
311	1	0.	R(152)
8876	1	5.9	SOLID(28)
8877	1	6.1	SOLID(29)

C DEBUG PRINT

C
708 DHNU=HNUP-HNU
 IF(R(152))713,712,713
713 IF (HNU-SOLID(29)) 712,714,714
714 IF (HNU-SOLID(28)) 715,715,712
715 WRITE (6,3) HNU,HNUP
717 WRITE (6,5) Y(JJ)
718 WRITE (6,6) JJ,IAX,IBX,ICX
 WRITE (6,8)
 IAXP1=MAX0(IAX,IAXP-1)
 DO 721 I=IAXP1,IBXP1
 IF(JJ.GT.1) GO TO 720

C PRINT Y=0 INTEGRATION

C
719 WRITE (6,7) I,C(I),X6(I),H2(I),H3(I),SUMX3(I),SUMX4(I),X2(I)
 GO TO 721
720 KKK=KK-I+IM+3

C PRINT REGULAR Y-LINE INTEGRATION

C
 WRITE (6,7)I,X(KKK),X6(I),H2(I),H3(I),SUMX3(I),SUMX4(I),X2(I)
721 CONTINUE
712 CONTINUE

Table 5.3
SAMPLE Y-LINE EDIT FOR STRANS

FREQUENCY BAND FROM 6.0000 TO 7.5000					
Y = 0.					
IAJ = 1 IAK = 1 IAL = 40 ICX = 10					
I	X	K6	M2	M3	SUMX4
1	0.	1.0211902+03	1.0479166-02	1.0479166-02	1.9314344+02
2	2.0000000+03	1.0211902+03	1.0479166-02	1.0479166-02	1.7559991+02
3	4.0000000+03	1.0211902+03	1.0479166-02	1.0479166-02	1.5768648+02
4	6.0000000+03	1.0211902+03	1.0479166-02	1.0479166-02	1.3938959+02
5	8.0000000+03	1.0211902+03	1.0479166-02	1.0479166-02	1.2070700+02
6	1.0000000+04	1.0211902+03	1.0479166-02	1.0479166-02	1.0162876+02
7	1.2000000+04	1.0211902+03	1.0479166-02	1.0479166-02	8.2146233+01
8	1.4000000+04	1.0211902+03	1.0479166-02	1.0479166-02	6.2250923+01
9	1.6000000+04	1.0211902+03	1.0479166-02	1.0479166-02	4.1934105+01
10	1.8000000+04	1.0211902+03	1.0479166-02	1.0479166-02	2.1186836+01
11	2.0000000+04	0.	2.4286433-05	2.4286433-05	0.
12	2.1000000+04	0.	2.4286433-05	2.4286433-05	0.
13	2.2000000+04	0.	2.4286433-05	2.4286433-05	0.
14	2.3000000+04	0.	2.4286433-05	2.4286433-05	0.
15	2.4000000+04	0.	2.4286433-05	2.4286433-05	0.
16	2.5000000+04	0.	2.4286433-05	2.4286433-05	0.
17	2.6000000+04	0.	2.4286433-05	2.4286433-05	0.
18	2.7000000+04	0.	2.4286433-05	2.4286433-05	0.
19	2.8000000+04	0.	2.4286433-05	2.4286433-05	0.
20	2.9000000+04	0.	2.4286433-05	2.4286433-05	0.
21	3.0000000+04	0.	2.4286433-05	2.4286433-05	0.
22	3.1000000+04	0.	2.4286433-05	2.4286433-05	0.
23	3.2000000+04	0.	2.4286433-05	2.4286433-05	0.
24	3.3000000+04	0.	2.4286433-05	2.4286433-05	0.
25	3.4000000+04	0.	2.4286433-05	2.4286433-05	0.
26	3.5000000+04	0.	2.4286433-05	2.4286433-05	0.
27	3.6000000+04	0.	2.4286433-05	2.4286433-05	0.
28	3.7000000+04	0.	2.4286433-05	2.4286433-05	0.
29	3.8000000+04	0.	2.4286433-05	2.4286433-05	0.
30	3.9000000+04	0.	2.4286433-05	2.4286433-05	0.
31	4.0000000+04	0.	2.4286433-05	2.4286433-05	0.
32	4.1000000+04	0.	2.4286433-05	2.4286433-05	0.
33	4.2000000+04	0.	2.4286433-05	2.4286433-05	0.
34	4.3000000+04	0.	2.4286433-05	2.4286433-05	0.
35	4.4000000+04	0.	2.4286433-05	2.4286433-05	0.
36	4.5000000+04	0.	2.4286433-05	2.4286433-05	0.
37	4.6000000+04	0.	2.4286433-05	2.4286433-05	0.
38	4.7000000+04	0.	2.4286433-05	2.4286433-05	0.
39	4.8000000+04	0.	2.4286433-05	2.4286433-05	0.
40	4.9000000+04	0.	2.4286433-05	2.4286433-05	0.
41	5.0000000+04	0.	0.	0.	0.

Table 5.4

FREQUENTLY BAND FCM 0.660 10' 7.5000

SECTION VI

TIMING AND ACCURACY COMPARISONS

A timing and accuracy study was made on the new radiation and transport subroutines, SRADTN and STRANS, so that the new routines could be compared with the old routines to obtain a quantitative estimate of the improvements. It was estimated that the reorganization of the subroutines would reduce the calculational time by 50 percent.

6.1. CALCULATIONS FOR TIMING AND ACCURACY

1. Initial formulation of sources, including source at $icx + 1$, and characteristic y-lines was made with the faster exponential subroutine FREXP. (This is compared with the same calculation using the library exponential subroutine.)
2. In the subsequent calculations, the FREXP was used and sources at $icx + 1$ were set to 0.
3. The index for setting the initial y-line distribution (all y-lines are not necessarily used) was improved. A calculation was made where the input number, CVB, that controls the initial number of y-lines was set to 0 (i. e., generate all y-lines).
4. The above calculations were done with thick/thick (i. e., Rosseland) opacities used throughout (SOLID(10) = 10.). A two-cycle run was completed to check that the calculation recycles correctly.
5. The main accuracy and timing comparisons were made with calculations having normal y-line and all-y-line configurations and with the thick/thick and thick/thin approximations (set of 4). The thick/thin approximation used here differs from the Planck and Rosseland averages used in the old subroutines.

The comparison in calculation time was obtained by using timing calls at selected locations in the logic of the code. To use the timing calls, it was necessary to establish a fiducial time from the system clock and then print the location of the time call, the time, and the difference in time between calls for each call. The subroutine that carries out these steps is CLOCK.

In the calculations described above, the subroutine CLOCK was called at the following locations in SRADTN and STRANS:

SRADTN

- 13.105 - After setting $\log_{10}$ of θ and SV
- 13.118 - After calculating x-array
- 13.140 - After call KAPPA on merge
- 13.700 - End of merge and source
- 13.701 - After call KAPPA on main frequency loop
- 13.151 - After calculating general sources
- 13.180 - Before call transport (STRANS)
- 13.292 - After edit (normal) end of frequency loop
- 13.286 - After last frequency start time step
- 13.289 - End of cycle

STRANS

- 14.708 - Before debug print

6.2. COMPARISON FOR TIMING

The general conclusions from the timing study are summarized as follows:

1. The use of the faster exponential subroutine FREXP in comparing a normal y-line problem showed an improvement of approximately 2.5 percent.
2. The all-y-line calculations did not increase the calculational time in proportion to the increase in y-lines, i. e., a factor of 5 increase in y-lines increased the running time by only 80 percent.
3. The normal setup times and typical frequency-group-dependent calculational times for a number of runs (in units of 1/60 sec) are:

Set up $\log_{10}$ Q and SV	~4
Calculate x-array (36 y-lines)	~32
Call KAPPA first group	~34
Call KAPPA second group	~23
Merge above and calculate source	~10
Total setup time, including merging two groups	~103

4. A breakdown of the times required for a normal frequency loop (i. e. , normal y-lines) is as follows:

Bring in new absorption coefficients (call KAPPA)	~18
Source calculation (PLNKUTT)	~5 - 8
Calculations before "call trans. " mostly diffusion fluxes	~2
y-line calculation of intensities	~7
Normal print (X2, H3, etc.)	~35
Total time per frequency group with normal EDIT	~68
Brightness print	~11

The radiation cycle is completed by calculating a minimum time step from the grey absorption coefficients obtained at this time from a fit in KAP8.

The total times for a radiation cycle with ~60 zones (36 are active) and 21 frequency groups require for

Normal editing	$\sim 1.49 \times 10^3$ (1/60 sec)
Brightness editing	$\sim 1.2 \times 10^3$ (1/60)
No special editing	$\sim 1.00 \times 10^3$ (1/60)

The all-y-line calculation with normal editing takes $\sim 2.40 \times 10^3$ (1/60 sec).

In comparison, with the old subroutines the calculation times (in units of 1/60 sec) for a particular frequency group require:

All y-line	~200
KAPPA	~17
Source	~13-30
Normal prints	~17
Brightness print	~13

The setup time for all groups, including the monofrequency time step, is ~30 (1/60 sec). The total times for a radiation cycle with 60 zones, 21 frequency groups, and all y-lines require for

All prints	$\sim 5.40 \times 10^3$ (1/60 sec)
Normal editing	$\sim 5.19 \times 10^3$ (1/60 sec)

6. 3. COMPARISON FOR ACCURACY

The new SRADTN and STRANS subroutine calculations are compared to an all-y-line, all-transport result from HA5. In general, the results all agree within 5 to 8 percent either from a flux versus radius comparison (Fig. 6.1) or from a central brightness comparison (Fig. 6.2). The differences are qualitatively understood and are within acceptable limits. The close agreement (within 1 percent) of the new all-trans, all-y-line calculations with the standard routines indicates that the normal y-line calculation for Rosseland averages (~5 to 8 percent) gives very good results with fewer y-lines. This result can probably be improved.

6. 4. CONCLUSIONS

The over-all computational time has been reduced by a factor of two from the old standard transport calculation without apparent loss in accuracy. The new formulation will allow for fewer y-lines and subsequent further decrease in running time from the old calculation with estimated differences of only 5 to 8 percent.

