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FIREBALL PHENOMENOLOGY
AND CODE DEVELOPMENT

Volume IV

SPUTTER Subroutines for Radiation Transport in Planes

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 IV

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Research and Technology Division
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Kirtland Air Force Base
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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.

This 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 planes described in Volume IV 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.

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* Volume II has been withdrawn, and will not be published.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

The radiation-transport subroutines of the SPUTTER code for plane slab geometry have been supplemented by an alternative formulation based on integration along sampling ray paths through the slab. Angular integrations are performed by the Gaussian quadrature method which determines the ray angles. Options may be exercised to determine the number of angles and the nature of the radiation boundary condition at one boundary of the transport region. The characteristic ray code differs from the current integral method in performing problems having a large number of zones more rapidly and in having more general boundary conditions. For most applications a small number of angles give adequate accuracy. The numerical method used in the ray code is described. In addition, the organization of the code is discussed and subroutines are listed.
The SPUTTER code subroutines for radiation transport in planes described herein are as they existed on July 30, 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 new routines for radiation transport in planes closely parallel the spherical radiation transport subroutines (Volume III) in mathematical formulation and code organization. This parallelism is especially close between the SRADTN (for spheres) and PRADTN (for planes) subroutines in which calculations peripheral to the transport integration are performed. In fact, it is likely that these subroutines can be condensed to form a single subroutine for spheres and planes, although currently they are separate.

The routines reported here are to be considered as alternatives to the routines based on the integral formulation of the transport equation currently in use. By comparison, the current integral version is more accurate in the performance of angular integrations of the intensity, but for problems requiring a large number of zones it requires more computation time. Boundary conditions on the radiation intensity, however, are much more naturally incorporated into the new version.

Conditions suggesting a preference for using the new routines are: (1) a large number of zones and a desire to reduce calculation time and (2) the necessity of specifying a radiation intensity incident on the slab surface which has arbitrary angular and frequency dependence.

The numerical sequences used in solving the transport equation are discussed in Section II. A description of the diffusion approximation used in conjunction with the transport solution is given in Section III and a brief description of the methods of frequency integration is given in Section IV. Section V includes the actual code description in terms of code organization and economics. Section VI includes some initial studies on timing and accuracy in the angular integrations.
SECTION II
NUMERICAL SOLUTION OF THE TRANSPORT EQUATION

The radiation routines described herein contain a formulation based on the numerical solution of the radiation transport equation along a selection of sampling rays through the slab. 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 plane geometry that describes the changes in the specific intensity $I_\nu$ of photons of frequency $\nu$ resulting from pure absorption and emission according to the local thermodynamic equilibrium assumption is

$$\mu \frac{\partial I_\nu}{\partial x} = \sigma'_\nu (B_\nu - I_\nu),$$  \hspace{1cm} (2.1)

where

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

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

and $\sigma'_\nu$ 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.

Defining the monochromatic optical depth, $\tau$, as

$$\tau = \frac{1}{\mu} \int_0^x \sigma'_\nu \, dx,$$  \hspace{1cm} (2.2)
the values

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

where

\[ a_- = \frac{B_{i-1} \tau - B_{i-\frac{1}{2}} \tau_{i-1}}{\tau - \tau_{i-\frac{1}{2}}}, \quad b_- = \frac{B_{i-\frac{1}{2}} - B_{i-1}}{\tau - \tau_{i-\frac{1}{2}}} \]  \hspace{1cm} (2.4)

and

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

where

\[ a_+ = \frac{B_{i-\frac{1}{2}} \tau - B_{i} \tau_{i-\frac{1}{2}}}{\tau - \tau_{i-\frac{1}{2}}}, \quad b_+ = \frac{B_i - B_{i-\frac{1}{2}}}{\tau - \tau_{i-\frac{1}{2}}} \]

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

\[ I_1 = \alpha_{1-\frac{1}{2}} + [(I_{i-1} + \gamma_{1-\frac{1}{2}})e^{-\Delta/2} + \beta_{1-\frac{1}{2}}]e^{-\Delta/2} \]  \hspace{1cm} (2.5)

where

\[ \alpha_{1-\frac{1}{2}} = a_+ + b_+(\tau_i - 1) \]
\[ \beta_{1-\frac{1}{2}} = a_- + b_+(\tau - \frac{\Delta}{2} - 1) \]
\[ \gamma_{1-\frac{1}{2}} = b_- (1 + \Delta - \tau_i) - a_- \]

In these expressions, \(\Delta = \tau_i - \tau_{i-1}\). The coefficients of Eq. (2.5) can be re-expressed by using the definitions of Eq. (2.4):
The terms in Eq. (2.6) may be interpreted as containing combinations of numerical approximations to the values of the source function and the $\tau$ 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. (2.3). Two successive integrations by parts transforms the expression for $I_i$ into the following equivalent form:

$$I_i = \left( B - \frac{\partial B}{\partial\tau}_i \right) + \left[ I_{i-1} - \left( B - \frac{\partial B}{\partial\tau}_{i-1} \right) \right] e^{-\Delta} + \int_{\tau_{i-1}}^{\tau_i} \frac{\partial^2 B}{\partial\tau^2} e^{-(\tau_1 - \tau)} d\tau,$$

in terms of values of the source function and the first two derivatives of the source function with respect to $\tau$.

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. (2.3). 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. (2.7).

If $\Delta$ is not too large, a representative mean value of the exponential in the interval may be taken to give for the integral of Eq. (2.7)

$$\int_{\tau_{i-1}}^{\tau_i} \frac{\partial^2 B}{\partial\tau^2} e^{-(\tau_1 - \tau)} d\tau \cong e^{-\Delta/2} \left[ \frac{\partial B}{\partial\tau}_i - \frac{\partial B}{\partial\tau}_{i-1} \right],$$

and thus the expression for intensity becomes
\[ I_i = \left( B - \frac{\partial B}{\partial \tau} \right) + \left\{ \left( I_{i-1} - \left( B - \frac{\partial B}{\partial \tau} \right)_{i-1} \right) e^{-\Delta/2} + \left[ \frac{\partial B}{\partial \tau} - \frac{\partial B}{\partial \tau} \right]_{i-1} \right\} e^{-\Delta/2}. \]

(2.8)

This expression has just the form of Eqs. (2.5) and (2.6) when the difference expressions are identified with the derivatives.

It is clear from the derivation of Eq. (2.5) 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, only quantities at interface \( i \) will survive, and

\[ I_i = B_i - \frac{\partial B}{\partial \tau} \]

which can be evaluated as

\[ \frac{\partial B}{\partial \tau} = \mu \frac{\partial B}{\partial h}, \]

(2.9)

where

\[ h = \int_0^x \sigma' dx. \]

The independent variable \( h \) depends only on \( x \), 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. (2.9). A difference approximation can also be based on this expression, assuming that \( B \) is linear in \( h \), i.e.,

\[ \frac{\partial B}{\partial \tau} \approx \frac{B_i - B_{i-1}}{h_i - h_{i-1}} \mu, \]

(2.10)

where \( \mu \) is the cosine of the angle which the ray makes with the slab normal. The corresponding equation for the intensity is Eq. (2.5), in which
If the optical depth is very small, the intensity expression in Eq. (2.3) takes a much simpler form,

\[
\alpha_{i-\frac{1}{2}} = \frac{B_i - B_{i-\frac{1}{2}}}{h_i - h_{i-\frac{1}{2}}},
\]

\[
\beta_{i-\frac{1}{2}} = \mu \frac{B_i - B_{i-\frac{1}{2}}}{h_i - h_{i-\frac{1}{2}}} - \frac{B_{i-\frac{1}{2}} - B_{i-1}}{h_{i-\frac{1}{2}} - h_{i-1}},
\]

\[
\gamma_{i-\frac{1}{2}} = -\left( \frac{B_{i-\frac{1}{2}} - B_{i-1}}{h_{i-\frac{1}{2}} - h_{i-1}} \right).
\]  

(2.11)

2.1.2. Small-optical-depth Expansion

Although this result is the limiting form of Eqs. (2.5) and (2.6), the terms must cancel through second order in an expansion in \( \Delta \) 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. (2.12) in the PTRANS 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.

2.1.3. Boundary Conditions

Integration of the transport equation to obtain intensities is performed through the thickness of a zone, called a "trans" region. At intersections of characteristic rays with the inner and outer surfaces of each layer it is necessary to supply the starting value of the intensity \( I_{i-1} \) required in Eq. (2.5). Three classes of boundary conditions occur:

1. The trans region outside boundary coincides with outside zones of the SPUTTER calculation and a prescribed function, \( I_0 \), is applied at the left boundary value:

\[
I(X_{i\alpha+1}, \mu) = I_0, \quad \mu \leq 0 \text{ or blackbody boundary condition.} \quad (2.13)
\]
2. The right-hand boundary of the slab provides for reflective and transmittal boundary conditions as well as special routines to establish prescribed intensities for angles with $\mu < 0$ at the boundary:

$$I(x_{IB'}, -\mu) = I(x_{IB'}, \mu), \quad I(B_{IB'}, \mu) = 0,$$

or

$$I(B_{IB'}, -\mu) = I_0(\mu, t), \quad \text{where} \quad I_0 \text{ is the prescribed negatively directed boundary intensity applied to the outer boundary as a function of angle, frequency, and time.}$$

Intensities at up to 50 frequencies and six angles can be accommodated in the table located in the array QINT1(N). The table entries are used as $I_0$ and are formed in the subroutine QUE4 where they are stored in the QINT1 array. Since this subroutine is appropriate to the thermal-interaction application, additional uses may require subroutines tailored to the specific application.