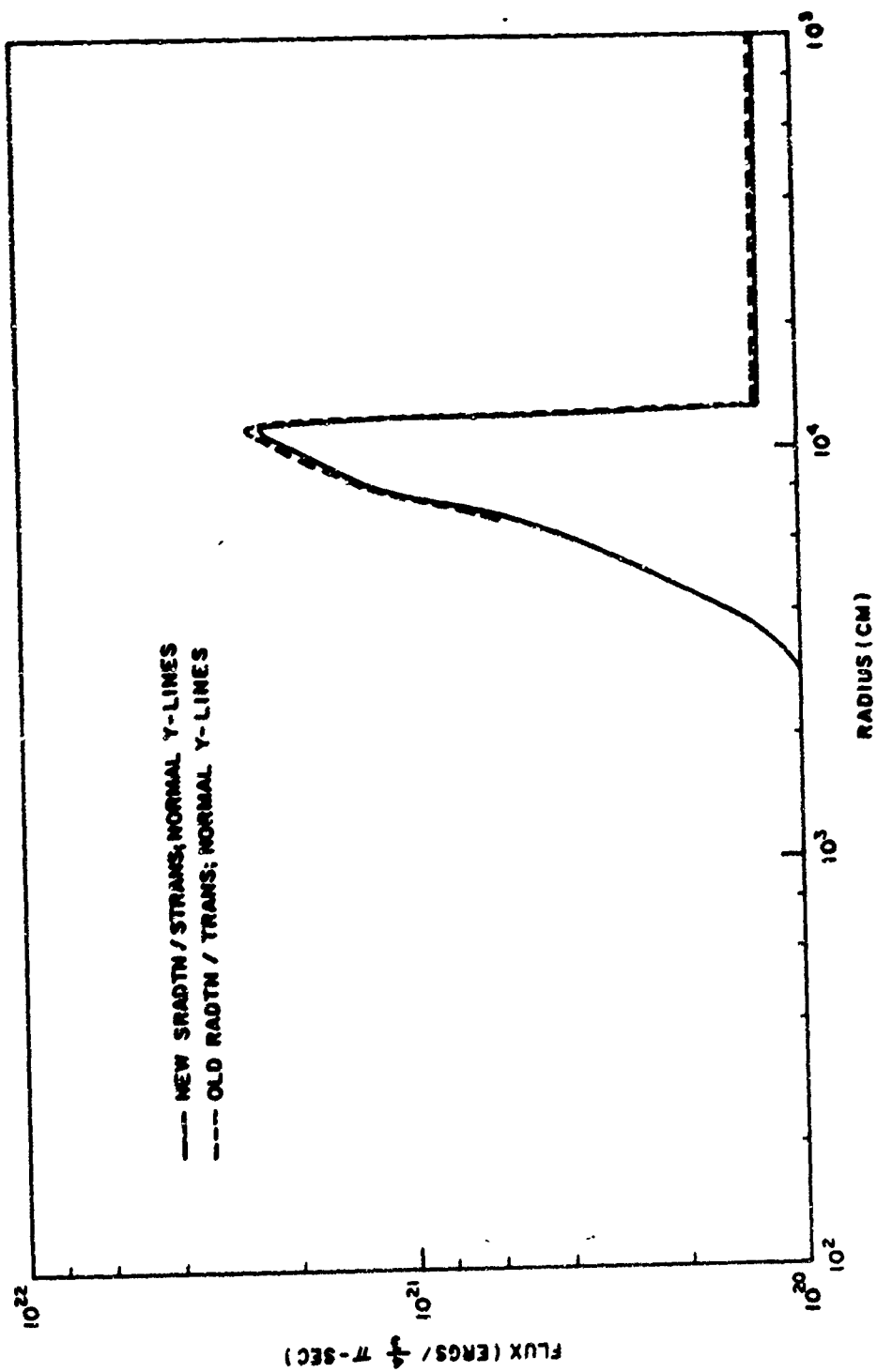


Fig. 6.1--Flux versus radius comparison with results from old version of code

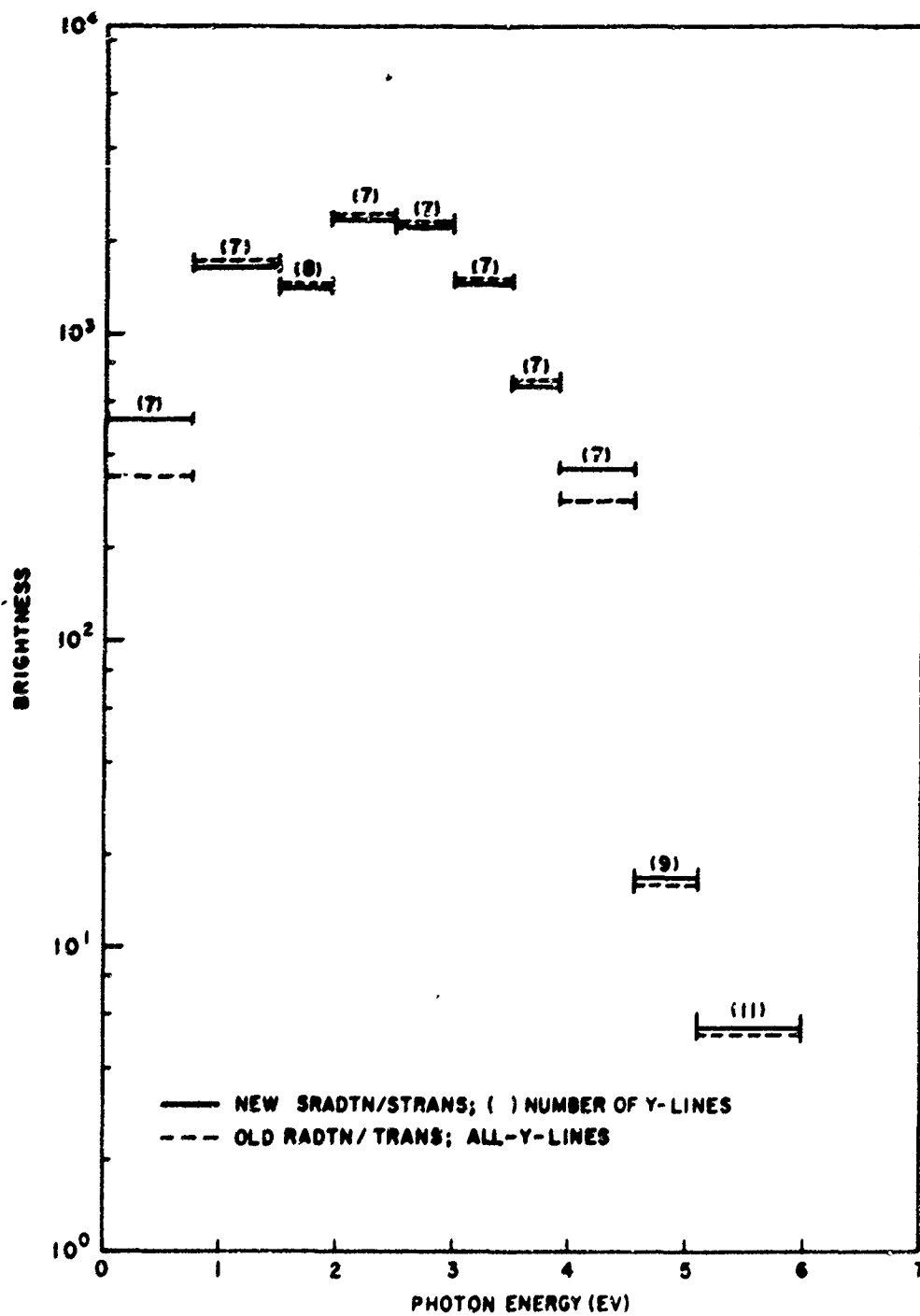


Fig. 6.2--Central brightness comparison with results from old version of code

REFERENCES

1. Optical Interactions, Vol. II, The SPUTTER Program (U), Air Force Special Weapons Laboratory, RTD-TDR-63-3128 (AD-440287), May 1964. (Vol. II Unclassified).
2. Lindley, W. B., PLNKUT, Evaluation of the Integral of the Planck Function in SPUTTER, General Atomic, Informal Report GAMD-6366, May 5, 1965.

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Appendix A
SRADTN

\$IBFTC SRADTN LIST,DECK,REF

SUBROUTINE RADTN

C DATE COMPILED 3 JUNE 1965

C SPECIAL EDIT ON S12

C REVISED SPHERICAL TRANSPORT (NEW 65)

C MUST USE WITH LATEST KAPPA FOR AVERAGE OPACITIES

C H2(1) NOW CONTAINS PLANCK MFP ON SOLID(10)=0.0

C*****

C* **

C* S P U T T E R C O M M O N **

C *

```
COMMON LMDA(37), NR , NSMLR , IA , IB , ICA , ICB ,
1 KMAX , BLANK1, BLANK2, BLANK3, IAP1 , IBP1 , ICAP1 , ICBP1 ,
2 II , IG , NRAD , BLANK4, IAM1 , IBM1 , ICAM1 , ICBM1 ,
3 IIP1 , IGM1 , IALPHA, BLANK5, TH , TMAX , BLANK6, DELPRT,
4 FREQ , CNTMAX, AR , ASMLR , PUSHA , PUSHB , BOILA , BOILB ,
5 CVA , CVB , SLUG , ALPHA , HVA , HVB , HCA , HCB ,
6 EMINA , EMINB , CA , CB , GA , GB , GL , GR ,
7 RHOL , RHOR , EPIO , EPSI , RIA , RIB , RDIA , RDIB ,
8 RPIA , RPIB , RPDIA , RPDIB , TPRINT, TA , TB , TC
COMMON TD , TE , DTH2 , DTH2P , DTH1 , DTRMIN, DTMAX ,
1 DTMAX1, DTMAX2, DTMAX3, DTR , SWITCH, CO , CMIN , DELTA ,
2 GAMA , WCRIT , SIGMAQ, AC , ACO3T4, CNVRT , SUMRA , SUMRB ,
3 ROIA , ROIAM1, ROIB , ROIBP1, GMS , S1 , S2 , S3 ,
4 S4 , S5 , S6 , S7 , S8 , S9 , S10 , S11 ,
5 S12 , S13 , S14 , S15 , S16 , S17 , S18 , S19 ,
6 S20 , EO , FO , TAU , ZERO , R (152), DELTAR(152),
7 ASQ (152), RD (152), VD (152), RDD (152), SMLR (152),
8 DELR ( 37), P (152), P1 (152), PB (152), PB1 (152)
COMMON P2 (152), SV (152), RHO (152), THETA (152),
1 W (152), E (152), EI (152), EK (152), A (152),
2 V (152), G (152), D (152), C (152), X2 (152),
3 X3 (152), X4 (152), X5 (152), X6 (152), X7 (152),
4 SMLA (152), SMLB (152), SMLC (152), SMLD (152), SMLE (152),
5 EC (152), ER (152), SMLQ (152), SMLH (152), BIGA (152),
6 BIGB (152), CV (152), BC (152), BR (152), CHIC (152),
7 CHIR (152), CAPAC (152), CAPAR (152), CRTC (152), CRTR (152),
8 CRTPC (152), GOFR (152), FEW (152), CAR (152), OKLM ( 37)
COMMON TELM ( 37), EKLM ( 37), ELM ( 37), FCLM ( 37),
1 FRLM ( 37), WLM ( 37), QLM ( 37), AMASNO( 37), CHRNO ( 37),
2 ZP1 ( 37), ZP2 ( 37), SOLID ( 37), ECHCK ( 37), RK (104),
3 RL ( 37), RHOK (104), RDK (104), THETAK(104), TEMP ( 16),
4 HEAD ( 12), MAXL , MAXLM
```

C* **

C*****

C *

COMMON /LINDLY/ HNU,SGNL, IHNU,NHNU,HNUP,NT, IH, IN, DHNU,THICK,NY

C

COMMON /CNTRL/ SCYCLE, JMULT

C

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COMMON /DAVIS/ FEX (152), ICX, IR, PR(152),
1 TG(152), X(2400), OX(152)

DIMENSION CSQD (1),ERR(1), FM (1), H (1), H2 (1),
1 H3 (1), H4 (1), PRR (1), Q1 (1), Q2 (1), Q3 (1),
2 Q37 (1), Q38 (1), SUMX2 (1), SUMX3 (1), SUMX4 (1), X8 (1),
3 Y (1), Y2 (1), YSQD (1), PHO (1), PH1 (1)

EQUIVALENCE (ACO3T4,TRDBG), (BC ,SUMX4), (BIGA ,Y),
1 (BIGB , H), (BR ,H3), (CAR ,Q37), (CHIC ,SUMX3),
2 (CHIR ,Q38), (CRTR ,SUMX2), (EC ,Q1), (GOFR ,Q3),
3 (RDD ,ERR), (S12 ,EDITMF), (SMLA ,H4), (SMLB ,FM),
4 (SMLC ,CSQD), (SMLD ,Y2), (SMLE ,H2), (SMLH ,X8),
5 (SMLR ,PRR), (V ,Q2), (X7 ,YSQD), (CRTC ,PH1),
6 (CRTPC,PHO)

OX CONTAINS X FROM THE PREVIOUS Y LINE

CSQD	SAME AS	SMLC
EDITMF	SAME AS	S12
ERR	SAME AS	RDD
FM	SAME AS	SMLB
H	SAME AS	BIGB
H2	SAME AS	SMLE
H3	SAME AS	BR
H4	SAME AS	SMLA
PHO	SAME AS	CRTPC
PH1	SAME AS	CRTC
PRR	SAME AS	SMLR
Q1	SAME AS	EC
Q2	SAME AS	V
Q3	SAME AS	GOFR
Q37	SAME AS	CAR
Q38	SAME AS	CHIR
SUMX2	SAME AS	CRTR
SUMX3	SAME AS	CHIC
SUMX4	SAME AS	BC
TRDBG	SAME AS	ACO3T4
X8	SAME AS	SMLH
Y	SAME AS	BIGA
Y2	SAME AS	SMLD
YSQD	SAME AS	X7

PHO SIDE FLUX (ERGS/CM**2-SEC)
PH1 FORWARD FLUX (ERGS/CM**2-SEC)

```

C          PH2      BACKWARD FLUX      (ERGS/CM**2-SEC)      *
C          PRR      RADIATION PRESSURE  (ERGS/CM**3)          *
C          RHO      RADIATION ENERGY   (ERGS)CM**3)          *
C
C*****
      NTIMES=BOILB
      IMP1=IB
      IM=IBM1
      IN=IA
      INH1=IN-1
      CALL DVCHK(KOOFX)
      GO TO(17,17),KOOFX
17  IR=IN
      THTAMX=.025
104 DO 105 I=IN,IM
      X3(I)=0.
      X4(I)=0.
      X5(I)=0.
      X6(I)=0.
      X7(I)=0.
C*****
C
C          SET UP FOR KAPPA INTERPOLATION
C
C*****
      Q1(I)=THETA(I)**4
      Q37(I)=ALOG(THETA(I))
      Q38(I)=ALOG(SY(I))
      CSQD(I)=C(I)**2
C
C          FIND IR LARGEST INDEX OF ZONE WITH THETA
C          GREATER THAN 0.05
C
      IF(THETA(I)-THTAMX)100,100,101
101 THTAMX=THETA(I)
100 IF(THETA(I)-0.05)105,105,106
106 IR=I
105 CONTINUE
      CSQD(IR)=C(IR)**2
C
C          PROBLEM STOPS IF MAX TEMP LESS THAN 0.05
C
      IF(THTAMX-0.05)108,108,107
108 S1=13.108
      CALL UNCLE
107 K=IFIX((FLOAT(IR)+2.0)/(2.4E3/FLOAT(IR)+(FLOAT(IR)+1.0)/2.))
C
C          DETERMINE WHETHER TO SKIP ZONES WITH Y-LINES
C
111 K1=K