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:

$$I_{IB'} = B_{IB'} - \mu \frac{\partial B}{\partial n},$$

where $I_0$ is the prescribed negatively directed boundary intensity applied to the outer boundary as a function of angle, frequency, and time. Intensities at up to 50 frequencies and six angles can be accommodated in the table located in the array QINT1(N). The table entries are used as $I_0$ and are formed in the subroutine QUE4 where they are stored in the QINT1 array. Since this subroutine is appropriate to the thermal-interaction application, additional uses may require subroutines tailored to the specific application.

2.2. ANGULAR INTEGRATION

Integrals over the polar angle of the intensity are required, as described in Section 2.2.1, to carry the calculation forward in time and to provide edits of informative derived quantities. These are formed by numerical quadrature using the intensities evaluated at a series of discrete values of polar angle by the integrations described in Section 2.2. Since in the plane calculation the value of the polar angle remains fixed along a characteristic ray and enters only parametrically in the equations, it is possible to exercise a choice of polar-angle values in order to optimize the accuracy of the resulting integrals.

The numerical quadrature method used for the PTRANS subroutine is the so-called double Gaussian. In this method the integrals of the radiation quantities (flux, energy, pressure, etc.) are approximated by

$$\int I f(\mu) \, d\mu = \sum_{0}^{n} A_m (if)_m,$$
where \((I_m)_{\mu_m}\) is the known value of the integrand at a chosen value \(\mu_m\) of the cosine of the polar angle, \(\mu\). In the method of Gaussian, not only are the coefficients \(A_m\) determined but the values of \(\mu_m\) are fixed to minimize the difference between the integral and the approximation. The result of this minimization is to relate the \(\mu_m\) to the zeros of the Legendre polynomial of order \(n + 1\).

For those integrals having the range \(-1 \leq \mu \leq 1\) it is frequently advantageous to treat the forward and backward hemispheres separately to allow for the possibility of a discontinuity in \(I\) at \(\mu = 0\). Such discontinuities or very abrupt changes in the values of the intensity between forward and backward directions may occur in systems which are transparent enough that strong source regions are accessible. In these cases, a better fit to the integrand is obtained by the two approximating functions which permit a discontinuity at \(\mu = 0\) than by a single approximating function which imposes a smooth behavior near \(\mu = 0\). The method used in PTRANS, based on separate integration regions for \(-1 \leq \mu \leq 0\) and \(0 \leq \mu \leq 1\), is called the double Gaussian quadrature method. Values of \(A_m\) and \(\mu_m\) are derived by a simple transformation from those for the single integration region.

Since the angles for a single integration region are arranged symmetrically about the interval midpoint, for double region integration it is possible to identify pairs of angles \(\pm \mu_m\) having the same weight \(A_m\). In Table 2.1, the values for the \(0 \leq \mu \leq 1\) interval are recorded for values of \(n = 1, 2, 3, 4, 5\). The total number of forward and backward angles, \(2n + 2\), for each \(n\) (also equal to the total number of entries in the table of \(\mu_m\) and \(A_m\) for each \(n\)) is also listed in the table.

The backward and the corresponding forward ray integrations in the PTRANS subroutine are performed sequentially. Since the same absolute values of \(\mu_m\) are required for these two calculations, many of the quantities formed in the backward integration pass can be used for the forward pass as well, and hence these quantities are saved to increase calculation efficiency. Contributions of the pair of forward and backward intensities to the weighted sums corresponding to the angular integrals are tallied at the same time that the forward integration pass is being calculated.
### Table 2.1

**GAUSSIAN WEIGHTS**

<table>
<thead>
<tr>
<th>n = LMDA(37)-1</th>
<th>Total No. of Angles, 2n+2</th>
<th>$\mu_m = RR(NMU)$</th>
<th>$A_m$</th>
<th>$\mu_m A_m = RR(NGS)$</th>
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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 $B_\nu$ about the point $r$ permits the intensity $I_\nu(\mu)$ of the radiation field in the direction making an angle, whose cosine is $\mu$, with the linear 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

$$I(r) = \int_{-\infty}^{T} B(\tau') e^{-\left(\tau - \tau'\right)} d\tau' ,$$

where $\tau = \int_0^x k_\nu \rho \, dx$, in which $k_\nu$ is the monochromatic absorption coefficient (in cm$^2$/g) at frequency $\nu$. By expanding $B(\tau')$ in series about the point $\tau$, i.e.,

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

the intensity becomes

$$I = B - \frac{\delta B}{\delta \tau} + \frac{1}{2} \frac{\delta^2 B}{\delta \tau^2} - \ldots$$

or

$$I = B - \frac{\mu}{k_\rho} \frac{\delta B}{\delta x} + \frac{\mu}{k_\rho} \frac{\partial}{\partial x} \left( \frac{1}{k_\rho} \frac{\delta B}{\delta x} \right) - \ldots$$

for plane slab geometry.

The diffusion approximation results from retention of only the first two terms, so that the diffusion intensity is
and the monochromatic diffusion flux $\phi_r$ and radiation energy $E_R$ are

$$\phi_r = 2\pi c \int_{-1}^{1} I \mu \, d\mu = -\frac{4\pi c}{3} \frac{1}{\kappa_0} \frac{\delta B}{\delta x} \quad \text{(3.2)}$$

$$E_R = 2\pi \int_{-1}^{1} I \, d\mu = 4\pi B \quad \text{(3.2)}$$

### 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 $\tau$ 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 derivatives approximations.

In the SPUTTER subroutine PRADTN, 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

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

is required. In this expression $h = \int \kappa_0 \, dx$ is the optical depth normal to the slab; the derivative is approximated by the centered first difference of $B$ between adjacent zones. The resulting expression, of course, contains some nonlocal 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:

$$|T_G| < HCB \times Y_2,$$  \hspace{1cm} (3.4)

where $T_G$ is the difference approximation to the gradient and $Y_2$ is the source function evaluated at the interface by interpolation. The second criterion uses the input number HVB (in mean free paths). If

$$|Q_3(\ ) - Q_3(J)| > HVB,$$ \hspace{1cm} (3.5)

then the interface with index $J$ which satisfies Eq. (3.4) is removed from the diffusion region. In Eq. (3.5), $Q_3$ is the normal 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 characteristic rays 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

$$I = B - \frac{\mu}{\kappa_p} \frac{\theta B}{\delta x}.$$  

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

$$\int_{v_j}^{v_{j+1}} I \, dv = \int_{v_j}^{v_{j+1}} B \, dv - \frac{\mu}{\rho} \frac{\delta \theta}{\delta x} \int_{v_j}^{v_{j+1}} \frac{\theta B}{\delta \theta} \frac{\delta v}{\delta \nu}.$$  

In terms of the partial Rosseland mean absorption coefficient
the frequency group intensity becomes

\[ I_j = \int_{\nu_j}^{\nu_{j+1}} I d\nu = \int_{\nu_j}^{\nu_{j+1}} B d\nu - \frac{\mu}{\rho} \int_{\nu_j}^{\nu_{j+1}} \frac{\partial B}{\partial x} \frac{1}{\kappa_j} \]

(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 \( \kappa_j \) and the integrated source functions \( \mathbf{X}_\mathbf{6} = \int B d\nu \) 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
and by forming the variable \( \tau = \int p \kappa_j \, dx \). In terms of these quantities, the intensity can be written as

\[
\frac{\partial}{\partial \tau} \int_{v_j}^{v_{j+1}} B \, dv = \frac{\partial}{\partial x} \int_{v_j}^{v_{j+1}} \frac{\partial B}{\partial \theta} \, dv
\]

and

\[
I_j = \int_{v_j}^{v_{j+1}} B \, dv - \mu \frac{\partial}{\partial \tau} \int_{v_j}^{v_{j+1}} B \, dv.
\]
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 $I_{ij}$:

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

Then, for example, this quantity can be integrated over angles to form $\phi_{ij}$, the contribution to the flux at position $i$ of frequency group $j$:

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

and thus the total radiant flux at position $i$ is

$$\phi_i = \sum_j \phi_{ij} .$$

Equation (2.8) gives the expression for the frequency-dependent intensity to be used in Eq. (4.1). The frequency integration of Eq. (2.8) has been reported recently, \(^{(4)}\) but the current SPUTTER code does not include the transmission functions. The first two terms of Eq. (2.8) which form the diffusion limit can be integrated, as in Section 3.3, to give
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 \( \sigma_{R,i} = \rho \kappa_i \). In this form, Eq. (4.2) correctly gives the frequency-group intensity for the optically thick limiting case. The remaining \( B_i \) and \( \sigma B/\sigma \tau \) terms of Eq. (2.8) are formed in the same way. Thus,

\[
I_{ij} = B_{ij} - \frac{\mu}{\sigma} \frac{\partial B_{ij}}{\partial x} \left( \int_{\nu_j}^{\nu_{j+1}} \frac{\mu}{\sigma} \frac{\partial B_i}{\partial x} \, d\nu \right)_{ij} - \left( \int_{\nu_j}^{\nu_{j+1}} \frac{\mu}{\sigma} \frac{\partial B_i}{\partial x} \, d\nu \right)_{i-1,j} \frac{e^{-\Delta/2}}{e^{-\Delta}} + \left[ I_{i-1,j} - B_{i-1,j} + \frac{\mu}{\sigma} \frac{\partial B_i}{\partial x} \right]_{i-1,j} \frac{e^{-\Delta}}{e^{-\Delta}} .
\]  

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

\[
e^{-\Delta} = e^{-\sigma \delta R} \quad \text{(4.4)}
\]

and the second is

\[
e^{-\Delta} = e^{-\sigma \delta P} ,
\]

where

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

and

\[
\delta = x_i - x_{i-1}.
\]
For small optical depth, the correct result makes use of the Planck mean absorption coefficient. From Eq. (2.12) the frequency integration then gives

\[ I_{ij} = I_{i-1,j} + \left[ \frac{1}{4} B_{ij} + \frac{1}{4} B_{i-1,j} + \frac{1}{2} B_{i-1,j} - I_{i-1,j} \right] \sigma P^6. \]  

(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 plane transport subroutines were written with the idea of removing unnecessary calculations from inside the frequency loop and characteristic ray integrations. These improvements required an increase in storage for the subroutines to attain a decrease in calculational time. The reorganized subroutines will be discussed in two sections, corresponding to the two major subroutines: (1) the radiation subroutine (PRADTN) in which most of the preliminary setup and the diffusion calculation is completed and (2) the transport subroutine (PTRANS) in which the intensity calculation and angular integrations are performed. The subroutines which execute the opacity interpolations (KAPPA), Planck function (PLNKUT), and fast exponential (FREXP) will be discussed in Section 5.4. The input numbers and the output edits will be presented in Sections 5.5 and 5.6.

5.1. THE PRADTN SUBROUTINE

In PRADTN, the 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 PRADTN will be discussed in subsequent paragraphs.

5.1.1. 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 $h_{v1}$ of the group in question ($h_{v1}, h_{v2}$) 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 equation for $d\sigma/d\theta^4$ and the appropriate sums:
\[
\frac{dB}{d\theta^4} \approx \frac{0.0384974}{\theta^4} \left[ \left( \frac{\frac{4}{\theta}}{1 - e^{-\frac{4}{\theta}}} \right) e^{-\frac{4}{\theta}} - \left( \frac{\frac{4}{\theta}}{1 - e^{-\frac{4}{\theta}}} \right) e^{-\frac{4}{\theta}} \right].
\]

\[
\sum b_j \theta^4, \sum \frac{dB}{d\theta^4}, \sum b_j \theta^4 \kappa_P, \text{ and } \sum \frac{dB}{d\theta^4} \kappa_R.
\]  

(5.1)

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

\[
\overline{\kappa_R} = \frac{\sum dB \nu / d\theta^4}{\sum dB \nu / (d\theta^4 \times \kappa_R)} \quad \text{(CAPAR)},
\]

\[
\overline{\kappa_P} = \frac{\sum b_j \theta^4 \kappa_P}{\sum b_j \theta^4} \quad \text{(CAPAC)}.
\]  

(5.2)

5.1.2. Set Up Sources and Derivatives

The frequency-dependent sources must be established at the interfaces from the zonal quantities \(b_j \theta^4 \) \((X6(i))\) and \(\tau_{i+4} \) \((H3(i))\). 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 \(\text{PLNKUT}\), a test is made to see if \(u_1\) (i.e., the reduced frequency \(hv_1/\theta\)) \(\geq 19\); 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 \((\text{ICX})\) 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 \(x\) (change greater than a factor of two), the derivative at that interface \((\text{TC}(i))\) is set equal to zero. The zero source derivative is used in \(\text{PTRANS}\), 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 \((I = \text{ICX})\) and at the outside of the mesh \((I = \text{IM})\) (see Section 2.1.3).
5.1.3. 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 \( (YZ) \) (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 \( x = 0 \) 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 \( PRADTN \), and if so, a \( PTRANS \) 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.

5.1.4. 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 \( (\kappa_P) \) and Rosseland \( (\kappa_R) \) in the DIANE code. The actual time step for radiation transfer is then obtained from the formula

\[
\Delta t_R = (0.5 + 1.5 H3(i) \frac{I^2}{(ac \kappa R \theta^3)} \times CV(i)) \quad (5.3)
\]

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 \( \varepsilon R(i) \) 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 \( \kappa_R \) and \( \kappa_P \) 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 PTRANS SUBROUTINE

The subroutine PTRANS is called by PRADTN 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 rays \( \left( \int_{-1}^{1} \mu \, d\mu \right) \). After the intensity transport along a typical ray in the outward direction \( (I_A \rightarrow I_B) \) is done, the flux is calculated while the inward pass of the intensity calculation is being completed. The angular integration is based on a linear interpolation of the intensities between rays. The logic in PTRANS is described in detail in the following sections.

5.2.1. Selection of Angles

At present, only five sets of Gaussian angles and weights are stored in the subroutine. These can be selected by setting an input number \( \text{LMDA}(37) \), the number of angles with \( \mu > 0 \) to the desired \( n+1 \). The selection from storage is made from the following indices

\[
\begin{align*}
NY &= \text{LMDA}(37) - 1 \\
NMU &= (NY-1) \times (NY+2) + 1 \\
NGS &= NMU+NY + 1
\end{align*}
\]

\( NMU \) selects the cosine of the angle \( (\mu_m^m) \); \( NGS \) selects the relation \( (\mu_m^m A_m^m) \), the cosine of the angle times the Gaussian weights for the flux formulation.
5.2.2. Intensity Integration along Characteristic Rays

The integration using Eq. (2.11) starts at the left boundary with the appropriate boundary condition and proceeds outward, storing the exponentials $e^{-\Delta \tau}$ in (H4(i)), the derivatives $\mu \partial B/\partial h_{i+\frac{1}{2}}$ in X8(i), and the calculated intensities in sum X3(i). The more general boundary conditions are established (see Section 2.1) and the stored quantities are now used except for the change of sign of $\mu \partial B/\partial h_{i+\frac{1}{2}}$ in Eq. (2.1) to calculate the intensities $I(F2)$, on the outward pass.

The regions where constant sources, and therefore zero boundary derivatives, should be used in the intensity integrations were established in PRADTN by setting TG(i) equal to zero. In the integration along a particular ray, 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 - $\frac{1}{2}$) respectively (see Fig. 2.1).

As discussed in Section 2.1.1, the accuracy of the exponential term and the effect of truncating 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 $\tau_1$ (the half optical depth $\tau$ is stored in H2(i)), and if $\tau < 10^{-2}$ a switch is made to the limiting form of the transport equation (Eq. (2.12) developed in Section II).

5.2.3. Angular Integration

The only integral over angle formed in PTRANS, at present, is the flux; $\int \mu \, d\mu$ the formula for energy (\$1d\mu) is included for possible use later. These integrals are formed on the outward pass from the intensity (sum X3(i)) stored on the inward pass and the intensity being calculated (F2). The difference forms of the equations are

$$X2(i) = \sum (F2 - \text{sum X3(i)}) \times \mu_m A_m$$

$$ER(i) = \sum (F2 + \text{sum X3(i)}) \times A_m$$

5.3. DIFFERENCES WITH INTEGRAL FORMULATION

The principal difference in the subroutines is in replacing the integration of angle done explicitly in the integral formulation by a sampling scheme of a double Gaussian nature. It is expected that accuracy can be achieved with a minimum number of rays (presumably less than $n = 6$, see Section 2.2). This result is in logical agreement with the use of the S4 approximation in the neutron-transport work. The advantage, therefore, will appear in problems with many zones, since the integral method will
increase as the number of zones squared whereas the present method will only increase linearly with zones. Furthermore, the present method makes it possible to have special boundary conditions depending on angle (see Section 2.1.3).

5.4. AUXILIARY SUBROUTINES

In addition to the two new basic subroutines PRADTN and PTRANS, 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 FREXP 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

\[ b(u_1, u_2) = \frac{1}{B} \int_{u_1}^{u_2} \frac{\hbar \nu^3}{c^2} \frac{1}{e^{\hbar \nu/kT} - 1} \, d\nu = b_j . \]  

(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^-6 normal to 10 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 steps in PRADTN. KAPPA reads in first the tape name, the number of frequency groups, and the size of the records. If the sentinel for multifrequency is set to KMAX = 1, then the first frequency group, \( \hbar \nu_1 \), and its absorption coefficients are read into storage. The interpolations in log \( \theta_i \) and log \( \rho_i \) are performed and a return to PRADTN 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.

5.5. INPUT NUMBERS

The input quantities used in the radiation-transport subroutines and their functions are listed in Table 5.1. The entries in it are as follows: column 1 is the storage location number used for entering the quantity into storage with the CARDS subroutine, column 2 lists the FORTRAN name of the stored quantity, column 3 gives the range of admissible values of the input quantity, column 4 describes its function and identifies special values it may assume, and column 6 records a set of values of the quantities which might be typical of those for a normal problem. Included is a set of values for the input quantities selected for solving typical problems.

5.6. EDITS

The editing of such frequency-dependent quantities as H3, the optical depth (Rosseland), X6, the source \( b_j \sigma^4 \), X2, the flux (in ergs/4/3 \( \pi \) sec) \( X2/DHNU \), the flux divided by the frequency group, THETA, the temperature (eV), and EI, the energy (ERGS/G) versus radius is accomplished by setting S12 to the desired number of cycles between prints. These multi-frequency edits have been used to evaluate the criteria for the subroutines as well as for diagnostics during the calculations.