```

```

Y(1)=0.0
YSQD(1)=0.0
IRM1=IR-1
JK=1

```

```

C*****
C
C           S E T   U P   Y   L I N E S
C
C*****

```

```

C
C           D R A W   Y   L I N E S --- O N E   F O R   E A C H   L A R G E   T E M P E R A T U R E   C H A N G E
C
C           N O   Y   G R E A T E R   T H A N   C ( I R )
C

```

```

DO 112 I=IN,IRM1
IF (ABS(Q37(I+1)-Q37(I))-CVB) 113,113,114
114 JK=JK+1
Y(JK)=C(I+1)
YSQD(JK)=CSQD(I+1)
K1=K
GO TO 112
113 IF(K1)114,114,115
115 K1=K1-1
112 CONTINUE
NY=JK
GO TO 116
117 K=K+1
GO TO 111

```

```

C*****
C
C           F I N D   C O M P L E T E   S E T   O F   X   V A L U E S
C           ( I N T E R S E C T I O N S   O F   R A D I I   W I T H   Y   L I N E S )
C
C*****

```

```

C
C           F O R M A T = - Y S Q D , - N U M B E R   O F   I N T E R S E C T I O N S , X * S .
C

```

```

116 K2=1
DO 118 J=2,NY
I=IMP1
X(K2)=-YSQD(J)
K2=K2+2
KK=1
120 TS1=CSQD(I)-YSQD(J)
IF(TS1)122,122,119
119 X(K2)=SQRT(TS1)
K2=K2+1
IF(K2-2400)1191,1191,117
1191 I=I-1
KK=KK+1

```

```

GO TO 120
122 KKK=K2-KK
X(KKK)=-X(KK-1)
118 CONTINUE
C
C      FINISH X-BLOCK WITH NEG NUMBER
C
X(K2)=-1.0
C*****
C
C      S E T U P   F R E Q U E N C Y   L O O P
C*****
HNUP=4000.
C
C      S E T   U P   M A X   F R E Q   B O U N D A R Y
C
HNUP4=2.56E14
IHNU=1
DO 121 I=IN,IMP1
ERR(I)=0.0
PRR(I)=0.0
121 SUMX2(I)=0.0
C*****
C
C      T E S T   F O R   M O N O F R E Q U E N C Y
C*****
IF (KMAX .EQ. 0) GO TO 150
140 CALL KAPPA(IN,IM)
HNU4=HNU**4
C*****
C
C      M E R G E   G R O U P S   H A V I N G   H N U   L E S S
C      T H A N   T E N   T I M E S   L A R G E S T   T H E T A
C*****
IF(THTAXX-0.1*HNU) 142,141,141
C
C      R E J E C T   T A P E   I F   M O R E   T H A N   H A L F   O F   G R O U P S   M E R G E
C
142 IF(IHNU+IHNU-NHNU)143,144,144
144 S1=13.0144
C
C      U S E   S T A T E M E N T   A S   I N   P L A N E   C O D E   N O W
C
C      W I L L   H O P E   T O   C A L L   N E X T   T A P E   I N   F U T U R E
C
CALL UNCLE
143 DO 145 I=IN,IM

```

```

BETA=HNU/THETA(I)
BETAP=HNUP/THETA(I)
DFB=PLNKUT(BETA,BETAP)
IF(DFB .EQ. 0.) GO TO 145
TEMP(1)=DFB*Q1(I)
EMB1=EXP(-BETA)
EMB2=EXP(-BETAP)
TEMP(2)=DFB+0.0384974/Q1(I)*(HNU4/(1.0-EMB1)
1*EMB1-HNUP4/(1.0-EMB2)*EMB2)

```

```

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)
145 CONTINUE
HNUP=HNU
IHNU=IHNU+1
HNUP4=HNU4
IF(IHTAMX-0.1*HNU) 140,703,703

```

```

C*****

```

```

C
C      MONOFREQUENCY CALCULATION
C

```

```

C*****

```

```

150 NHNU=1

```

```

C
C      CALLS KAPPA ONE TIME ON RESTART (S15=1.0) FOR
C      AVERAGE OPACITIES FROM DIANNE TAPE AND STORED
C      IN KAPPA FOR FUTURE INTERPOLATIONS
C

```

```

CALL KAPPA(IN,IM)
DO 704 I=IN,IM
X5(I)=1.
704 X6(I)=Q1(I)
ICX=IR
GO TO 139
141 IF(IHNU-1) 153,702,143

```

```

C
C      FORM MERGED KAPPAS
C

```

```

703 DO 700 I=IN,IM
IF (X6(I)) 210,700,200
210 S1=13.210
CALL UNCLE
200 CAPAR(I)=X4(I)/X3(I)
215 CAPAC(I)=X5(I)/X6(I)
700 CONTINUE
HNUP=4000.

```

```

      HNUP4=2.56E14
      IHNU=IHNU-1
      GO TO 702
C*****
C
C          TYPICAL GROUP CALCULATIONS OF SOURCES
C
C*****
      701 CALL KAPPA(IN,IM)
          HNU4=HNU**4
      702 ICX=IN
          DO 151 I=IN,IR
              BETA=HNU/THETA(I)
              EMB1=EXP(-BETA)
C
C          AVOID CALCULATION OF DFB LESS THAN 1E-5
C
          IF(BETA-19.)146,147,147
      146 BETAP=HNUP/THETA(I)
          EMB2=EXP(-BETAP)
          IF(BETAP-.01)147,147,148
      147 IF(ICX-IR)149,157,157
      157 ICX=I-1
      149 X6(I)=0.0
C
C          X5(I)=0.0
C
          GO TO 151
C
C          FORM SOURCES X6 AND X5
C
      148 DFB=PLNKUT(BETA,BETAP)
          X6(I)=DFB*Q1(I)
      132 ICX=IR
      151 CONTINUE
      139 Q31=0.0
C*****
C
C          FORM ROSS AND PLANCK OPTICAL DEPTHS
C
C*****
          DO 152 I=IN,IM
              IF(CAPAR(I))153,153,154
      154 IF(CAPAC(I))153,153,155
      153 S1=13.153
          CALL UNCLE
C
C          CHOOSE ALL ROSS IF SOLID 10 IS POS.
C
      155 IF(SOLID(10).EQ.0.)GO TO 167

```

```

H2(I)=CAPAR(I)/SV(I)
GO TO 169
167 H2(I)=CAPAC(I)/SV(I)
169 H(I)=CAPAR(I)/SV(I)
H3(I)=CAPAR(I)/SV(I)*DELTAR(I)
Q31=Q31+H3(I)
Q3(I+1)=Q31
H(I)=0.5*H(I)
H2(I)=0.5*H2(I)
H3(I)=0.5*H3(I)

```

```

C
C      ZERO DIFF INDICATORS AND X2
C

```

```

X2(I)=0.0
X3(I)=0.0
X4(I)=0.0
Y2(I)=0.0
TG(I)=0.0
SUMX3(I)=0.0
SUMX4(I)=0.0
PH1(I)=0.0
PH0(I)=0.0
PR(I)=0.0
152 RHO(I)=0.0
X2(IMP1)=0.0
PH0(IMP1)=0.0
PH1(IMP1)=0.0
X3(IMP1)=0.0
X4(IMP1)=0.0

```

```

C
C      X6(IR+1)=0.0
C

```

```

C
C      X5(IR+1)=0.0
C

```

```

TG(IN)=0.0
Y2(IN)=X6(IN)
X3(IN)=-1.0

```

```

C*****

```

```

C
C      S E T   U P   S O U R C E S
C

```

```

C*****

```

```

C
C      FORM Y2 AND TG
C

```

```

C      SET X3=-1 IF DIFFUSION CRITERION MET USING HCB
C

```

```

C
DO 156 I=IN,ICX
IF (I-IM) 135,136,136

```

```

135 TEMP(1)=H3(I+1)+H3(I)
    IF (AMIN1(H3(I),H3(I+1))-CMIN) 1157,1157,1156
1157 IF(ABS((H3(I)-H3(I+1))/TEMP(1))-GA) 1156,1156,1158
1158 IF (X6(I) .EQ. 0.0) GO TO 1159
    IF(ABS((X6(I)-X5(I+1))/(X6(I)+X6(I+1)))-GA) 1156,1156,1159
1159 TG(I+1)=0.0
    GO TO 156
1156 TG(I+1)=(X6(I+1)-X6(I))/TEMP(1)
C
C          TG(I+1)=(Q1(I+1)-Q1(I))/TEMP(1)*(X5(I+1)+X5(I))/2.0
C
    Y2(I+1)=(X6(I+1)*H3(I)+X6(I)*H3(I+1))/TEMP(1)
    IF(ABS(TG(I+1))-HCB*Y2(I+1)) 158,158,156
158 X3(I+1)=-1.0
156 CONTINUE
C
C          RADIATION BOUNDARY CONDITIONS AT ICX
136 Y2(IMP1)=X6(ICX)
    TG(IMP1)=0.0
C
C          ENLARGE TRANSPORT REGION BOUNDRIES BY HVB
C          MEAN FREE PATHS
C
137 I=IN+1
159 IF(X3(I))160,161,162
160 I=I+1
    IF(I-ICX-1)159,161,172
162 S1=13.162
    CALL UNCLE
161 J=I-1
165 IF(Q3(I)-Q3(J)-HVB)163,163,164
163 X4(J)=-1.0
    J=J-1
    IF(J-IN)164,165,165
164 I=I+1
    IF(I-ICX-1)166,172,172
166 IF(X3(I))168,164,162
168 J=I
171 IF(Q3(J)-Q3(I-1)-HVB)170,170,160
170 X4(J)=-1.0
    J=J+1
    IF(J-ICX-1)171,160,160
172 I=IN+1
C
C          TEST TO FORM TRANS REGIONS
C
    IF(X3(IN))173,174,162
173 IF(X4(IN))174,175,162
174 IAX=IN
176 IF(X3(1))177,178,162

```

```

177 IF(X4(I))178,179,162
C
C      REMOVE ONE ZONE DIFF REGION
C
178 I=I+1
    IF(I-ICX-1)176,180,180
179 I=I+1
    IF(I-ICX-1)187,180,180
187 IF(X3(I))188,176,162
188 IF(X4(I))176,189,162
189 IBX=I-3
    GO TO 181
175 X2(IN)=0.0
    PR (IN)=Y2(IN)*45.666
    RHO(IN)=Y2(IN)*137.0
    PH0(IN)=Y2(IN)*1.E12
    PH1(IN)=PH0(IN)
185 IF(X3(I))182,183,162
182 IF(X4(I))183,184,162
C
C      FORM X2 FOR DIFF ZONES IN ORDER
C
184 X2(I)=-4.12E12*TG(I)*CSQD(I)
    PR (I)=Y2(I)*45.666
    RHO(I)=Y2(I)*137.0
    PH0(I)=1.E12*Y2(I)
    PH1(I)=PH0(I)
    I=I+1
    IF(I-ICX-1)185,186,186
C
C      DO TRANS TO IM IN REGION OF NO SOURCE
C
183 IAX=I
    GO TO 178
180 IBX=IM
181 CALL TRANS(IAX,IBX)
    IF(IBX-IM)190,760,760
190 I=IBX+2
    GO TO 184
186 IAX=I
    GO TO 180
C*****
C
C      O P T I O N A L   E D I T   O F   X 2   E T C
C
C*****
760 IF (EDITMF)282,282,280
280 IARG1=SOLID(18)+0.001
    IARG2=EDITMF*0.001
    IF (MOD(IARG1, IARG2)) 282,281,282

```

```

281 WRITE (3) HNU, IN, IM, IMP1, SOLID(18), TH, DHNU
    WRITE (3) (C(I), I=IN,IMP1), (H3(I), I=IN,IM), (X6(I), I=IN,IMP1),
1   (X2(I), I=IN,IMP1), (PHO(I), I=IN,IMP1), (PH1(I), I=IN,IMP1),
2   (RHO(I), I=IN,IMP1), (PR(I), I=IN,IMP1), (CSQD(I), I=IN,IMP1)
    XX=-2.0
    WRITE (3) XX,XX,XX,XX,XX,XX,XX
    BACKSPACE 3
    JMUL=1.0
282 DO 292 I=IN,IMP1
    SUMX2(I)=SUMX2(I)+X2(I)
    ERR(I)=ERR(I)+RHO(I)
    PRR(I)=PRR(I)+PR(I)
292 CONTINUE
C
C           ADVANCE FREQUENCY AND STORE EMERGENT FLUX
C
C           TEST FOR COMPLETION OF GROUPS
C
    HNUP=HNU
    HNUP4=HNU4
    CRTPC(IHNU+50) = X2(IMP1)
    IHNU = IHNU + 1
    IF (IHNU - NHNU) 283, 283, 285
283 CALL DVCHK (K000FX)
    GO TO(284,701),K000FX
C*****
C
C           E N D   F R E Q U E N C Y   L O O P
C
C*****
284 S1 = 13.0284
    CALL UNCLE
285 DO 286 I=INM1,IMP1
288 X2(I)=SUMX2(I)
286 ER(I) = SUMX2(I) - SUMX2(I+1)
C
C           FORM MONOFREQUENCY QUANTITIES AND FIND MIN TIME STEP
C
    WSB=0.0
    DO 81 I=1,MAXLM
81  WSB=WSB+ELM(I)
    DTR1=1.E10
    DTR2=1.E10
C
C           FOR MULTIFREQUENCY WILL CALL KAPPA ONCE MORE FOR
C           AVERAGED OPACITIES
C
    IF (KMAX .EQ. 0) GO TO 1110
    CALL KAPPA(IN,IM)
1110 DO 124 I=IN,IM

```

```

C
C      IF ROSS IS ZERO EXIT
C
      IF(CAPAR(I))1111,1111,1112
1111 S1=13.1111
      CALL UNCLE
C
C      THICK - THIN ETC
C
1112 TEMP(3)=CAPAR(I)
      IF(SOLID(10))1113,1114,1113
1113 TEMP(1)=CAPAR(I)
      GO TO 1117
1114 TEMP(1)=SQRT(CAPAR(I)*CAPAC(I))
1117 IF(TEMP(1))1111,1111,1118
1118 H(I)=0.5*TEMP(1)/SV(I)
      H3(I) = H(I) * DELTAR(I)
      IF(0.05-THETA(I)) 1120,1201,1201
1120 IF (H3(I) .GT. 0.1) GO TO 1201
      IF (ER(I) .EQ. 0.0) GO TO 1201
      WSBB=E(I)*G(I)
      IF (TELM(37) .EQ. 0.0) GO TO 1201
      IF (WSBB-TELM(37)*WSB) 1201,1203,1203
1203 TEMP(2)=0.5*CV(I)*THETA(I)*G(I)/ABS(ER(I))
      GO TO 1202
1201 TEMP(2) = (.5 + 1.5 * H3(I)**2) * CV(I) / (AC*TEMP(3)*THETA(I)**3)
      TEMP(2)=TEMP(2)*TELM(25)
C*****
C
C      F I N D   M I N I M U M   T I M E   S T E P
C
C*****
1202 IF(TEMP(2))124,124,1211
1211 CONTINUE
      IF(TEMP(2)-DTR1)1122,1130,1130
1122 DTR2=DTR1
      IMN2=IMN1
      DTR1=TEMP(2)
      IMN1=I
      GO TO 124
1130 IF(TEMP(2)-DTR2)1140, 124,124
1140 DTR2=TEMP(2)
      IMN2=I
124 CONTINUE
      DTRMIN=DTR1
      EQ=IMN1
C
C      PRINT MINIMUM TIME STEPS BETWEEN EDITS
C
      IF(DTR1-TELM(26))150,1160,1160

```

```

1150 TELM(26)=DTR1
      TELM(27)=IMN1
      TELM(28)=DTR2
      TELM(29)=IMN2
      TELM(30)=SOLID(18)+1.0
1160 CONTINUE
C
C          DETERMINE IF RADIATION OR HYDRO WILL SUBCYCLE
C
      IF (DTRMIN-DTR) 125,240,1165
1165 BLANK3=TH+AMIN1(DTRMIN,GR*DTH2)
      IF (S17) 240,123,240
123 S9 = 1.0
C*****
C
C          R E D U C E   T I M E   S T E P
C
C*****
125 NRAD=ZP1(18)/DTRMIN+1.0
      DTR=ZP1(18)/FLOAT(NRAD)
      IF(NRAD-NTIMES) 240,240,238
238 S1=13.238
      CALL UNCLE
240 RETURN
      END

```

Appendix B

STRANS

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SIBFTC STRANS LIST,DECK,REF

SUBROUTINE TRANS(N,M)

C DATE COMPILED 3 JUNE 1965

C ANGULAR INTEGRATIONS ON LINEAR FORM

C CONNECTED LINEAR-QUADRATIC INTERPOLATION AT X=0.

C EDITING OF VARIOUS M.F. QUANTITIES ON S12 CYCLES

C TRDBG USED TO TRANSFER FROM THIN-PLANCK TO THICK-ROSSELAND

C*****

C*

C*

C

S P U T T E R C O M M O N

```
COMMON LMDA(37), NR , NSMLR , IA , IB , ICA , ICB ,
1 KMAX , BLANK1, BLANK2, BLANK3, IAP1 , IBP1 , ICAP1 , ICBP1 ,
2 II , IG , NRAD , BLANK4, IAM1 , IBM1 , ICAM1 , ICBM1 ,
3 IIP1 , IGM1 , IALPHA, BLANK5, TH , TMAX , BLANK6, DELPRT,
4 FREQ , CNTMAX, AR , ASMLR , PUSHA , PUSHB , BOILA , BOILB ,
5 CVA , CVE , SLUG , ALPHA , HVA , HVB , HCA , HCB ,
6 EMINA , EMINB , CA , CB , GA , GB , GL , GR ,
7 RHOL , RHOR , EPIO , EPSI , RIA , RIB , RDIA , RDIB ,
8 RPIA , RPIB , RPDIA , RPDIB , TPRINT, TA , TB , TC
COMMON TD , TE , DTH2 , DTH2P , DTH1 , DTRMIN, DTMAX ,
1 DTMAX1, DTMAX2, DTMAX3, DTR , SWITCH, CO , CMIN , DELTA ,
2 GAMA , WCRIT , SIGMAQ, AC , ACO3T4, CNVRT , SUMRA , SUMRB ,
3 ROIA , ROIAM1, ROIB , ROIBP1, GMS , S1 , S2 , S3 ,
4 S4 , S5 , S6 , S7 , S8 , S9 , S10 , S11 ,
5 S12 , S13 , S14 , S15 , S16 , S17 , S18 , S19 ,
6 S20 , EO , FO , TAU , ZERO , R (152), DELTAR(152),
7 ASQ (152), RD (152), VD (152), RDD (152), SMLR (152),
8 DELR ( 37), P (152), P1 (152), PB (152), PB1 (152)
COMMON P2 (152), SV (152), RHO (152), THETA (152),
1 W (152), E (152), EI (152), EK (152), A (152),
2 V (152), G (152), D (152), C (152), X2 (152),
3 X3 (152), X4 (152), X5 (152), X6 (152), X7 (152),
4 SMLA (152), SMLB (152), SMLC (152), SMLD (152), SMLE (152),
5 EC (152), ER (152), SMLQ (152), SMLH (152), BIGA (152),
6 BIGB (152), CV (152), BC (152), BR (152), CHIC (152),
7 CHIR (152), CAPAC (152), CAPAR (152), CRTC (152), CRTR (152),
8 CRTPC (152), GOFR (152), FEW (152), CAR (152), OKLM ( 37)
COMMON TELM ( 37), EKLM ( 37), ELM ( 37), FCLM ( 37),
1 FRLM ( 37), WLM ( 37), QLM ( 37), AMASNO( 37), CHRNO ( 37),
2 ZP1 ( 37), ZP2 ( 37), SOLID ( 37), ECHCK ( 37), RK (104),
3 RL ( 37), RHOK (104), RDK (104), THETAK(104), TEMP ( 16),
4 HEAD ( 12), MAXL , MAXLM
```

C*

C*****

C

COMMON /LINDLY/ HNU,SGNL,IHNU,NHNU,HNUP,NT,IM,IN,DHNU,THICK,NY

C

COMMON /CNTRL/ SCYCLE, JMUL

C

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COMMON /DAVIS/ FEX (152), ICX, IR, PR(152),
1 TG(152), X(2400), OX(152)

DIMENSION CSQD (1),ERR(1), FM (1), H (1), H2 (1),
1 H3 (1), H4 (1), PRR (1), Q1 (1), Q2 (1), Q3 (1),
2 Q37 (1), Q38 (1), SUMX2 (1), SUMX3 (1), SUMX4 (1), X8 (1),
3 Y (1), Y2 (1), YSQD (1), PHO (1), PH1 (1)

EQUIVALENCE (AC03T4,TRDBG), (BC ,SUMX4), (BIGA ,Y ,
1 (BIGB , H), (BR ,H3), (CAR ,Q37), (CHIC ,SUMX3),
2 (CHIR ,Q38), (CRTR ,SUMX2), (EC ,Q1), (GOFR ,Q3),
3 (RDD ,ERR), (S12 ,EDITMF), (SMLA ,H4), (SMLB ,FM),
4 (SMLC ,CSQD), (SMLD ,Y2), (SMLE ,H2), (SMLH ,X8),
5 (SMLR ,PRR), (V ,Q2), (X7 ,YSQD), (CRTC ,PH1),
6 (CRTPC,PHO)

OX CONTAINS X FROM THE PREVIOUS Y LINE

CSQD	SAME AS	SMLC
EDITMF	SAME AS	S12
ERR	SAME AS	RDD
FM	SAME AS	SMLB
H	SAME AS	BIGB
H2	SAME AS	SMLE
H3	SAME AS	BR
H4	SAME AS	SMLA
PHO	SAME AS	CRTPC
PH1	SAME AS	CRTC
PRR	SAME AS	SMLR
Q1	SAME AS	EC
Q2	SAME AS	V
Q3	SAME AS	GOFR
Q37	SAME AS	CAR
Q38	SAME AS	CHIR
SUMX2	SAME AS	CRTR
SUMX3	SAME AS	CHIC
SUMX4	SAME AS	BC
TRDBG	SAME AS	AC03T4
X8	SAME AS	SMLH
Y	SAME AS	BIGA
Y2	SAME AS	SMLD
YSQD	SAME AS	X7

PHO	SIDE FLUX	(ERGS/CM**2-SEC)
PH1	FORWARD FLUX	(ERGS/CM**2-SEC)
PH2	BACKWARD FLUX	(ERGS/CM**2-SEC)

```

C          FRR      RADIATION PRESSURE      (ERGS/CM**3)      *
C          RHO      RADIATION ENERGY      (ERGS/CM**3)      *
C                                                     *
C*****
C          H(1)=0.5/ROSSELAND MFP      *
C          TEMP(1)=DELTAX*H(1)      *
C          H2(1)=0.5/PLANCK MFP      *
C          TEMP(2)=DELTAX*H2(1)      *
C          H3(1)=(TAU SUB R)      *
C*****
C
C          IAX=N
C          ISX=M
C          DO 99 I=IN,IM
C          99 Q2(I)=0.
C             CALL DVCHK(KCOOFX)
C             GO TO(100,101),KCOOFX
C          100 S1=14.0100
C             CALL UNCLE
C          101 IBXPI=IBX+1
C             IALPHA=ALPHA
C
C          ERROR IF NOT SPHERE
C
C          GO TO (102,102,103) , IALPHA
C          102 S1=14.0102
C             CALL UNCLE
C
C          SPHERE ONLY
C
C          103 I=IBXPI
C             F2=0.0
C          113 IF(IBX-IM) 106,108,110
C
C          ERROR IF INDEX EXCEEDS NORMAL RANGE
C
C          110 S1=14.0110
C             CALL UNCLE
C*****
C          CALCULATE Y = 0 RAY      *
C*****
C          LHS OF RAY FIRST, STORE F2 IN SUMX3.
C
C          111 TEMP(2)=H2(1)*DELTAR(1)
C             IF (TEMP(2)-TRD8G) 131,131,132

```

```

C
C      SMALL OPTICAL DEPTH EXPANSION
C
131 F2=F2+((Y2(I)+Y2(I+1))*0.5+X6(I)-F2-F2)*TEMP(2)
    GO TO 112
C
C      GENERAL EXPRESSION FOR F2(Y=0.)
C
C      SAVE EXP
C
132 H4(I)=FREXP(-H3(I))
    F2=Y2(I)+TG(I)+((F2-Y2(I+1)-TG(I+1))
      1 *H4(I)+TG(I+1)-TG(I))*H4(I)
112 IF(F2.LT.0.) GO TO 115
C
C      SAVE LHS INTENSITIES IN SUMX3
C
114 SUMX3(I)=F2
    IF(TG(I).EQ.0.) Y2(I)=X6(I-1)
    I=I-1
    IF(TG(I).EQ.0.) Y2(I)=X6(I)
    IF(I-ICX) 116,111,111
C
C      F2=0. IF I GREATER THAN ICX
C
105 I=I-1
108 SUMX3(I)=0.0
    IF(I-1-ICX) 110,114,105
C
C      DIFFUSION BOUNDARY CONDITION AT IBXP1
C
106 IF(TG(I).EQ.0.) Y2(I)=X6(I)
    TEMP(2)=H2(I)*DELTAR(I)
    IF (TEMP(2)-TRDBG) 133,133,134
C
C      SMALL OPTICAL DEPTH EXPANSION(DIFF)
C
133 F2=Y2(I+1)+TG(I+1)+((Y2(I)+Y2(I+1))*0.5+X6(I))*TEMP(2)
    GO TO 112
C
C      GENERAL EXPRESSION FOR F2(DIFF)Y=0.,LHS
C
134 H4(I)=FREXP(-H3(I))
    F2 = Y2(I)+TG(I)+(TG(I+1)-TG(I))*H4(I)
    GO TO 112
C
C      NEGATIVE F2 ZEROED
C
115 F2=0.0
    GO TO 114