A list of sample editing for a particular frequency group is given on page 27. The HNU is in electron volts. The quantities found useful to display for each frequency group and for a characteristic ray are listed on page 28. The format statements, in the listings appended, have been revised for the debug print from those used on page 28.
### Table 5.1

**PLANE RADIATION INPUT QUANTITIES**

<table>
<thead>
<tr>
<th>Card No.</th>
<th>Quantity</th>
<th>Range of Values</th>
<th>Description</th>
<th>Typical Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>37</td>
<td>LMDA(37)</td>
<td>2, 3, 4, 5, 6</td>
<td>Number of angles with ( \mu &gt; 0 ).</td>
<td>2</td>
</tr>
<tr>
<td>44</td>
<td>KMAX</td>
<td>----</td>
<td># 0, performs multigroup frequency approximation; = 0, performs single-group frequency approximation.</td>
<td>0</td>
</tr>
<tr>
<td>81</td>
<td>HVB</td>
<td>( \geq 0 )</td>
<td>Number of optical mean free paths by which a transport region is extended at the expense of each adjacent diffusion region. (See Section 3.2.)</td>
<td>5</td>
</tr>
<tr>
<td>83</td>
<td>HCB</td>
<td>( \geq 0 )</td>
<td>Criterion to define a diffusion region in terms of relative gradient of the source function. Diffusion regions are eliminated if 0. (See Section 3.2.)</td>
<td>0.1</td>
</tr>
<tr>
<td>87</td>
<td>CB</td>
<td>( \geq 0 )</td>
<td>Criterion to combine frequency groups. If the lower frequency of the group is more than CB times the temperature of the hottest zone, that group is combined with the adjacent group of lower frequency. A half-integer value presents termination of the problem when half or more of the groups have been combined. (See Section 5.1.1.)</td>
<td>10.5</td>
</tr>
<tr>
<td>88</td>
<td>GA</td>
<td>( \geq 0 )</td>
<td>One of two criteria for choice of linear or stepwise constant source within a zone. (See Section 5.1.2.)</td>
<td>0.333</td>
</tr>
<tr>
<td>90</td>
<td>GL</td>
<td>Neg., 0, ( \frac{1}{2} ), pos. integer</td>
<td>Indicator for radiation boundary condition at IB. GL = negative, total reflection; GL = 0, intensity for ( \mu &lt; 0 ) is zero; GL = ( \frac{1}{2} ), blackbody intensity based on temperature located in THETA(IB) for ( \mu &lt; 0 ); GL = positive integer, intensity for ( \mu &lt; 0 ) obtained from source routine. GL must equal number of frequency groups. (See Section 2.1.3.)</td>
<td>0</td>
</tr>
<tr>
<td>121</td>
<td>AC</td>
<td>( \geq 0 )</td>
<td>One of two criteria for choice of linear or stepwise constant source. Minimum value for using a linear source. (See Section 5.1.2.)</td>
<td>0.3</td>
</tr>
<tr>
<td>127</td>
<td>ACO3T4</td>
<td>----</td>
<td>Transport debug edit criterion. Edit occurs if # 0 and &lt; cycle number.</td>
<td>9</td>
</tr>
<tr>
<td>147</td>
<td>S12</td>
<td>----</td>
<td>Number of cycles between multifrequency edits.</td>
<td>10</td>
</tr>
<tr>
<td>150</td>
<td>S15</td>
<td>0, 1</td>
<td>Trigger controlling call of DIANE tape. Must have value # 0 on starts or restarts.</td>
<td>1</td>
</tr>
<tr>
<td>8466</td>
<td>TELM(25)</td>
<td>( \geq 0 )</td>
<td>Constant multiplying the radiation time step. Can be used to modify the stability criterion.</td>
<td>1</td>
</tr>
<tr>
<td>8478</td>
<td>TELM(37)</td>
<td>( \geq 0 )</td>
<td>Maximum permissible fractional energy in any zone due to radiation. Time step may be reduced to meet this requirement.</td>
<td>0.05</td>
</tr>
<tr>
<td>8858</td>
<td>SOLID(10)</td>
<td>----</td>
<td>Thick-thin criterion. If 0, Planck mean is used to form HZ; otherwise, Rosseland mean. (See Section 4.)</td>
<td>1</td>
</tr>
</tbody>
</table>
### Table 5.1

**SAMPLE EDIT FOR A CHARACTERISTIC DIRECTION FOR PTRANS**

<table>
<thead>
<tr>
<th>FREQUENCY BAND FROM 17,8000 TO 29,1000</th>
<th>J1 = 0</th>
<th>IAX = 1</th>
<th>IBX = 31</th>
<th>ICX = 31</th>
<th>ICY = 23</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>X</td>
<td>X4</td>
<td>H3 SUMX3</td>
<td>SUMX4</td>
<td>X2</td>
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<tr>
<td>1</td>
<td>1.75964889-08</td>
<td>0.</td>
<td>2.4339197+02</td>
<td>2.4339197+02</td>
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</tr>
<tr>
<td>2</td>
<td>9.3999999+00</td>
<td>0.</td>
<td>2.4339192-01</td>
<td>2.4339192-01</td>
<td>0.</td>
</tr>
<tr>
<td>3</td>
<td>1.0000000+01</td>
<td>0.</td>
<td>2.4339192-01</td>
<td>2.4339192-01</td>
<td>0.</td>
</tr>
<tr>
<td>4</td>
<td>1.0002000+01</td>
<td>0.</td>
<td>2.4339192-01</td>
<td>2.4339192-01</td>
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<tr>
<td>5</td>
<td>1.0030000+01</td>
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<td>2.4339192-01</td>
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<tr>
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<td>1.0040000+01</td>
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<td>2.4339192-01</td>
<td>2.4339192-01</td>
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<tr>
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<tr>
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<td>2.4339192-01</td>
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</tr>
<tr>
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<td>2.4339192-01</td>
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<tr>
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<tr>
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<tr>
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<tr>
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<tr>
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<tr>
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<tr>
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<tr>
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<tr>
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<tr>
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</tr>
<tr>
<td>24</td>
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<td>0.</td>
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</tr>
<tr>
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</tr>
<tr>
<td>26</td>
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<td>0.</td>
<td>2.4339192-01</td>
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<tr>
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<td>2.4339192-01</td>
<td>2.4339192-01</td>
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<tr>
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</tr>
</tbody>
</table>
## Table 5.2

**SAMPLE MULTIFREQUENCY EDIT FOR PTRANS**

<table>
<thead>
<tr>
<th>CYCLE</th>
<th>TIME</th>
<th>HNU FROM 17.8000 TO 20.1000</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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<tr>
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<td></td>
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</tr>
</tbody>
</table>
SECTION VI
TIMING STUDIES AND ACCURACY IN
ANGULAR INTEGRATION

6.1. TIMING CALLS

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 PRADTN and PTRANS:

PRADTN

13, 105 - Before frequency loop
13, 140 - After call KAPPA on merge
13, 701 - After call KAPPA on main frequency loop
13, 151 - After calculating general sources
13, 180 - Before calling PTRANS
13, 292 - After EDIT (normal) end of frequency loop
13, 286 - After last frequency start time step
-13, 239 - End of cycle (return to main program)

PTRANS

14, 708 - Before debug print

The following calculation was timed in units of 1/60 sec for the above breakdown in computing time.

The calculation described here did not use the TG criteria (see Section 5.1.2) nor the special boundary conditions (see Section 5.2.4). Three ray passes were completed for each frequency group for a total of six angles, forward and back, and with 32 active zones. The total time for 21 frequency groups was ~14.9 sec. The breakdown in time for a
single frequency group (in units of 1/60 sec) are the following:

<table>
<thead>
<tr>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Call KAPPA for absorption coefficient</td>
<td>14</td>
</tr>
<tr>
<td>After sources</td>
<td>1</td>
</tr>
<tr>
<td>Characteristic ray passes (3)</td>
<td>3</td>
</tr>
<tr>
<td>After call PTRANS with EDIT</td>
<td>23</td>
</tr>
<tr>
<td>Average time required</td>
<td>~41/νν</td>
</tr>
</tbody>
</table>

The start and merge of KAPPA is ~32
Total time with EDIT ~869 (1/60 sec)
Total time without EDIT ~515 (1/60 sec)

6.2. **ACCURACY IN ANGULAR INTEGRATIONS**

Comparisons have been made between calculations for two sets of angles for a radiation shock problem. The problem consists of a hot (5 ev) shock moving into cold low-density air. The effect on the flux versus linear zones for a set of four and eight angles is given in Fig. 6.1. This result indicates that as few as six and probably even four angles would be sufficient for reasonable accuracy.
Fig. 6.1 -- Flux vs linear zones for six and ten angles
REFERENCE

Appendix A

PRADTN
SUBROUTINE RADTN

COMMON OCTOBER 7, 1965 WBL
C PLANE CHARACTERISTIC TRACe WITH DOUBLE GAUSSIAN INTEGRATION

C SPUTTEr COMMON

COMMON LMDA(37), NR, NSMLR, IA, IB, ICA, ICB, PRADO0060
1 KNAX, BLANK1, BLANK2, BLANK3, IAPI, IBPI, ICAP1, ICBP1, PRADO0000
2 II, IG, NRAD, BLANK4, IAM1, IM1, ICAML, ICAM1, PRADO80
3 IPI, IGML, IALPHA, BLANK5, TH, TMAX, BLANK6, DEPR, PRADO1000
4 FREQ, CNTMAX, AR, ASMLR, PUSHA, PUSHB, BOILA, BOILB, PRADO1100
5 CVA, CVB, SLUG, ALPHA, HVA, HVB, HCA, HCB, PRADO1200
6 EMINA, EMINB, CA, CB, GA, GB, GL, GR, PRADO1300
7 RHOL, RHRD, EPSI, EPSI, RIA, RB, RIA, RDIB, PRADO1400
8 RPIA, RPIB, RPOIA, RPOIB, RPRINT, TA, TB, TC, PRADO1500