```

```

C
C
C          RHS OF RAY
C
116 I=IAX
    IAXP=IAX
    IF(IAX-IN)110,222,119
222 IAXP=IN+1
    RHQ(1)=SUMX3(1)*137.0
    PR (1)=SUMX3(1)*45.66
    PHQ(1)=1.026E12*SUMX3(1)
    PH1(1)=PHQ(1)
    GO TO 223
C
C
C          DIFFUSION BOUNDARY CONDITION AT IAX
C
119 TEMP(2)=H2(I-1)*DELTAR(I-1)
    IF (TEMP(2)-TRDBG) 135,135,136
C
C
C          SMALL OPTICAL DEPTH EXPANSION(DIFF)
C
135 F2=Y2(I-1)-TG(I-1)+((Y2(I)+Y2(I-1))*0.5 +X6(I-1))*TEMP(2)
    GO TO 121
C
C
C          GENERAL EXPRESSION FOR F2 (DIFF,Y=0,RHS)
C
136 H4(I-1)=FREXP(-H3(I-1))
    F2=Y2(I)-TG(I)+((TG(I)-TG(I-1))*H4(I-1)
    GO TO 121
C
C
C          REGULAR INTEGRATION STEP (Y=0,RHS)
C
120 TEMP(2)=H2(I-1)*DELTAR(I-1)
    IF (TEMP(2)-TRDBG) 137,137,138
C
C
C          SMALL OPTICAL DEPTH EXPANSION FOR F2
C
137 F2=F2+((Y2(I)+Y2(I-1))*0.5+X6(I-1)-F2-F2)*TEMP(2)
    GO TO 121
C
C
C          GENERAL EXPRESSION FOR F2(Y=0,RHS)
C
138 F2=Y2(I)-TG(I)+((F2-Y2(I-1)+TG(I-1))*H4(I-1)
    1 +TG(I)-TG(I-1))*H4(I-1)
121 IF(F2.LT.0.)GO TO 221
C
C
C          SAVE RHS INTENSITIES IN SUMX4
C
223 SUMX4(I)=F2
    OX(I)=C(I)
    IF(TG(I).EQ.0.) Y2(I)=X6(I)

```

```

      I=I+1
      IF(TG(I).EQ.0.) Y2(I)=X6(I-1)
      IF(I-IBXP1)122,122,126
122  IF(I-ICX) 120,120,124
C
C      NEGATIVE F2 ZEROED
C
221  F2=0.0
      GO TO 223
124  IF(F2.EQ.0.) GO TO 223
      F2=F2*FREXP(-H3(I-1)-H3(I-1))
      GO TO 223
C*****
C
C      COMPLETE Y = 0 RAY
C
C*****
126  YSQD1=0.0
      JJ=1
      JJJ=1
      KK=1
C
C      SEARCH FOR Y-LINE NEAR HALF OF C(IAX)
C
      C1=0.50*C(IAX)
      II=IAX+1
      GO TO 708
C*****
C
C      SET UP Y - L I N E S
C
C*****
C
C      FIRST, TEST IF Y LIES OUTSIDE OF ACTIVE MESH.
C
127  IF(JJ-NY) 129,129,308
128  IF(C(II)-Y(JJ))152,150,150
152  II=II+1
      GO TO 128
129  IF(C(ICX)-Y(JJ))307,151,151
146  IF(C(IAX)-Y(JJ))128,145,130
130  IF(C1-Y(JJ))141,141,142
142  IF(C1-Y(JJ+1))144,140,140
140  JJ=JJ+1
      KK=KK-IFIX(X(KK+1))+2
      GO TO 127
C
C      SEARCH FOR Y-LINE NEAR THREE QUARTERS OF C(IAX)
C
141  C1=C1+0.25*C(IAX)

```

```

GO TO 145
144 IF(Y(JJ)+Y(JJ+1)-C1-C1)140,141,141
145 YSQDP=-X(KK)
      K=KK+IM-IBX+2
      TEMP(5)=YSQDP-YSQD1
      GO TO 503
151 IF(C(IBXP1)-Y(JJ))300,300,146
C
C      SEARCH FOR Y-LINE NEAR C(IAx)
C
150 IF(C(IAx)-Y(JJJ-1))153,153,145
153 TEMP(1)=X6(II)+X6(II-1)
      IF(TEMP(1).EQ.0.)GO TO 154
C
C      SKIP Y-LINES (UP TO 4) IF SOURCE (X6) AND MFP (H) ARE
C      FLAT (CRITERION BASED ON GL)
C
      IF(ABS((X6(II)-X6(II-1))/TEMP(1))-GL)154,145,145
154 IF(ABS((H(II)-H(II-1))/(H(II)+H(II-1))-GL)155,145,145
155 IF(JJ=JJJ-4)157,145,145
157 JJ=JJ+1
      KK=KK-IFIX(X(KK+1))+2
      GO TO 127
307 TEMP(1)=CSQD(ICX+1)
      GO TO 305
308 TEMP(1)=CSQD(IR+1)
      GO TO 305
C*****
C
C      COMPLETE X2 INTEGRATION WHEN LAST Y-LINE USED
C*****
300 DO 310 I=IAXP,IBXP1
C
C      ANGULAR INTEGRATION OF X2 USING LINEAR INTERPOLATION
C
      X2(I)=X2(I)+(OX(I)+OX(I))*(SUMX4(I)-SUMX3(I))*OX(I)
C
C      OPTIONAL CALCULATION ON S12
C
      IF(EDITMF)310,310,625
625 IARG1=SOLID(18)+0.001
      IARG2=EDITMF+0.001
      IF(MOD(IARG1,IARG2))310,627,310
627 IF(1BX-1M)315,317,510
315 IF(1-IAXP)510,312,340
312 XS=SQRT(CSQD(IBXP1+1)-CSQD(1BXPI))
      FM(1BXPI)=Y2(1BXPI)+XS/C(1BXPI+1)*TG(1BXPI+1)*
1      EXP(-XS*H(1BXPI))
      GO TO 340

```

```

317 FM(IBXP1)=0.0
340 TEMP(5)=CSQD(IBXP1)-YSQD1
    TEMP(11)= CSQD(I)-YSQD1
    FU=(TEMP(11))*(FM(IBXP1)+FM(IBXP1))+(CSQD(IBXP1)-
1    CSQD(I))*(SUMX4(IAXP)+SUMX3(IAXP))/TEMP(5)
    FL=SUMX3(I)+SUMX4(I)
    TEMP(6)=OX(I)*OX(I)
    FP=FL+FL
    FPL=FP+FL
    RHO(I)=RHO(I)+OX(I)*FP
    PR(I)=PR(I)+TEMP(6)*(FPL+FL)*OX(I)
    PHO(I)=PHO(I)+FU*(OX(I)*TEMP(9)+CSQD(I)*ARSIN(OX(I)/C(I)))
1    +.667*(FL-FU)*(C(I)*CSQD(I)-TEMP(9)*YSQD1)/OX(I)
    PH1(I)=PH1(I)+FPL*TEMP(6)

```

```

310 CONTINUE

```

```

C*****
C
C      C O M P L E T I O N   O F   X 2   I N T E G R A T I O N   A T
C      E N D   O F   T R A N S   R E G I O N
C
C*****

```

```

C
C      B R I G H T N E S S   P R I N T
C

```

```

320 IF(CB) 726,725,726
726 IARG1=SOLID(18)+0.001
    IF (IARG1 .EQ. 0) GO TO 725
    IARG2=CB+0.001
    IF (MOD(IARG1,IARG2)) 725,727,725
727 XX = -1.0
    WRITE (3)  XX, IAX, IBX, NY, SOLID(18), TH, XX
    WRITE (3)  (Y(J), J=1,NY), (Q2(J), J=1,NY)
    XX = -2.0
    WRITE (3)  XX, XX, XX, XX, XX, XX, XX
    BACKSPACE 3
725 DO 321 I=IAx,IBXP1

```

```

C
C      O P T I O N A L   C A L C U L A T I O N   O N   S 1 2
C

```

```

    IF(EDITMF) 321,321,730
730 IARG1=SOLID(18)+0.001
    IARG2=EDITMF+0.001
    IF(MOD(IARG1,IARG2))321,731,321
731 IF(I.EQ.1) GO TO 321
    RHO(I)=RHO(I)*34.25/C(I)
    PR(I)=PR(I)*5.71/(CSQD(I)*C(I))
    PHO(I)=PHO(I)*0.327E12/CSQD(I)
    PH1(I)=PH1(I)*0.343E12/CSQD(I)
321 X2(I)=X2(I)*1.026E12
322 RETURN

```

C
C
C

COMPLETE X2 INTEGRATION WHEN NO MORE SOURCES

```
305 F2=0.0
    TEMP(5)=TEMP(1)-YSQD1
    DO 306 I=IAXP,IBXP1
    TEMP(15)=TEMP(1)-CSQD(I)
    IF(TEMP(15)) 318,319,319
318 FM(I)=0.0
```

C
C
C

ANGULAR INTEGRATION OF X2 USING LINEAR INTERPOLATION

```
    XM=SQRT(-TEMP(15))
    X2(I)=X2(I)+(OX(I)-XM)*(OX(I)+OX(I)+XM)*(SUMX4(I)-SUMX3(I))
    IF(EDITMF) 306,306,323
323 IARG1=SOLID(18)+0.001
    IARG2=EDITMF+0.001
    IF(MOD(IARG1,IARG2)) 306,324,306
324 FL=SUMX3(I)+SUMX4(I)
    TEMP(6)=OX(I)*OX(I)
    TEMP(7)=-TEMP(15)
    FCA=SQRT(TEMP(1))
    FXM=OX(I)-XM
    FXP=OX(I)+XM
    RHO(I)=RHO(I)+FXM*FL
    PR(I)=PR(I)-FXP*(TEMP(6)+TEMP(7))*FL
1    +4.0*FL*OX(I)*TEMP(6)
    PHO(I)=PHO(I)-(FL*XM*(OX(I)*TEMP(9)-XM*FCA+CSQD(I)*
1 (ARSIN(OX(I)/C(I))-ARSIN(XM/C(I)))-0.667*FL*(FCA*TEMP(1)
2 -TEMP(9)*YSQD1)))/FXM
    PH1(I)=PH1(I)+FXM*FL*(FXP+OX(I))
    GO TO 306
```

C
C
C

ANGULAR INTEGRATION OF X2 USING LINEAR INTERPOLATION

```
319 X2(I)=X2(I)+(OX(I)+OX(I))*(SUMX4(I)-SUMX3(I))*OX(I)
```

C
C
C

OPTIONAL CALCULATION ON S12

```
    IF(EDITMF) 306,306,635
635 IARG1=SOLID(18)+0.001
    IARG2=EDITMF+0.001
    IF(MOD(IARG1,IARG2)) 306,637,306
637 TEMP(5)=TEMP(1)-YSQD1
    FU=TEMP(15)*(SUMX4(IAXP)+SUMX3(IAXP))/TEMP(5)
    FL=SUMX3(I)+SUMX4(I)
    TEMP(6)=OX(I)*OX(I)
    FP=FL+FU
    FPL=FP+FPL
    RHO(I)=RHO(I)+OX(I)*FP
```

```

PR(I)=PR(I)+TEMP(6)*(FPL+FL)*OX(I)
PHO(I)=PHO(I)+FU*(OX(I)*TEMP(9)+CSQD(I)*ARSIN(OX(I)/C(I)))
1   +.667*(FL-FU)*(C(I)*CSQD(I)-TEMP(9)*YSQD1) / OX(I)
PH1(I)=PH1(I)+FPL*TEMP(6)
306 CONTINUE
GO TO 320

```

```

C*****

```

```

C

```

```

C      T Y P I C A L   Y - L I N E   I N T E G R A T I O N

```

```

C

```

```

C*****

```

```

C

```

```

C      LHS CALCULATION FIRST,STORE F2 IN FM

```

```

C

```

```

503 I=IBXP1

```

```

    F2=0.0

```

```

502 IF (IBX-1M) 506,508,510

```

```

C

```

```

C      ERROR IF INDEX EXCEEDS NORMAL RANGE

```

```

C

```

```

510 S1=14.0510

```

```

    CALL UNCLE

```

```

C

```

```

C      DIFFUSION BOUNDARY CONDITION AT IBXP1

```

```

C

```

```

506 IF (TG(I) .EQ. 0.0) Y2(I)=X6(I)

```

```

    X8(I)=X(K)/C(I)*TG(I)

```

```

    TEMP(2)=(X(K-1)-X(K))*H2(I)

```

```

    IF (TEMP(2)-TRDBG) 533,533,534

```

```

C

```

```

C      SMALL OPTICAL DEPTH EXPANSION (DIFF)

```

```

C

```

```

533 F2=Y2(I+1)+X(K-1)/C(I+1)*TG(I+1)+((Y2(I)+Y2(I+1))*0.5+X6(I))

```

```

1   *TEMP(2)

```

```

    GO TO 512

```

```

C

```

```

C      GENERAL EXPRESSION FOR F2 (DIFF,LHS)

```

```

C

```

```

534 TEMP(1)=(X(K-1)-X(K))*H(I)

```

```

    H4(I)=FREXP(-TEMP(1))

```

```

    F2=Y2(I)+X8(I)+(X(K-1)/C(I+1)*TG(I+1)-X8(I))*H4(I)

```

```

    GO TO 512

```

```

C

```

```

C      SAVE X8 FOR RHS=(DIFF INTENSITY)

```

```

C

```

```

511 X8(I)=X(K)/C(I)*TG(I)

```

```

    TEMP(2)=(X(K-1)-X(K))*H2(I)

```

```

C

```

```

C      REGULAR INTEGRATION STEP(LHS)

```

```

C

```

```

      IF (TEMP(2)-TRDBG) 531,531,532
C
C      SMALL OPTICAL DEPTH EXPANSION (LHS)
C
531 F2=F2+((Y2(I)+Y2(I+1))*0.5+X6(I)-F2-F2)*TEMP(2)
      GO TO 512
C
C      GENERAL EXPRESSION FOR F2(LHS)
C
C      SAVE EXP FOR RHS
C
532 TEMP(1)=(X(K-1)-X(K))*H(I)
      H4(I)=FREXP(-TEMP(1))
      F2=Y2(I)+X8(I)+((F2-Y2(I+1)-X8(I+1))*H4(I)
1      +X8(I+1)-X8(I))*H4(I)
512 IF(F2.LT.0.) GO TO 515
C
C      SAVE F3 OF LHS IN FM FOR INTEGRATION.
C
613 FM(I)=F2
      IF(TG(I).EQ.0.) Y2(I)=X6(I-1)
      I=I-1
      K=K+1
      IF(TG(I).EQ.0.) Y2(I)=X6(I)
      IF(I-1AX)516,513,513
513 IF(X(K))514,509,511
514 TEMP(3)=SQRT(DELTA(I)*(4.0*C(I)+DELTA(I))*H(I)
      IF (TEMP(3) .GT. 0.0) GO TO 517
      S1=14.0517
      CALL UNCLE
517 TEMP(2)=X(K-1)*H2(I)
      IF (TEMP(2)-TRDBG) 535,535,536
535 TEMP(16)=(Y2(I+1)+X6(I))*TEMP(2)+(0.667*Y2(I)-0.5*Y2(I+1)
1      -0.167*X6(I))*TEMP(3)*H2(I)/H(I)
      F2=F2*(1.0-2.0*TEMP(2))+TEMP(16)
      GO TO 521
536 TEMP(1)=2.0*X(K-1)*H(I)
      H4(I)=FREXP(-TEMP(1))
      TEMP(7)=FREXP(-TEMP(3))
      TEMP(13)=(X6(I)-Y2(I))/TEMP(3)**2*2.0
      TEMP(15)=(X6(I)-Y2(I+1))/(TEMP(1)-TEMP(3))
      F2=Y2(I)+TEMP(13)+TEMP(7)*(-TEMP(15)-TEMP(13)*(TEMP(3)+1.0))
1      +H4(I)*(F2-Y2(I+1)+TEMP(15))
      GO TO 521
C
C      NEGATIVE F2 ZEROED
C
515 F2=0.0
      GO TO 613
C

```

```

C          FIRST TRANSPORT ZONE ON LHS
C
507 X8(I)=X(K)/C(I)*TG(I)
    GO TO 613
C
C          X = ZERO ERROR
C
509 S1=14.0509
    CALL UNCLE
508 FM(I)=0.0
    I=I-1
    K=K+1
    IF(I-1-ICX) 510,507,508
523 F2=0.0
    GO TO 522
C
C          DO Y-INTEGRATION TO X=0
C
521 IF(F2.LT.0.)GO TO 523
522 FM(I)=F2
C
C          FORM TOP SLICE CONTRIBS TO X2
C
    DO 524 J=IAXP,I
333 TEMP(11)=CSQD(J)-YSQD1
    X2(J)=X2(J)+(OX(J)+OX(J))*(SUMX4(J)-SUMX3(J))*OX(J)
C
C          OPTIONAL CALCULATION ON S12
C
    IF(EDITMF) 524,524,331
331 IARG1=SOLID(18)+0.001
    IARG2=EDITMF+0.001
    IF(MOD(IARG1,IARG2)) 524,332,524
332 FU=(TEMP(11)*(FM(I)+F2)+(YSQD1-CSQD(J))*(SUMX4(IAXP)
1      +SUMX3(IAXP)))/TEMP(5)
    FL=SUMX3(J)+SUMX4(J)
    TEMP(6)=OX(J)*OX(J)
    FP=FL+FU
    FPL=FP+FL
    RHO(J)=RHO(J)+OX(J)*FP
    PR(J)=PR(J)+TEMP(6)*(FPL+FL)*OX(J)
    PH0(J)=PH0(J)+FU*(OX(J)*TEMP(9)+CSQD(J)*ARSIN(OX(J)/C(J)))
1      +0.667*(FL-FU)*(C(I)*CSQD(I)-TEMP(9)*YSQD1)/OX(I)
    PH1(J)=PH1(J)+FPL*TEMP(6)
524 CONTINUE
    IAXP=I+1
    SUMX3(I)=F2
    SUMX4(I)=F2
    I=IAXP
    K=K-1

```

```

      IF (TEMP(2)-TRDBG) 538,538,700
C
C      SMALL OPTICAL DEPTH EXPANSION (X=0,RHS)
C
538 F2=F2*(1.0-2.0*TEMP(2))+TEMP(16)
      GO TO 704
700 F2=Y2(I)+TEMP(15)+FREXP(-TEMP(1)+TEMP(3))*(-TEMP(15)
1    +TEMP(13)*(1.0-TEMP(3)))+H4(I-1)*(F2-Y2(I-1)-TEMP(13))
      GO TO 704
C
C      CALCULATE RHS Y-LINE INTEGRATION
C
516 IAXP=IAX
      I=IAX
      K=K-1
      IF(X(K+1))525,509,526
526 X8(I-1)=X(K+1)/C(I-1)*TG(I-1)
      TEMP(2)=(X(K)-X(K+1))*H2(I-1)
C
C      DIFFUSION BOUNDARY CONDITION AT IAX
C
      IF (TEMP(2)-TRDBG) 537,537,702
C
C      SMALL OPTICAL DEPTH EXPANSION (DIFF,LHS)
C
537 F2=Y2(I-1)-X8(I-1)+((Y2(I)+Y2(I-1))*0.5 + X6(I-1))*TEMP(2)
      GO TO 704
C
C      GENERAL EXPRESSION FOR F2(DIFF,RHS)
C
702 TEMP(1)=(X(K)-X(K+1))*H(I-1)
701 F2=Y2(I)-X8(I)+(X8(I)-X8(I-1))*FREXP(-TEMP(1))
      GO TO 704
710 TEMP(2)=(X(K)-X(K+1))*H2(I-1)
      IF (TEMP(2)-TRDBG) 539,539,540
C
C      SMALL OPTICAL DEPTH EXPANSION(RHS)
C
539 F2=F2+((Y2(I)+Y2(I-1))*0.5+X6(I-1)-F2-F2)*TEMP(2)
      GO TO 704
540 F2=Y2(I)-X8(I)+((F2-Y2(I-1)+X8(I-1))*H4(I-1)
1    +X8(I)-X8(I-1))*H4(I-1)
704 IF(F2.LT.0.)GO TO 705
C
C      FORM CONTRIB TO X2
C
706 CONTINUE
C
C      ANGULAR INTEGRATION OF X2 USING LINEAR INTERPOLATION
C

```

```

703 X2(I)=X2(I)+((X(K)+X(K)+OX(I))*F2-FM(I))
1    +(OX(I)+OX(I)+X(K))*(SUMX4(I)-SUMX3(I))*(OX(I)-X(K))

```

C
C
C
OPTIONAL CALCULATIONS OF H.F. QUANTITIES ONLY ON EDITMF

```

IF(EDITMF)735,735,736
736 IARG1=SOLID(18)+0.001
IARG2=EDITMF+0.001
IF (MOD(IARG1,IARG2)) 735,732,735
732 FU=FM(I)+F2
FL=SUMX3(I)+SUMX4(I)
TEMP(6)=OX(I)*OX(I)
TEMP(7)=X(K)*X(K)
FXM=OX(I)-X(K)
FXP=OX(I)+X(K)
FM1=FU-FL
RHO(I)=RHO(I)+FXM*(FU+FL)
PR(I)=PR(I)+FXP*(TEMP(6)+TEMP(7))*FM1
1    +4.0*(FL*OX(I)*TEMP(6)-FU*X(K)*TEMP(7))
PHO(I)=PHO(I)+((OX(I)*FU-X(K)*FL)*(OX(I)*TEMP(9)-X(K)*Y(JJ)
1    +CSQD(I)*(ARSIN(OX(I)/C(I))-AFSIN(X(K)/C(I))))-0.667*FM1
2    *(Y(JJ)*YSQDP-TEMP(9)*YSQD1))/FXM
PH1(I)=PH1(I)+FXM*(F2*(FXP+X(K))+SUMX4(I)*(FXP+OX(I)))

```

C
C
C
SAVE F2 AND FM FOR NEXT Y-LINE

```

735 SUMX4(I)=F2
SUMX3(I)=FM(I)
OX(I)=X(K)
IF(TG(I).EQ.0.) Y2(I)=X6(I)
I=I+1
K=K-1
IF(TG(I).EQ.0.) Y2(I)=X6(I-1)
IF(I-1BXPL)707,707,706
707 IF(I-1-ICX)710,710,711

```

C
C
C
NEGATIVE F2 ZEROED

```

705 F2=0.0
GO TO 706
711 IF(F2.EQ.0.) GO TO 706
TEMP(1)=(X(K)-X(K+1))*H(I-1)
H4(I-1)=FREXP(-TEMP(1)-TEMP(1))
F2=F2*H4(I-1)
GO TO 706

```

C
C
C
DIFFUSION BOUNDARY CONDITION WHEN X=0.

```

525 X8(I-1)=0.0
TEMP(1)=X(K)*H(I-1)

```

```

GO TO 701
708 OHNU=HAUP-HAU
712 IF(JJ.EQ.1) GO TO 722

```

```

C*****
C
C      EDIT AND Y-LINE ADVANCE
C
C*****

```

```

      KK=KK-IF(IX(KK+1)).*2
722 YSQD1=YSQD(JJ)
      TEMP(9)=Y(JJ)
      JJ=JJ+1
724 JJJ=JJ
      Q2(JJ-1)=F2*3.274E4
GO TO 127
END