COMMON TO, TE, DTNUM, DTNUM, DPRT, SWITCH, CO, CMIN, DELTA, PRADO1700
2 GANA, WCRIT, SIGMAQ, AC, AGOST4, CNVRT, SUMRA, SUMRB, PRADO1800
3 ROIA, ROIA, ROIB, ROIB, GM5, SI, S2, S3, PRADO1900
4 SQ, SS, S6, S7, S8, S9, S10, S11, PRADO2000
5 S12, S13, S14, S15, S16, S17, S18, S19, PRADO2100
6 S20, EO, (!), TAU, ZERO, R (152), DELTAR(152), PRADO2200
7 ASQ (152), RO (152), VO (152), RRO (152), SMLR (152), PRADO2300
8 DELR (37), P (152), P1 (152), PB (152), PB1 (152), PRADO2400
9 COMMON P2 (152), SV (152), RHD (152), THETA (152), PRADO2500
1 W (152), E (152), EI (152), EK (152), A (152), PRADO2600
2 V (152), G (152), D (152), C (152), X2 (152), PRADO2700
3 X3 (152), X4 (152), X5 (152), X6 (152), PRADO2800
4 SMLA (152), SMLB (152), SMLC (152), SMLD (152), PRADO2900
5 EC (152), ER (152), SMLE (152), SMLH (152), SIGMA (152), PRADO3000
6 BIG (152), CV (152), BC (152), BR (152), CHIC (152), PRADO3100
7 GHIN (152), GHPAR (152), GCTC (152), GTR (152), PRADO3200
8 GTPC (152), GOFR (152), FEN (152), CAR (152), OCLM (37), PRADO3300
9 COMMON TELM (37), ELM (37), ELM (37), FLM (37), PRADO3400
10 FLM (37), LML (37), QM (37), AQMOS (37), CHROM (37), PRADO3500
11 ZIP1 (37), ZIP2 (37), SIGMA (37), ECH (37), RK (104), PRADO3600
12 RL (37), ROH (1104), VDK (104), THETA (104), TEMP (16), PRADO3700
13 HEAD (121), MAXL, MAXL, MAXL, PRADO3800

C DIMENSION Q3(1), T6G1(1), H2(1), Q1(1), X8(1), SUMX3(1), SUMX4(1)
PRADO4000
1 DIMENSION H4(1), Y2(1), H1(1), SUMX2(1), Q2(1)
PRADO4200
2 DIMENSION Q3(1), Q3(1), H3(1)
PRADO4300
3 COMMON /LINCOLN, HNU, HNNU, HNNU, HNHP, NT, IM, IN, DHNU, THICK, NY
PRADO4400
4 COMMON /CNTRL/ SCYCLE, JMLUT
PRADO4500
5 COMMON /DAVIS/ ICX, ICY
PRADO4600
6 COMMON /TQ/ QINT1(300), QINT2(300), TITLE(12)
PRADO4700

C EQUIVALENCE(SMLH, H4), (SMLD, Y2)
PRADO4900
1 EQUIVALENCE (BG, TG), (BIGB, H), (CCTR, SUMX1), (CICH, SUMX3)
PRADO5000
2 EQUIVALENCE (SMLH, X8), (CAR, Q37), (CHR, Q38), (SMLC, H3)
PRADO5100
3 EQUIVALENCE (ACOST4, TROBG), (S12, EDITMF)
PRADO5200
4 EQUIVALENCE (EC, Q1), (X7, H2), (BIGA, SUMX4), (GOFR, Q3)
PRADO5300
5 C

35
C*** EDITMF SAME AS S12
H SAME AS BIGB
C H2 SAME AS X7
C H3 SAME AS SMLC
H4 SAME AS SMLA
Q1 SAME AS EC
Q2 SAME AS GOFR
Q3 SAME AS CAR
Q37 SAME AS CHIK
Q38 SAME AS SMLB
SUMX2 SAME AS CRTA
SUMX3 SAME AS CHIC
SUMX4 SAME AS BIGS
WS6 SAME AS BC
TRDBG SAME AS ACOJ74
X0 SAME AS SMLH
Y2 SAME AS SMLD
C
C*******************************************************************************
C
C PRADO550
C PRADO560
C PRADO570
C PRADO580
C PRADO590
C PRADO600
C PRADO610
C PRADO620
C PRADO630
C PRADO640
C PRADO650
C PRADO660
C PRADO670
C PRADO680
C PRADO690
C PRADO700
C PRADO710
C PRADO720
C PRADO730
C
C*******************************************************************************
C
C PRADO740
C PRADO750
C PRADO760
C PRADO770
C PRADO780
C PRADO790
C
C*******************************************************************************
C
C PLANES ONLY
C
C*******************************************************************************
C
C PRADO800
C PRADO810
C PRADO820
C PRADO830
C PRADO840
C PRADO850
C PRADO860
C
C*******************************************************************************
C
C BOUNDARY CONDITIONS
C
C*******************************************************************************
C
C PRADO870
C PRADO880
C PRADO890
C PRADO900
C PRADO910
C PRADO920
C PRADO930
C PRADO940
C PRADO950
C PRADO960
C
C*******************************************************************************
C
C N TIMES=501LB
IM=IM1
IN=IA
IF(ZP1(26).EQ.0) GO TO 15
C SAVE STUFF FROM EIONX FOR NDNEQ AND RESET IN OR IM
IF (PUSHA .LT. 0.0) GO TO 100
IM = NR - 1
WS2=BC(IM+1)
WS23=BR(IM+1)
WS24 = CRTA(IM+1)
WS25=RHO(IM+1)
GO TO 15
100 IN = NR
WS22 = BC(IN-1)
WS23 = BR(IN-1)
WS24 = CRTA(IN-1)
WS25 = RHO(IN-1)
CONTINUE
IMPI=IM+1
INM=IN-1
CALL DVCHK (KOOOFX)
IF (IMPI-IN) 190,190,125

NO VAPOR ZONES

190 X2(IMPI) = 1.0283E12 * A(IM) * (THETA(IM)**4 - THETA(IMPI)**4)
ER(IM)=-X2(IMPI)
GO TO 1300

125 IR=IN
THTAX=.025
IF (IALPHA-1) 130,140,130
130 S1 = 13.0130
CALL UNCLE

DO 180 I=IN,IM
X3(I)=0.
X4(I)=0.
X5(I)=0.
X6(I)=0.
CRTR(I)=0.

SET UP FOR KAPPA INTERPOLATION

Q1(I)=THETA(I)**4
Q37(I)=ALOG(THETA(I))
Q38(I)=ALOG(SV(I))

FIND IR, RIGHTMOST ZONE WITH THETA GREATER THAN 0.05 EV

IF (THETA(I)-THTAX) 160,160,150
150 THTAX=THETA(I)
160 IF (THETA(I)-0.05) .LT. .80,170
170 IR=I
180 CONTINUE
IF (THTAX .LT. THETA(IB)) THTAX = THETA(IB)

SET UP MAX FREQ BOUNDARY

HNUP4 = 6.1E13
IMNU=1
DO 210 I=IN,IMPI
210 SUMX2(I)=0.0
IF (KMAX.EQ.0.0) GO TO 280

THIS CODING WONT WORK IF HNU NOT EVALUATED
C 220 CALL KAPPA(IN,IM)
   HNU = HNU**4
   DHNUP = DHNU
   DHNU = HNU - HNU
C
C MERGE GROUPS WITH HNU MORE THAN CB TIMES LARGEST THETA
C
C IF (THTAMX-HNU/CB) 240,300,300
C
C REJECT TAPE IF MORE THAN HALF OF GROUPS MERGE
C
C 240 IF ((HNU+IHNU-NHU) 260, 250, 250
C 250 IF (MOD(CB1.0, .EQ. 0.5)) GO TO 260
   31=13.0250
   CALL UNCLE
C 260 DO 270 IM=IN,IM
   BETA = HNU/THETA(I)
   BETAP = HNU/THETA(I)
   DFB=PLNKUT(BETA, BETAP)
   IF (DFB.EQ.0.0) GO TO 270
   TEMP(1)=DFB*Q1(I)
   EMB1=EXP(-BETA)
   EMB2=EXP(-BETAP)
   TEMP(2)=DFB*0.0384974/0.1(HNU4/(1.0-EMB1)
1*EMB1-HNU4/(1.0-EMB2)*EMB2)
C
C FORM NUMERATORS AND DENOMINATORS OF MERGED KAPPAS
C
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)
C 270 CONTINUE
C
C MERGE FREQUENCY-DEPENDENT EXTERNAL INPUT INTENSITIES
C
C IF (GL .LT. 1. OR. IHNU .EQ. 1) GO TO 275
C 275 QINT=QINT(I)
   CALL UNCLE
C 276 QINT=Q1NT2
C 277 QINT=Q1NT2+QINT1
C 278 QINT=QINT+QINT2
C 279 QINT=QINT(QINT2)
C 280 QINT=QINT(QINT1)
C 281 QINT=QINT(QINT1)+QINT2
C 282 QINT=QINT(QINT1)+QINT2
C 283 QINT=QINT(QINT1)+QINT2
C 284 QINT=QINT(QINT1)+QINT2
C 285 QINT=QINT(QINT1)+QINT2
C 286 QINT=QINT(QINT1)+QINT2
C 287 QINT=QINT(QINT1)+QINT2
C 288 QINT=QINT(QINT1)+QINT2
C 289 QINT=QINT(QINT1)+QINT2
C 290 QINT=QINT(QINT1)+QINT2
C
C MONOFREQUENCY CALCULATION
C
C 290 CALL KAPPA(IN,IM)
C 291 DO 300 IN=IN,IM
C 292 X5(I)=1.
C 293 X6(I)=Q1(I)
C 294 300 CONTINUE
C
DFB=1.0
HHU = .001
ICX=IR
IF (GL.GT. 0.0) ICX = IM
ICY=IN
GO TO 480
300 IF (IHNNU-1) 550,370,260
C FORM MERGED KAPPAS
C
310 DC 350 I=IN,IM
IF (X6(I)) 320,350,330
320 S1=13.0320
CALL UNCLE
330 CAPAR(I)=X4(I)/X3(I)
340 CAPACII)=X5(I)/X6(I)
350 CONTINUE
HNU=3.E3
HNUP4=8.1E13
HNUP = HNUP - HNU
IHNNU=IHNNU-1
IF(GL.LT.1.) GO TO 370
DO 355 I=1,NMU
IGN2 = IGN + I + NMU
355 QINT(I) = QINT(I)+QINT2)/DHNU
GO TO 370
C TYPICAL GROUP CALCULATION OF SOURCES
C
360 CALL KAPPA(IN,IM)
DHNU=HNUP-HNU
HNUP4=HNUP#4
370 IF (GL-1.) 390,380,380
380 IF (HNU.NE.RDX(IHNNU+52)) GO TO 490
IF (GL.NE.FLOAT(NHNU)) GO TO 490
CALCULATE ICX, ICY
390 ICX=IN
ICY=IN
IF (GL.LE. 0.) GO TO 395
ICX = IM
DO 392 I=IN,IM
DFB = PLNKUT(HNU / THETA(I), HNUP / THETA(I))
392 X6(I)=DFB*Q1(I)
GO TO 480
395 DO 470 I=IN,IR
BETA=HNU/THETA(I)
C AVOID CALCULATION OF DFB LESS THAN 1E-5
C
400 IF (BETA-19.0) 400,410,410
400 BETAP=HNUP/THETA(I)
C EMB2=EXP(-BETAP)
410 IF (BETAP=0.01) 410,410,410
410 IF (ICX=IR) 430,420,420
420 ICX=IR-1
430 IF (ICY-I) 440,440,450
440 ICY=ICY+1
C ICX IS INDEX OF LAST ZONE WITH SIGNIFICANT SOURCE
C I CY IS INDEX OF FIRST ZONE WITH SIGNIFICANT SOURCE
C
450 X6(I)=0.0
X5(I)=0.0
GO TO 470
C FORM SOURCES X6 AND X5
C
460 DFB=PLNKUT(BETA,BETAP)
X6(INM)=DFB*Q1(INM)
TEMP(2)=0.0384974/Q1(INM)*(HNU4/Q1(INM)-1.0)
1 = -HNU4/Q1(INM)*EMB2
C X5(I)=DFB*TEMP(2)
ICX=IR
470 CONTINUE
480 IF (INM1) 490,520,500
C SET BLACKBODY CONDITION FOR IA GREATER THAN 1
C
490 K1=13.0490
CALL UNCLE
500 DFB = PLNKUT (HNU/THETA(INM1),HNU/THETA(INM1))
X6(INM1) = DFB * THETA(INM1)**4
C SET BLACKBODY CONDITION IF DESIRED FOR IMPI
520 IF (GLNE0.5) GO TO 530
DFB = PLNKUT (HNU/THETA(IMPI),HNU/THETA(IMPI))
X6(IMPI) = DFB * THETA(IMPI)**4
530 Q1 = 0.0
C FORM ROSCELAND AND PLANCK OPTICAL DEPTHS
C
DO 590 I=INM,IM
IF (CAPAR(I)) 550,550,540
540 IF (CAPAC(I)) 550,550,560
550 S1=13.0550
CALL UNCLE
C
C CHOOSE ALL ROSCELAND IF SOLID 10 IS POSITIVE
C
560 IF (SOLID(10).EQ.0.) GO TO 570
H(I)=CAPAR(I)/SV(I)
GO TO 580
570 H(I)=CAPAC(I)/SV(I)
580 H(I)=H(I)*DELTAR(I)
IF (ALPHA.GT.1.) GO TO 586
H3(I) = CAPAR(I) * G(I)
GO TO 588
C CAVEAT. ASYNCHRONISMS IN SV AND DEFTAR LEAD TO ERRONEOUS FLUCTUATIONS
C IN H3. THIS CAN BE FIXED BY SUBSTITUTING G IN PLANES, BUT SPHERES
C WILL STILL HAVE THIS TROUBLE.
586 H3(I)=CAPAR(I)/SV(I)*DELTAR(I)
588 Q3(I)=Q3(I-1)+H3(I)
   Q3(I+1)=Q3(I)
   H(I)=0.5*H(I)
   H2(I)=0.5*H2(I)
   H3(I)=0.5*H3(I)