```

Appendix C

FREXP

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```

$IBMAP FREEMA LIST,DECK,REF
*
* DECK FREEMA EVALUATES FUNCTION FREXP(ARG)
*
* EVALUATE THE NEGATIVE POWER OF E(E**X) FOR X BETWEEN
*
* 0.0 AND -10.0 TO FOUR SIGNIFICANT FIGURES. WHEN X LIES
*
* OUTSIDE THE RANGE, THE STANDARD ROUTINE(EXP) IS USED.
*
* THE METHOD IS AS FOLLOWS, E**X=E**N+E**P-E**2,
*
* WHERE N IS THE INTEGRAL PART OF THE EXPONENT AND P IS THE
*
* MULTIPLE OF 2**-7 CONTAINED IN THE FRACTIONAL PART.
*
* R=X-N-P. THE VALUES OF E**N AND E**P ARE FOUND BY
*
* TABLE LOOK-UP IN ITAB AND FTAB RESPECTIVELY, E**R IS FOUND
*
* AS 1.0-R.
*
* ENTRY FREXP
*
* EXTERN EXP
*
* AXT **,2 RESTORE
*
* AXT **,4 INDICES 2 AND 4
*
* FREXP TRA ** RETURN ADDRESS
*
* SXA *-3,4 SAVE INDICES 2 AND 4
*
* LAC FREXP,4 LOCATE ARGUMENT
*
* CLA* 2,4 PICK UP THE ARGUMENT
*
* CAS =-9.99 SELECT THE
*
* TMI **3 NUMBERS BETWEEN
*
* TMI **2 0.0 AND -9.99
*
* TRA NORMAL OUTSIDE THAT RANGE
*
* ARGUMENT IN THE RIGHT RANGE
*
* UFA =0633000000000 EXTRICATE THE INTEGER PART
*
* CAS =0633000000000
*
* TRA NORMAL
*
* TRA SIMPLE
*
* PAC 0,4 PUT THE INTEGER PART IN THE INDEX
*
* STQ T1 PUT THE FRACTIONAL PART
*
* SXA FREXP-2,2 SAVE INDEX 2
*
* CLA T1 IN THE AC
*
* UFA =0624000000000 EXTRICATE THE 2**-7 MULTIPLE
*
* PAC 0,2 PUT IT IN INDEX 2
*
* REMAINDER LEFT IN MQ
*
* FMP FTAB,2 FIND THE FRACTIONAL
*
* FAD FTAB,2 POWER
*
* STO T1 PUT IT
*
* LDQ T1 IN THE AC
*
* FMP ITAB,4 MULTIPLY IT BY THE INTEGRAL POWER
*
* TRA FREXP-2 RETURN WITH ANSWER IN THE AC
*
* THE EXPONENT LIES BETWEEN 0.0 AND -1.0
*
* SIMPLE STQ T1
*
* CLA T1
*
* UFA =0624000000000
*
* PAC 0,4
*
* FMP FTAB,4
*
* FAD FTAB,4
*
* TRA FREXP-1

```

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NORMAL	CLA	2,4	
	STA	N1	
	TSL	EXP	
	TXI	*+3,,1	
	BCI	1,FREXP	
N1	PZE	**	
	TRA	FREXP-1	
T1	PZE		
ITAB	DEC	1.0	0
	DEC	0.3678794411	1
	DEC	0.1353352832	2
	DEC	0.0497870683	3
	DEC	0.0183156388	4
	DEC	0.0067379469	5
	DEC	0.0024787521	6
	DEC	0.0009118819	7
	DEC	0.0003354626	8
	DEC	0.0001234098	9
FTAB	DEC	1.0	0
	DEC	.99221794	
	DEC	.98449644	
	DEC	.97683503	
	DEC	.96923324	
	DEC	.96169060	
	DEC	.95420668	
	DEC	.94678098	
	DEC	.93941307	
	DEC	.93210250	
	DEC	.92484882	
	DEC	.91765159	
	DEC	.91051038	
	DEC	.90342472	
	DEC	.89639421	
	DEC	.88941842	
	DEC	.88249691	
	DEC	.87562926	
	DEC	.86881506	
	DEC	.86205389	
	DEC	.85534534	
	DEC	.84868899	
	DEC	.84208444	
	DEC	.83553128	
	DEC	.82902913	
	DEC	.82257757	
	DEC	.81617622	
	DEC	.80982469	
	DEC	.80352259	
	DEC	.79726952	
	DEC	.79106511	
	DEC	.78490900	

DEC	.77880079
DEC	.77274011
DEC	.76672660
DEC	.76075989
DEC	.75483961
DEC	.74896540
DEC	.74313691
DEC	.73735377
DEC	.73161563
DEC	.72592215
DEC	.72027299
DEC	.71466778
DEC	.70910619
DEC	.70358787
DEC	.69811252
DEC	.69267976
DEC	.68728928
DEC	.68194076
DEC	.67663385
DEC	.67136824
DEC	.66614361
DEC	.66095965
DEC	.65581602
DEC	.65071242
DEC	.64564854
DEC	.64062406
DEC	.63563868
DEC	.63069209
DEC	.62578401
DEC	.62091413
DEC	.61608213
DEC	.61128774
DEC	.60653067
DEC	.60181060
DEC	.59712727
DEC	.59248041
DEC	.58786967
DEC	.58329484
DEC	.57875560
DEC	.57425170
DEC	.56978284
DEC	.56534874
DEC	.56094916
DEC	.55658382
DEC	.55225246
DEC	.54795480
DEC	.54369058
DEC	.53945954
DEC	.53526144
DEC	.53109600

DEC .52696298
DEC .52286212
DEC .51879318
DEC .51475589
DEC .51075003
DEC .50677535
DEC .50283159
DEC .49891852
DEC .49503590
DEC .49118350
DEC .48736108
DEC .48356841
DEC .47980525
DEC .47607137
DEC .47236656
DEC .46869057
DEC .46504319
DEC .46142419
DEC .45783336
DEC .45427047
DEC .45073532
DEC .44722766
DEC .44374731
DEC .44029404
DEC .43686765
DEC .43346792
DEC .43009464
DEC .42674762
DEC .42342664
DEC .42013151
DEC .41686203
DEC .41361798
DEC .41039918
DEC .40720543
DEC .40403653
DEC .40089229
DEC .39777252
DEC .39467703
DEC .39160563
DEC .38855813
DEC .38553435
DEC .38253409
DEC .37955719
DEC .37660345
DEC .37367270
DEC .37076476
DEC .36787944
END

Appendix D

KAPPA

\$IBFTG KAPPA FULIST,DECK,REF
SUBROUTINE KAPPA(N,M)

C
C THIS ROUTINE WAS RECOMPILED JANUARY 11, 1965
C T W O - D I A N E - T A P E V E R S I O N
C ASSUMES EXTRA CALL FOR GREY DATA -- NO GOOD WITH STANDARD RADTN
C DOES MONOFREQUENCY WITH AVERAGE KAPPAS
C

C*****

C
C* S P U T T E R C O M M O N **
C* **
C* **

COMMON	LMDA(37),	NR	, NSMLR ,	IA	, IB	, ICA	, ICB	,
1 KMAX	, BLANK1,	BLANK2,	BLANK3,	IAP1	, IBP1	, ICAP1	, ICBP1	,
2 II	, IG	, NRAD	, BLANK4,	IAM1	, IBM1	, ICAM1	, ICBM1	,
3 IIP1	, IGM1	, IALPHA,	BLANK5,	TH	, TMAX	, BLANK6,	DELPRT,	
4 FREQ	, CNTMAX,	AR	, ASMLR ,	PUSHA	, PUSHB	, BOILA	, BOILB	,
5 CVA	, CVB	, SLUG	, ALPHA	, HVA	, HVB	, HCA	, HCB	,
6 EMINA	, EMINB	, CA	, CB	, GA	, GB	, GL	, GR	,
7 RHOL	, RHOR	, EPIO	, EPSI	, RIA	, RIB	, RDIA	, RDRB	,
8 RPIA	, RPIB	, RPDIA	, RPDIB	, TPRINT,	TA	, TB	, TC	,
COMMON	TD	, TE	, DTH2	, DTH2P	, DTH1	, DTRMIN,	DTMAX	,
1 DTMAX1,	DTMAX2,	DTMAX3,	DTR	, SWITCH,	CO	, CMIN	, DELTA	,
2 GAMA	, WCRIT	, SIGMAQ,	AC	, ACO3T4,	CNVRT	, SUMRA	, SUMRB	,
3 ROIA	, ROIAM1,	ROIB	, ROIBP1,	GMS	, S1	, S2	, S3	,
4 S4	, S5	, S6	, S7	, S8	, S9	, S10	, S11	,
5 S12	, S13	, S14	, S15	, S16	, S17	, S18	, S19	,
6 S20	, EO	, FO	, TAU	, ZERO	, R	(152),	DELTAR(152),	
7 ASQ	(152),	RD	(152),	VD	(152),	RDD	(152),	SMLR (152),
8 DELR	(37),	P	(152),	PI	(152),	PB	(152),	PBI (152)
COMMON		P2	(152),	SV	(152),	RHO	(152),	THETA (152),
1 W	(152),	E	(152),	EI	(152),	EK	(152),	A (152),
2 V	(152),	G	(152),	D	(152),	C	(152),	X2 (152),
3 X3	(152),	X4	(152),	X5	(152),	X6	(152),	X7 (152),
4 SMLA	(152),	SMLB	(152),	SMLC	(152),	SMLD	(152),	SMLE (152),
5 EC	(152),	ER	(152),	SMLQ	(152),	SMLH	(152),	BIGA (152),
6 BIGB	(152),	CV	(152),	BC	(152),	BR	(152),	CHIC (152),
7 CHIR	(152),	CAPAC	(152),	CAPAR	(152),	CRTC	(152),	CRTR (152),
8 CRTPC	(152),	GOFR	(152),	FEW	(152),	CAR	(152),	OKLM (37)
COMMON		TELM	(37),	EKLM	(37),	ELM	(37),	FCLM (37),
1 FRLM	(37),	WLM	(37),	QLM	(37),	AMASNO(37),	CHRNA (37),	
2 ZP1	(37),	ZP2	(37),	SOLID	(37),	ECHCK	(37),	RK (104),
3 RL	(37),	RHOK	(104),	RDK	(104),	THETAK(104),	TEMP	(16),
4 HEAD	(12),	MAXL		, MAXLM				

C* **
C*****

DIMENSION CSQD(1), FM(1), H4(1), Y2(1), X(1), Y(1), H(1), SUMX2(1)
DIMENSION SUMX3(1), SUMX4(1), SUMRHO(1), Q37(1), Q38(1), H3(1)
DIMENSION THETAT(23), KAMAX(23), KCNT(23), BUFS(750,1), ID(12)

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COMMON /LINDLY/ HNU,SGNL,IHNU,NHNU,HNUP,NT,IM,IN,DHNU,THICK,NY

C

EQUIVALENCE (SMLC,CSQD), (SMLB,FM), (SMLA,H4), (SMLD,Y2), (GOFR,X)
EQUIVALENCE (BIGA,Y), (BIGB,H), (CRTR,SUMX2), (CHIC,SUMX3), (BC,SUMX4)
EQUIVALENCE (SMLH,SUMRHO), (CAR,Q37), (CHIR,Q38), (BR,H3)
EQUIVALENCE (ECHCK(18),ID(1))

C

CAVEAT: KAPPA WILL FAIL ON ANY TWO LAMBDA REGIONS OF THE SAME MATERIAL
C IF THERE IS BETWEEN THEM AT LEAST ONE REGION OF A DIFFERENT MATERIAL
C FOR WHICH A DIANE TAPE IS TO BE READ.

C AMASNO(17-29) RESERVED FOR DESIGNATION OF DIANE TAPE UNIT.

100 FORMAT (I12, 12A6)

IN=N

IM=M

NT = 0

NMAT = 0

110 DO 600 J=1,MAXLM

IK=LMDA(J)

IL=LMDA(J+1)-1

IF (IL-IN) 600,130,120

120 IF (IK-IN) 130,140,140

130 IK=IN

GO TO 170

140 IF (IK-IM) 150,160,600

150 IF (IL-IM) 170,170,160

160 IL=IM

170 CONTINUE

SOLID(20)=IK

SOLID(21)=IL

SOLID(22)=J

L=OKLM(J)

180 IF (AMASNO(L+17)) 190,190,320

C DONT READ A DIANE TAPE. CALL A KAP INSTEAD.

190 GO TO (200,210,220,230,240,250,260,270,280,290,300,310), L

200 CALL KAP1

GO TO 590

210 CALL KAP2

GO TO 590

220 CALL KAP3

GO TO 590

230 CALL KAP4

GO TO 590

240 CALL KAP5

GO TO 590

250 CALL KAP6

GO TO 590

260 CALL KAP7

GO TO 590

270 CALL KAP8

GO TO 590

```

280 CALL KAP9
    GO TO 590
290 CALL KAP10
    GO TO 590
300 CALL KAP11
    GO TO 590
310 CALL KAP12
    GO TO 590
320 I = AMASNO(L+17)
    IF (NT-1) 330,460,330
C   READ DIANE TAPE
330 NT = AMASNO(L+17)
    NHAT = NHAT + 1
C   LIMIT ON NHAT SET BY DIMENSION OF BUFS
    IF (NHAT-1) 345,345,340
340 S1 = 15.0931
    CALL UNCLE
345 IF (KMAX) 370,350,370
350 IF (S15.EQ.0.) GO TO 420
    READ (NT,100) IDA,(ID(I),I=1,12)
    READ(NT) THNU,FNWD
    NWD=FNWD
    NHNU=THNU
    DO 360 I=1,NHNU
    READ(NT)
360 READ(NT)
    READ(NT) HNU,FJAMAX
    JAMAX=FJAMAX
    IF(HNU.GT.0.) GO TO 365
    READ(NT) (BUFS(I,NHAT),I=1,NWD)
    NHNU=1.
    REWIND NT
    GO TO 420
365 S1=15.0365
    CALL UNCLE
370 IF (IHNU-1) 380,380,390
380 READ (NT,100) IDA,(ID(I),I=1,12)
    READ (NT) THNU, FNWD
    NHNU = THNU
    NWD = FNWD
390 READ (NT) HNU, FJAMAX
    JAMAX = FJAMAX
    READ (NT) (BUFS(I,NHAT), I=1,NWD)
    IF (IHNU-NHNU-1) 420,410,400
400 S1 = 15.0957
    CALL UNCLE
410 REWIND NT
420 DO 430 JA=1,23
430 KENT(JA) = 0
    NCNT = 1

```

```

DO 450 JA=1,JAMAX
  THETAT(JA) = BUFS(NCNT,NMAT)
  KAMAX(JA) = BUFS(NCNT+1,NMAT)
  IF (JA-JAMAX) 440,450,450
440 KCNT(JA+1) = KCNT(JA) + 3 * KAMAX(JA) + 2
450 NCNT = NCNT + 3 * KAMAX(JA) + 2
460 IL = SOLID(21)
  IK = SOLID(20)
  DO 580 I=IK,IL
    TTST = Q37(I)
    RTST = Q38(I)
  DO 470 JA=2,JAMAX
    IF (TTST-THETAT(JA)) 480,480,470
470 CONTINUE
    JAT = JAMAX
    GO TO 490
480 JAT = JA
490 KAM = KAMAX(JAT)
    KAM1 = KAMAX(JAT-1)
    DO 500 KA=2,KAM
      NCNT = KCNT(JAT) + 3 * KA - 1
      IF (RTST-BUFS(NCNT+3,NMAT)) 510,510,500
500 CONTINUE
      KAT2 = KA - 1
      GO TO 520
510 KAT2 = KA
520 DO 530 KA=2,KAM1
      NCNT2 = KCNT(JAT-1) + 3 * KA - 1
      IF (RTST-BUFS(NCNT2+3,NMAT)) 540,540,530
530 CONTINUE
      KAT1 = KA - 1
      GO TO 550
540 KAT1 = KA
550 NCNT1 = KCNT(JAT-1) + 3 * KAT1 - 1
      NCNT4 = KCNT(JAT) + 3 * KAT2 - 1
      AA1 = BUFS(NCNT1-2,NMAT)
      AA2 = BUFS(NCNT1+1,NMAT)
      AA3 = BUFS(NCNT4-2,NMAT)
      AA4 = BUFS(NCNT4+1,NMAT)
      AA5 = BUFS(NCNT1,NMAT)
      AA6 = BUFS(NCNT1+3,NMAT)
      AA7 = BUFS(NCNT4,NMAT)
      AA8 = BUFS(NCNT4+3,NMAT)
      AA9 = THETAT(JAT)
      AA10 = THETAT(JAT-1)
      AA11 = BUFS(NCNT1-1,NMAT)
      AA12 = BUFS(NCNT1+2,NMAT)
      AA13 = BUFS(NCNT4-1,NMAT)
      AA14 = BUFS(NCNT4+2,NMAT)
      IF (AMIN1(ABS(AA6-AA5),ABS(AA8-AA7),ABS(AA10-AA9))) 570,560,570

```

```

560 S1 = 15.0915
    CALL UNCLE
570 AAC = AA1 + (RTST - AA5) * (AA2 - AA1) / (AA6 - AA5)
    AAE = AA11 + (RTST - AA5) * (AA12 - AA11) / (AA6 - AA5)
    AAD = AA3 + (RTST - AA7) * (AA4 - AA3) / (AA8 - AA7)
    AAF = AA13 + (RTST - AA7) * (AA14 - AA13) / (AA8 - AA7)
    CAPAR(I) = EXP(AAC + (AAD - AAC) * (TTST - AA10) / (AA9 - AA10))
    CAPAC(I) = EXP(AAE + (AAF - AAE) * (TTST - AA10) / (AA9 - AA10))
580 CONTINUE
590 CONTINUE
600 CONTINUE
    S15=0.0
C    INDUCED EMISSION CORRECTION FOR KAPPAS OBTAINED FROM KAP ROUTINES,
C    NOT DIANNE TAPES, IN MULTIFREQUENCY CASE
    IF (KMAX) 610,650,610
610 IF(HNU) 650,650,615
615 DO 640 J=1,MAXLM
    IK = LMDA(J)
    IL = LMDA(J+1) - 1
    L = OKLM(J)
    IF (AMASNO(L+17)) 620,620,640
620 DO 630 I=IK,IL
630 CAPAR(I)=CAPAR(I)*(1.-EXP(-HNU/THETA(I)))
640 CONTINUE
650 CALL DVCHK(KDMY)
    GO TO (660,670), KDMY
660 S1 = 15.0152
    CALL UNCLE
670 RETURN
    END

```

Appendix E

PLNKUT

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C
SIBFTC PLNKUT FULIST,DECK,REF
FUNCTION PLNKUT(BETA1, BETA2)
C
THIS ROUTINE WAS RECOMPILED NOVEMBER 19, 1964
C

DIMENSION CSQD(1), FM(1), H4(1), Y2(1), X(1), Y(1), H(1), SUMX2(1)
DIMENSION SUMX3(1), SUMX4(1), SUMRHG(1), Q37(1), Q38(1), H3(1)

C
C*****

C
C* S P U T T E R C O M M O N **
C* **
C* **

```
COMMON LMDA(37), NR      , NSMLR , IA      , IB      , ICA      , ICB      ,
1 KMAX , BLANK1, BLANK2, BLANK3, IAP1 , IBP1 , ICAP1 , IC6P1 ,
2 SI   , IG    , NRAD  , BLANK4, IAM1 , IBM1 , ICAM1 , ICBM1 ,
3 IIP1 , IGM1 , IALPHA, BLANK5, TH   , TMAX , BLANK6, DELPRT,
4 FREQ , CNTHAX, AR    , ASMLR , PUSHA , PUSHB , BOILA , BOILB ,
5 CVA  , CVB   , SLUG  , ALPHA , HVA   , HV8   , HCA   , HCB   ,
6 EMINA , EMINB , CA    , CB    , GA    , GB    , GL    , GR    ,
7 RHOL , RHOR , EPIO , EPSI  , RIA   , RIB   , RDIA  , RDIB  ,
8 RPIA , RPIB , RPDIA , RPDIB , TPRINT, TA    , TB    , TC
COMMON TD , TE , DTH2 , DTH2P , DTH1 , DTRMIN, DTMAX ,
1 DTMAX1, DTMAX2, DTMAX3, DTR , SWITCH, CO , CMIN , DELTA ,
2 GAMA , WCRIT , SIGMAQ, AC    , ACO3T4, CNVRT , SUMRA , SUMRB ,
3 ROIA , ROIAM1, ROIB , ROI8P1, GMS , S1 , S2 , S3 ,
4 S4 , S5 , S6 , S7 , S8 , S9 , S10 , S11 ,
5 S12 , S13 , S14 , S15 , S16 , S17 , S18 , S19 ,
6 S20 , EO , FO , TAU , ZERO , R (152), DELTAR(152),
7 ASQ (152), RD (152), VD (152), RDD (152), SMLR (152),
8 DELR ( 37), P (152), P1 (152), P8 (152), PB1 (152)
COMMON P2 (152), SV (152), RHO (152), THETA (152),
1 W (152), E (152), EI (152), EK (152), A (152),
2 V (152), G (152), D (152), C (152), X2 (152),
3 X3 (152), X4 (152), X5 (152), X6 (152), X7 (152),
4 SMLA (152), SMLB (152), SMLC (152), SMLD (152), SMLE (152),
5 EC (152), ER (152), SMLQ (152), SMLH (152), SIGA (152),
6 BIGB (152), CV (152), BC (152), BR (152), CHIC (152),
7 CHIR (152), CAPAC (152), CAPAR (152), CRTC (152), CRTR (152),
8 CRTPC (152), GOFR (152), FEW (152), CAR (152), OKLM ( 37)
COMMON TELM ( 37), EKL ( 37), ELM ( 37), FCLM ( 37),
1 FRLM ( 37), WLM ( 37), QLM ( 37), AMASNO( 37), CHRNO ( 37),
2 ZP1 ( 37), ZP2 ( 37), SOLID ( 37), ECHCK ( 37), RK (104),
3 RL ( 37), RHOK (104), RDK (104), THEIAK(104), TEMP ( 16),
4 HEAD ( 12), MAXL , MAXLM
```

C
C* **
C*****
EQUIVALENCE (SMLC,CSQD), (SMLB,FM), (SMLA,H4), (SMLD,Y2), (GOFR,X)
EQUIVALENCE (BIGA,Y), (BIGB,H), (CRTR,SUMX2), (CHIC,SUMX3), (BC,SUMX4)

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EQUIVALENCE (SMLH,SUMRHO),(CAR,Q37),(CHIR,Q38),(BR,H3)

C

COMMON /TBLC/ TBL(120)

C

C*****

C WARNING//DO NOT COMPILE AND GO//TABLES MUST BE *

C SUPPLIED *

C*****

C

ASSUME BETA2 MORE THAN BETA1

IF (BETA2 - TBL(1))10, 15, 15

10 PLNKUT = .05132911 * (BETA2**3 * (1.0- BETA2 * (.375 - BETA2 *
1 .05)) - BETA1**3 * (1.0- BETA1 * (.375 - BETA1 * .05)))

RETURN

15 J = 1

BETA = BETA1

17 IF (BETA - TBL(1))18, 21, 21

18 FCN = 1.0- .05132911 * BETA**3 * (1.0- BETA * (.375 - BETA *
1 .05))

GO TO 35

21 IF (BETA - 10.) 19, 30, 30

19 I = 1

16 IF (BETA-TBL(I+1)) 20,20,25

20 FCN =TBL(I+60)+(BETA-TBL(I))*(TBL(I+61)-TBL(I+60))
1 /(TBL(I+1)-TBL(I))

GO TO 35

25 I = I + 1

IF (I - 60) 16, 30, 30

30 FCN = .153989733 * EXP(-BETA) * (((BETA + 3.0) * BETA + 6.0) *
1 BETA + 6.0)

35 GO TO (37, 40), J

37 J = 2

OFCN = FCN

BETA = BETA2

GO TO 17

40 PLNKUT = OFCN - FCN

RETURN

END

SIDMAP PLNKTT LIST,DECK,REF

* THIS ROUTINE WAS ASSEMBLED NOVEMBER 9, 1964

TBL C NTRL TBL,TBL+112

TBL DEC 1.0,1.04,1.08,1.12,1.16,1.20,1.26,1.32,1.38,1.44,1.50
DEC 1.6,1.7,1.8,1.9,2.0,2.1,2.2,2.4,2.6,2.9,3.2,3.5,3.8,4.0
DEC 4.2,4.4,4.6,4.8,5.0,5.2,5.4,5.6,5.8,6.0,6.16,6.32,6.48
DEC 6.64,6.80,6.96,7.12,7.28,7.44,7.60,7.76,7.92,8.08,8.24
DEC 8.40,8.56,8.72,8.88,9.04,9.20,9.36,9.52,9.68,9.84,10.0
DEC .965382,.961696,.957807,.953716,.949426,.944936,.937836
DEC .930303,.922348,.913982,.905220,.88978,.87334,.85598
DEC .83779,.81886,.79926,.77909,.73736,.69435,.62882,.56372
DEC .50062,.44071,.40298,.36721,.33353,.30201,.27266,.24547
DEC .22041,.19740,.17637,.15722,.13984,.12714,.11544,.10469
DEC .05482,.08579,.07753,.06999,.06311,.05686,.05117,.04601
DEC .04134,.03710,.03327,.02981,.02669,.02388,.02135,.01907
DEC .01702,.01518,.01354,.01206,.01074,.00955

ENTRY PLNKTT

PLNKTT BSS 0

END

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13. ABSTRACT The radiation transport subroutines of the SPUTTER code for spherical geometry have been revised. The DIFFU subroutine has been eliminated and RADTN, TRANS, and KAPPA have been recoded. The results of this work on the codes are (1) improved logical organization, (2) more efficient and rapid calculation, (3) improved accuracy, (4) more complete documentation, and (5) comparisons with test problems. The much simpler and more accurate diffusion approximation is exploited when a new diffusion criterion is satisfied in shells within the sphere. A more accurate angular integration of the intensity makes use of the y-line integration results more efficiently to give improved fluxes. Reorganization of the calculation, saving of quantities to be used again, and use of a fast exponential routine have resulted in speeding up the routines by approximately a factor of 2. The diffusion and angular integration improvements apparently have resulted in an additional factor of 2 speedup for the same accuracy.		

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Numerical routines for radiation transport Spherically symmetric systems Fireball diffusion approximation Radiation multifrequency transport						

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