C C ZERO DIFFUSION INDICATORS AND X2
C C
X2(I+1)=0.0
X3(I+1)=0.0
X4(I+1)=0.0

590 RHQ(I)=0.0
   K2(IM)=0.0
   X4(IM)=0.0
   IF (ICY .GT. ICX) GO TO 990
C C
   STEP LINEAR CRITERION AT ICY
   UNCONDITIONAL STEP AS BOUNDARY CONDITION IF ICY = IN
C C
IF (ICY-IN) 675,660,610
600 Y2(IN)=X6(IN)
   TG(IN)=0.0
   GO TO 620
610 TEMP(1)=H3(ICY-1)+H3(ICY)
   TG(ICY)=X6(ICY)/TEMP(1)
   Y2(ICY)=TG(ICY)*H3(ICY-1)
C C
   FORM Y2 AND TG SET X3=-1 IF A DIFFUSION CRITERION MET USING HCB
C C
620 ICM1=ICY-1
IF (ICY .GT. ICM1) GO TO 672
   DG 670 I=ICY,ICMX
   TEMP(1)=H3(I+1)+H3(I)
   IF (ANAXI(X6(I), X6(I+1)) .LE. 0.) GO TO 640
   IF (AMMIN1(H3(I), H3(I+1)) .GT. AC) GO TO 650
   IF (ABS((H3(I)-H3(II))/TEMP(I) .GT. GA) GO TO 640
   IF (ABS((X6(I)-X6(I+1))/X6(I+1)/X6(I)) .GT. GA) 650,650,640
640 TG(I+1)=0.0
   GO TO 670
650 TG(ICY)=X6(ICY)/TEMP(1)
C C
   RADIATION BOUNDARY CONDITION AT ICX
   (VACUUM IF ICX = IM AND GL NOT 1/2)
C C
672 IF (ICX-IM) 680,690,675
675 S1 = 13.0675
CALL UNCLE
680 TEMP(1)+H3(ICX+1)+H3(ICX)
TG(ICX+1)=X6(ICX)/TEMP(1)
Y2(ICX+1)=TG(ICX+1)*H3(ICX+1)
GC TO 700
690 IF (GL .EQ. 0.5) GO TO 700
Y2(IMPI)=X6(ICX)
TG(IMPI)=0.0
C EXTEND TRANSPORT REGION BOUNDARIES, IF NEEDED, TO PROVIDE HVR MEAN
C FREE PATHS
C 700 I=IN+1
710 IF (X3(I)) 720,740,730
720 I=I+1
IF (I-ICX-1) 710,740,820
730 S1=13.0730
CALL UNCLE
740 J=I-1
750 IF (Q3(I)-Q3(J)-HV8) 760,760,770
760 X4(J)=-1.0
J=J-1
IF (J-IN) 770,750,750
770 I=I+1
IF (I-ICX-1) 780,780,820
780 IF (X3(I)) 790,770,730
790 J=I
800 IF (Q3(J)-Q3(I)-HV8) 810,810,720
810 X4(J)=-1.0
J=J+1
IF (J-ICX-1) 800,720,720
820 I=IN+1
C TEST TO FORM TRANSPORT REGIONS
C 830 IAX=IN
840 IF (X3(I)) 850,860,730
850 IF (X4(I)) 860,07C.77
C REMOVE ONE ZONE DIFFUSION REGION
C 860 I=I+1
IF (I-ICX-1) 840,950,950
870 I=I+1
IF (I-ICX-1) 850,950,950
880 IF (X3(I)) 890,840,730
890 IF (X4(I)) 840,900,730
900 IF (I-3) GO TO 960
910 IF (X3(I)) 920,940,730
920 IF (X4(I)) 940,930,730
C FORM X2 FOR DIFFUSION ZONES IN ORDER
930 X2(I) = -1,37E12 * TG(I)
I=I+1
IF (I ICX-1) 910,980,980

42
C DO TRANSPORT TO IM IN REGION OF NO SOURCE
940 IAX=I
   GO TO 860
950 IBX=IM
960 CALL TRANS(IAX,IBX)
   IF (IBX-IM) 970,990,990
970 I=IBX+2
   GO TO 930
980 IF (I.GT.IM) GO TO 990
   IAX=I
   GO TO 950
C OPTIONAL EDIT OF X2 ETC.
C
990 IF (EDITMX) 1020,1020,1000
1000 IARG1=SOLID(18)+0.001
   IARG2=EDITMF+0.001
1010 IF (MOD(IARG1,IARG2)) 1020,1010,1020
1020 WRITE (3) HNU, IN, IM, IMP1, SOLID(18), TH, DHNU
C IN SPHERICAL VERSION, REDIST IS GIVEN RHO.
C REPLACED HERE BY CAPAR.
   WRITE (3) (C(I), I=IN,IMP1), (H(I), I=IN,IM), (X6(I), I=IN,IMP1),
   (LX2(I), I=IN,IMP1),
   2 (CAPAR(I), I=IN,IMP1), (THETA(I), I=IN,IMP1), (E(I), I=IN,IM)
   XX=-2.0
   WRITE (3) XX,XX,XX,XX,XX,XX
   BACKSPACE 3
   JMULT=1
   1020 DO 1030 I=IM,IMP1
      SUMX2(I)=SUMX2(I)*X2(I)
   1030 CONTINUE
C ADVANCE FREQ, STORE EMERGENT FLUX, TEST FOR COMPLETION OF GROUPS
C
   HNUP=HNU
   HNUP4=HNU4
   IHNU = IHNU + 1
   IF ((IHNU-NHNU) 1040,1040,1060
1040 CALL DVCHK (KOOOFX)
   GO TO (1050,360), KOOOFX
C******************************************************
C******************************************************
C END FREQUENCY LOOP
C******************************************************
1050 51 = 13.050
   CALL UNCLE
1060 SUMX2(INP1) = 0.0
   DO 1070 I=INP1,IMP1
      A2(I) = SUMX2(I)
1070 ERI(I) = SUMX2(I) - SUMX2(I+1)
C FORM MCNDFREQUENCY QUANTITIES AND FIND MIN TIME STEP
C
PRAD4220
PRAD4240
PRAD4250
PRAD4260
PRAD4270
PRAD4280
PRAD4290
PRAD4300
PRAD4310
PRAD4320
PRAD4330
PRAD4340
PRAD4350
PRAD4360
PRAD4370
PRAD4380
PRAD4390
PRAD4400
PRAD4410
PRAD4420
PRAD4430
PRAD4440
PRAD4450
PRAD4460
PRAD4470
PRAD4480
PRAD4490
PRAD4500
PRAD4510
PRAD4520
PRAD4530
PRAD4540
PRAD4550
PRAD4560
PRAD4570
PRAD4580
PRAD4590
PRAD4600
PRAD4610
PRAD4620
PRAD4630
PRAD4640
PRAD4650
PRAD4660
PRAD4670
PRAD4680
PRAD4690
PRAD4700
PRAD4710
PRAD4720
PRAD4730
PRAD4740
PRAD4750
C
WSB = 0.0
DO 1075 I = 1, MAXLM
1075 WSB = WSB + ELM(I)
DTR1 = 1.0E0
DTR2 = 1.0E0
IF (KMAX.EQ.0) GO TO 1080
CALL KAPPA(IN, IM)
1080 DO 1230 I = IN, IM
C
IF ROSS IS ZERO EXIT
C
IF (CAPAR(I)) 1090, 1090, 1100
1090 S1 = 13.090
ALL UNCLE
1100 TEMP(I) = CAPAR(I)
IF (SCLID(10)) 1110, 1120, 1110
1110 TEMP(I) = CAPAR(I)
GO TO 1130
1120 TEMP(I) = SQRT(CAPAR(I) * CAPAC(I))
1130 IF (TEMP(I)) 1090, 1090, 1140
1140 H(I) = 0.5 * TEMP(I) / SV(I)
H3(I) = H(I) * DELTAR(I)
IF (.001 < THETA(I)) 1160, 1230, 1230
1160 IF (H3(I) > 0.1) GO TO 1170
IF (ER(I).EQ.0.) GO TO 1170
WSBB = E(I) * G(I)
IF (TELMI(37) .EQ. 0.0) GO TO 1170
IF (WSBB .EQ. WSB) 1170, 1165, 1165
1165 TEMP(2) = 1.5 * CV(I) * THETA(I) * G(I) / ABS(ER(I))
GO TO 1180
1170 TEMP(2) = 1.4 + 0.5 * H3(I) * 2 * CV(I) / 1.413212 * TEMPI(3) * THETA(I)) * 3
TEMP(2) = TEMPI(2) * TELMI(25)
C
FIND MINIMUM TIME STEP
C
PRINT MINIMUM TIME STEPS BETWEEN EDITS
C
44
IF ( DTR1 - TELM(26) ) .LT. 1240, 1250, 1250
1240 TELM(26) = DTR1
TELM(27) = IMIN1
TELM(28) = DTR2
TELM(29) = IMIN2
TELM(30) = SOLID(18) + 1.0
1250 CONTINUE
C
C DETERMINE IF RADIATION OR HYDRO WILL SUBCYCLE
C
C IF ( DTRMIN - DTR ) .LT. 1280, 1300, 1260
C
1260 BLANK3 = TH+AMIN1(DTRMIN, GR* DTH2)
C
1270 S9 = .5
GC TO 1360
C
C**********************************************************************
C
C REDUCE TIME STEP
C
C**********************************************************************

1280 NRAD = ZPI(18)/ DTRMIN+1.0
DTR = ZPI(18)/ FLOAT(NRAD)
IF (NRAD-NTIMES) .LT. 1300, 1300, 1290
C
1290 S1 = 13.1290
CALL UNCLE
C
5 ZERO OUT STRAY QUANTITIES FROM PREVIOUS CYCLES
C
1300 DC 1310 I = IMPI, IG
CAPAR(I) = 0.
CAPAC(I) = 0.
X2(I+1) = 0.
X3(I+1) = 0.
X4(I+1) = 0.
SUMX2(I+1) = 0.
SUMX3(I+1) = 0.
SUMX4(I+1) = 0.
C
1310 ER(I+1) = 0.
IF ( ZPI(26) = .EQ. 0.0) GO TO 1400
C
C RESTORE GOODIES FOR NONEQ
C
GPUSH "+LT* 0.0) GO TO 1350
BC IMPI=WSZ2
BR( IMPI)=WSZ3
CFTR(IMPI) = WSZ4
RQ( IMPI) = WSZ5
GO TO 1400
C
BC(INM1) = WSZ2
BR(INM1) = WSZ3
CFTR(INM1) = WSZ4
RHC(INM1) = WSZ5
C
1400 RETURN
END
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$IBFC PTRANS FULIST,DECK,REF
SUBROUTINE TRANS(N,M)
C COMPILED JULY 1, 1965 WBL
C PLANE CHARACTERISTIC TRACE WITH DOUBLE GAUSSIAN INTEGRATION
C DECK DBLLOG REQUIRED FOR INTEGRATION COEFFS.
C
C******************************************************************************
PTRA0050
C
C
C COMMON LMA0(37), NR, NMLR, IA, IB, ICA, ICB, PTRA080
1 KMAX , BLANK1, BLANK2, BLANK3, IAP1, IBP1, ICAPI, ICBP1, PTRA090
2 II, IG, NRAIN, BLANK4, IAM1, IMN1, IACM1, ICBM1, PTRA100
3 IPI1, IGM1, IALPHA, BLANK5, TH, TMAX, BLANK6, DELPTRT, PTRA110
4 FREQ, CNTMAX, AR, ASMLR, PUSHA, PUSHB, BOILTA, BOILTB, PTRA120
5 CVB, CVB, SLEY, ALPHI, MVA, NVB, HCA, NCART, PTRA130
6 EMMA, EMINH, CA, CB, GA, GB, GL, GR, PTRA140
7 RHCL, RHOR, EPIO, EPS1, RIJA, RIB, RIOL, RDI1, PTRA150
8 RP1IA, RPIB, RPDI1A, RPDIB, TPRTI1, TA, TB, TC, PTRA160
C COMMON TD, TE, DTU2, DTU2P, DTU1, DTU4N, DTU4M, PTRA170
1 DTMAX1, DTMAX2, DTMAX3, DTR, SWITCH, CO, CMN, DELTA, PTRA180
2 GAMA, WCRT, SINGA, AC, AC03T1, CVNTRT, SUMRA, SUMRB, PTRA190
3 ROIA, ROIAM1, ROIB, ROIBP1, GMS, SL, S2, S3, PTRA200
4 S4, S5, S6, S7, S8, S9, S10, S11, PTRA210
5 S12, S13, S14, S15, S16, S17, S18, S19, PTRA220
6 S20, E0, FD, TAU, ZERO, R, T, T, DELTAR, PTRA230
7 ASQ (152), RD (152), VA (152), RRO (152), SMLR (152), PTRA240
8 DELR (37), P (152), P1 (152), PB (152), PBL (152), PTRA250
C COMMON P2 (152), SV (152), RHO (152), THETA (152), PTRA260
1 W (152), E (152), EI (152), EK (152), A (152), PTRA270
2 V (152), X1 (152), X2 (152), C (152), X3 (152), PTRA280
3 X3 (152), X4 (152), X5 (152), X6 (152), X7 (152), PTRA290
4 SMLA (152), SMLB (152), SMLC (152), SMLO (152), SMLE (152), PTRA300
5 EC (152), ER (152), SMLQ (152), SMLH (152), BIGA (152), PTRA310
6 BIGB (152), CV (152), BC (152), BR (152), CHIC (152), PTRA320
7 CHIR (152), CAPC (152), CAR (152), CRTC (152), CRTR (152), PTRA330
8 CRTPC (152), GOFR (152), FEW (152), CAR (152), OKLM (37), PTRA340
C COMMON TELM (77), EKLM (37), ELM (37), FCLM (37), PTRA350
1 PALM (37), MLM (37), QLM (37), AMASNO (37), CRRDQ (37), PTRA360
2 ZP1 (37), ZP2 (37), SOLID (37), ECHCK (37), RK (104), PTRA370
3 RL (37), RHOK (104), RDQ (104), THEAT (104), TEMP (16), PTRA380
4 HEAD (12), MAXL, MAXL, PTRA390
C******************************************************************************
PTRA040
C
C DIMENSION Q3(1),TG(1),H2(1),Q11(1),X8(1),SUMX3(1),SUMX4(1)
PTRA040
DIMENSION H(1),Y2(1),H(1),SUMX2(1),Q2(1)
PTRA040
DIMENSION Q3(1), Q3(1), H3(1)
PTRA040
COMMON /LINDLY/ HNU, SNGL, HNUH, HNU, HNUP, NT, IN, DHNU, THICK, NY
PTRA040
COMMON /CNTRL/ SCYCLE, JMULT
PTRA040
COMMON 'DAVUS/ ICX, ICY
PTRA040
COMMON 'STO/ QINT(1300), QINT(300), TITLE(12)
PTRA040
EQUIVALENCE (SMXL,H4),(SMXL,Y2)
PTRA040
EQUIVALENCE (BCTG,H10BG),(CCTR,SYMX2),(CHIC,SYM3)
PTRA040
EQUIVALENCE (SMXL,XY),(CAR,Q37),(CHIR,Q38),(SMLC,H3)
PTRA050
EQUIVALENCE (AC03T1,TRDBG),(S12,EDITM)
PTRA050
EQUIVALENCE (ECL,SL1),(X7,H2),(GIGA,SUM4X),COFR,G3
PTRA050
C******************************************************************************
PTRA0340
DIMENSION RR(40)
DATA RR/2.113248E-01,1.886752E-01,1.056624E-01,3.943376E-01/, PTRA0550
1 1.127017E-01,1.5.000000E-01,1.1.87983E-01,1.1.130600E-02/, PTRA0560
2 2.222222E-01,1.446718E-01,6.943180E-02,3.300995E-01/, PTRA0570
3 6.69005E-01,9.205682E-01,1.207610E-02,1.076071E-01/, PTRA0580
4 2.184655E-01,1.618513E-01,4.691010E-02,2.307653E-01/, PTRA0590
5 5.000000E-01,1.492347E-01,9.530899E-01,5.557100E-03/, PTRA0600
6 5.522540E-02,1.422222E-01,1.840889E-01,1.129063E-01/, PTRA0610
7 3.37620E-02,1.093953E-01,1.309096E-01,1.930962E-01/, PTRA0620
8 8.30647E-01,1.066234E-01,2.892400E-03,3.055570E-02/, PTRA0630
9 8.906520E-02,1.448918E-01,1.076071E-01,1.930962E-01/, PTRA0640
C EDITMF SAME AS S12
C H SAME AS BIGB
C H2 SAME AS XT
C H3 SAME AS SMLC
C H4 SAME AS SMLA
C Q1 SAME AS EC
C Q3 SAME AS GOFR
C Q37 SAME AS CAR
C Q38 SAME AS CHIR
C SUMX2 SAME AS CAR
C SUMX3 SAME AS CHIC
C SUMX4 SAME AS BIGA
C IG SAME AS BC
C 1RDBG SAME AS ACOST4
C X6 SAME AS SMLH
C Y2 SAME AS SMLD
C
******************************************************************************
C FEX, FM, SUMRHO, CSQ0, XSQ0, Y, YSQD, Q2, NOT USED
C******************************************************************************
C PLANES ONLY
C******************************************************************************
C IAX1=N
C IBX=M
C IN1=IN-1
C IM1 = IM + 1
C CALL DVCHK(KDOOFX)
C GO TO (100,110), KDOOFX
100 51=14, 0100
C CALL UNCLE
C 110 18XP1=IBX+1
I ALPHA=ALPHA
C ERROR IF NOT PLANE
C GO TO (130,120,120), I ALPHA

C
50
120 S1=14.0120
CALL UNCLE
130 NY = LMDA(37) - 1
    NMU = (NY - 1) * (NY + 2) + 1
    NGS = NMU + NY + 1
    JJ = 0

C DO POSITIVE ANGLES FIRST
C
140 I=IAX
F2=0.0
C IF IAX=IN TRANSFER TO 150 TO SET SPECIAL BOUNDARY CONDITIONS
C
IF (IAX-IN) 360,150,100
C
CALCULATE BOUNDARY SOURCE INTENSITY
C
150 IF (INW1) 160,310,170
C
SET BLACKBODY CONDITION FOR PUSHER
C
160 S1=14.0160
CALL UNCLE
170 F2=X6(INM1)
GO TO 310
C
DIFFUSION BOUNDARY CONDITION AT IAX

180 IF (TG(I) .EQ. 0.) Y2(I) = X6(I-1)
    TEMP(I)=H2(I-1)/RR(NMU)
    X8(I)=TG(I)*RR(NMU)
    IF (TEMP(I)-1.E-2) 190,190,200
190 F2 = (Y2(I-1) + Y2(I-1)) * 0.5 + X6(I-1) - F2+X2X)* TEMP(I) + F2X*PTRAI180
GO TO 250
200 H4(I-1)=FREXP(-TEMP(I))
F2=Y2(I-1)-X8(I-1)*RR(NMU)*TG(I-1)*H4(I-1)
GO TO 250
210 IF (TG(I-1) .EQ. 0.) Y2(I-1) = X6(I-1)
    X8(I-1)=TG(I-1)*RR(NMU)
C
REGULAR INTEGRATION STEP FOR F2, POSITIVE MU
C
220 IF (TG(I) .EQ. 0.) Y2(I) = X6(I-1)
    X8(I)=TG(I)*RR(NMU)
    TEMP(I)=H2(I-1)/RR(NMU)
    IF (TEMP(I)-1.E-2) 230,230,240
230 F2 = ((Y2(I) + Y2(I)) * 0.5 + X6(I-1) - F2+X2X)* TEMP(I) + F2X
GO TO 250
240 H4(I-1)=FREXP(-TEMP(I))
F2=Y2(I)+X8(I+1)*((F2-Y2(I+1))/X8(I-1))*H4(I-1)
GO TO 250
250 IF (F2.LT.0.0) GO TO 280
260 SUMX3(I)=F2
IF (TG(I) .EQ. 0.) Y2(I) = X6(I)  
I=I+1  
IF (I-IBXPI) 270, 270, 320  
270 IF (I-ICX-1) 220, 220, 290  
C  
NEGATIVE F2 ERROR  
C  
280 S1=14.0280  
CALL UNCLE  
C  
NO SOURCE IN ZONE GREATER THAN ICX  
C  
290 IF (F2.EQ.0.0) GO TO 260  
TEMP(I)=H2(I-1)/RR(NMUI)  
H4(I-1)=FREXP(TMP(I))-EXP(TMP(I))  
F2=F2*H4(I-1)  
GO TO 260  
300 IF (F2.EQ.C.0.0) GO TO 310  
TEMP(I)=H2(I-1)/RR(NMUI)  
H4(I-1)=FREXP(TMP(I))-EXP(TMP(I))  
F2=F2*H4(I-1)  
310 FUMX3(I) = F2  
I=I+1  
IF (I-ICY) 300, 300, 210  
C  
DO NEGATIVE ANGLES SECOND  
C  
320 I=IBXPI  
IF (IBX-IM) 370, 330, 340  
330 IF (GL) 480, 520, 340  
C  
GL = 1/2 MEANS BLACKBODY CONDITION SET AT IMP1  
C  
GL = POSITIVE INTEGER MEANS INTENSITIES FROM QINT1 TABLE AT IMP1  
C  
GL = 0 MEANS VACUUM AT IMP1  
C  
GL NEGATIVE MEANS REFLECTIVE CONDITION AT IMP1  
340 IF (GL.NE.0.5) GO TO 350  
F2 = X6(IMPI)  
GO TO 480  
350 IQNT = JJ + 1 + (NY + 1) * (NMUI - 1)  
F2 = QINT(IQNT) / 68.5 * DMNU  
GO TO 480  
C  
ERROR IF INDEX EXCEEDS NORMAL RANGE  
C  
360 S1=14.0360  
CALL UNCLE  
C  
DIFFUSION BOUNDARY CONDITION AT IBXPI  
C  
370 IF (TG(I) .EQ. 0.) Y2(I) = X6(I)  
TEMP(I)=H2(I)/RR(NMUI)  
IF (TEMP(I) .LE. 2) 380, 380, 390  
380 F2X = Y2(I+1) + TG(I+1) * RR(NMUI)  
F2 = (F2X - Y2(I)) + Y2(I+1) * 0.5 + X6(I) - F2X - F2X) * TEMP(I) + F2X  
GO TO 430  
390 H4(I)=FREXP(TEMP(I))
F2 = Y2(I) + X8(I) + (RR(NMU)*TG(I+1) - X8(I)) * H4(I)
GO TO 430
399 IF (TG(I+1) .EQ. 0.) Y2(I+1) = X6(I)
C REGULAR INTEGRATION STEP FOR F2, NEGATIVE MU
C 400 IF (TG(I) .EQ. 0.) Y2(I) = X6(I)
TEMP(I) = H4(I) / RR(NMU)
IF (TEMP(I) .LT. 1.E-2) GO TO 410
410 F2 = ((Y2(I) + Y2(I+1)) * 0.5 + X6(I) - F2 - F21) * TEMP(I) + F2
GO TO 430
420 F2 = Y2(I) + X8(I) + (F2 - Y2(I+1) - X8(I+1) + H4(I)) / X8(I+1) - X8(I) * H4(I)
430 IF (F2 .LT. 0.0) GO TO 460
440 SUMX4(I) = F2
C FORM CONTRIBUTION TO X2
X2(I) = X2(I) - (F2 - SUMX3(I)) * RR(NGS)
C RHO(I) = RHO(I) + (F2 + SUMX3(I)) * RR(NGS) / RR(NMU)
C 450 IF (TG(I) .EQ. 0.) Y2(I) = X6(I-1)
I = I - 1
IF (I .LT. ICY) GO TO 530, 470, 450
C 460 IF (F2 .LE. 0.0) GO TO 480
TEMP(I) = H2(I) / RR(NMU)
H4(I) = FREXP(-TEMP(I)) - TEMP(I)
F2 = F2 * H4(I)
480 SUMX4(I) = F2
490 X2(I) = X2(I) - (F2 - SUMX3(I)) * RR(NGS)
I = I - 1
IF (I .LT. ICX) GO TO 399, 470, 490
C NO SOURCE IN ZONE LESS THAN ICY
C 500 IF (F2 .EQ. 0.0) GO TO 510
TEMP(I) = H2(I) / RR(NMU)
H4(I) = FREXP(-TEMP(I)) - TEMP(I)
F2 = F2 * H4(I)
510 SUMX4(I) = F2
520 X2(I) = X2(I) - (F2 - SUMX3(I)) * RR(NGS)
I = I - 1
IF (I .LT. ICX) GO TO 330, 500, 520
C NO SOURCE IN ZONE LESS THAN ICY
C 530 CONTINUE
IF (TRDBG .EQ. 0.0 .OR. TRDBG .GE. SOLID(18)) GO TO 539
C STORE INTENSITIES FOR DEBUG PRINT
XX = -0.5
JJJ = JJ + 1

WRITE (3) XX, IAX, JJJ, IBXP1, SOLID(18), TH, RR(NMU)
WRITE (3) (SUMX3(I), SUMX4(I), I = IAX, IBXP1)
XX = -2.
WRITE (3) (XX, I = 1, 7)
BACKSPACE 3

539 DHNU=HNUP-HNU
540 JJ = JJ + 1
550 NMU = NMU + 1
550 NGS = NGS + 1
550 DO 560 I=IAX,IBXP1
560 X2(I) = X2(I)*2.052E12
RETURN
END
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KEY WORDS

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