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Numerical Methods for Solution of the Integral Equations of Multi-Dimensional Radiation Transport

(Title Unclassified)

UNITED STATES
ATOMIC ENERGY COMMISSION
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Numerical Methods for Solution of the Integral Equations of Multi-Dimensional Radiation Transport

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Director, Air Force Weapons Laboratory	12-14
Military Liaison Committee	15
DCS/Research and Development, Headquarters, USAF	16
Chief, R&D, Army	17
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Op-75, Navy	19
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Abstract

The radiation transport equation and the equation for the change of material energy through interaction with radiation are formulated as an integral equation for the temperature. Geometric aspects of the interaction of distant source regions are incorporated into energy exchange coefficients which are formulated for the case of pure absorption.

Primary consideration is of the form of the approximating difference equations for the evolution of the system in time. Given appropriate energy exchange coefficients, the equations are applicable to quite general configurations which may be subdivided into cells of arbitrary shape. Boundaries of the system receive special treatment based on the assumption that a very short mean free path exists there. Frequency dependence is treated in the group approximation. The time dependence of the equations includes the retardation of the sources and the centering of the energy difference equation. The resulting equations are solved by an iteration scheme.

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Introduction

A number of calculational methods for solution of transient radiation transport problems in plane and spherically symmetric configurations has been developed. Greatest emphasis has been placed on methods in which the energy equation and the transport equation for the intensity are approximated over a spatial cell and give difference equations for the radiation intensity and material temperature.[1] Smaller efforts have been applied to the Monte Carlo[2] and integral equation[3] methods. The techniques vary widely in accuracy and the amount of calculation and computer storage requirements. Furthermore, the dependence of these quantities on the number of spatial zones is different. Consequently, while extension of each of these methods to configurations of higher dimensionality is possible, considerable differences in code complexity and efficiency are to be expected.

In this report an outline is given of the generalization of the integral method.[3] The formulation depends on the geometry and dimensionality of the system only through coefficients which are assumed known. Primary consideration is given to specification of the difference equations in time, to methods for solution of the equations, and to general properties of the energy exchange coefficients. The boundaries of the system are given special treatment.

On the basis of comparisons between the difference and integral methods, it is expected that for small numbers of zones the integral method will be faster as well as more accurate. When the coefficients are simply calculated or do not change with time, considerable advantage in simplicity of the code is also realized.

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Experience in applying transport codes to multi-dimensional problems is still limited, however. In order to be able to choose the best method for a particular problem, additional calculations with the available techniques are needed.

The Integro-Differential Equations

The equation for the change of the intensity I of the radiation is

$$\frac{1}{c}\frac{\partial I}{\partial t} + \Omega \cdot \nabla I = \mu_a' (B-I) \quad , \qquad (1)$$

where the intensity is the radiation energy traveling in the direction Ω per unit area normal to Ω, per unit time, per unit frequency interval, and per unit solid angle. The absorption coefficient corrected for induced emission is μ_a', the Planck function is

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

associated with the material temperature θ, and c is the speed of light. A solution of Eq. (1) can be obtained in integral form in which the intensity in a particular direction is expressed in terms of sources along the backward drawn ray from the point at which the intensity is to be evaluated (see Fig. 1). Denoting distance along this ray by s,

$$I = \int_0^\infty e^{-\int_0^s \mu_a' \, ds'} \mu_a' B \, ds \quad . \qquad (2)$$

The quantities in the integrand depend on both position and time. While the position dependence is evident, the time dependence is through the retarded time t', that is, that earlier time such that the signal reaches

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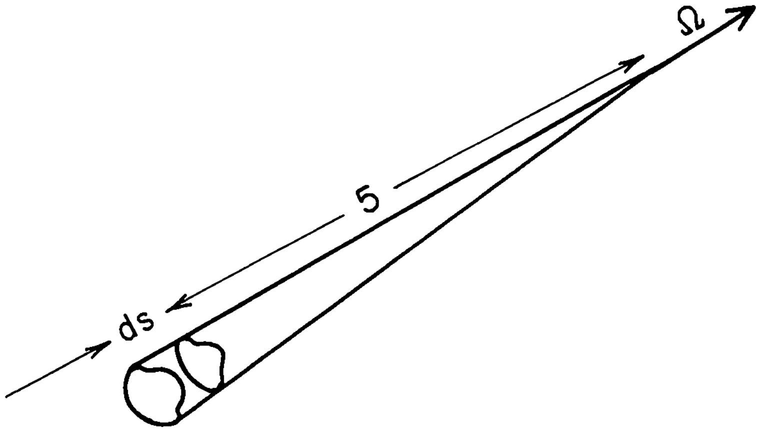

Figure 1

the point s = 0 at the current time t,

$$t' = t - \frac{s}{c} \quad .$$

The material energy E changes by virtue of hydrodynamics of the material which changes the specific volume τ, the pressure p, and the radiative terms which account for the emission and absorption of radiation,

$$\frac{dE}{dt} = - p \frac{d\tau}{dt} + c \int_0^\infty d\nu \; u_a' \left(\int I d\Omega - 4\pi B \right) \quad . \tag{3}$$

The absorption term is to be evaluated by using Eq. (2) for the intensity,

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$$\int I\,d\Omega = \int_0^\infty ds \int_{4\pi} d\Omega \; e^{-\int_0^s \mu_a'\, ds'} \mu_a' B$$

$$= \int_{\substack{\text{all}\\ \text{space}}} dV \, \frac{e^{-\int_0^s \mu_a'\, ds'}}{s^2} \, \mu_a' B \quad . \tag{4}$$

Since the system is considered to be bounded by regions in which the mean free path is very short (walls) and which have a temperature giving a Planck function B_w which is uniform several mean free paths into the wall (although varying along the wall), an especially simple result is obtained for the boundary. If the distance to the wall is s_w and the ray makes an angle θ_w with the wall normal, the integral over the wall volume is

$$\int_{\substack{\text{wall}\\ \text{volume}}} dV \, \frac{e^{-\int_0^s \mu_a'\, ds'}}{s^2} \, \mu_a' B$$

$$= \int_{\substack{\text{wall}\\ \text{area}}} d\sigma \, \frac{e^{-\int_0^{s_w} \mu_a'\, ds'}}{s_w^2} \, B_w \cos\theta_w \int_{s_w}^\infty ds \; e^{-\int_{s_w}^s \mu_a'\, ds'} \mu_a'$$

$$= \int_{\substack{\text{wall}\\ \text{area}}} d\sigma \, \frac{e^{-\int_0^{s_w} \mu_a'\, ds'}}{s_w^2} \, B_w \cos\theta_w \quad . \tag{5}$$

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Substituting these results in Eq. (3) gives

$$\frac{dE}{dt} = - p \frac{d\tau}{dt} + c\int_0^\infty d\nu \, \mu_a' \left(\int_{\text{volume}} dV \, \mu_a' B \, \frac{e^{-\int_0^s \mu_a' ds'}}{s^2} + \int_{\text{walls}} d\sigma \, B_w \cos\theta_w \, \frac{e^{-\int_0^{s_w} \mu_a' ds'}}{s_w^2} - 4\pi B \right) , \tag{6}$$

in which the volume integral ranges over all of the system inside the walls which can be reached by rays from the point P in question without intersecting the walls, and the surface integral ranges over all of the wall area first reached by these rays (see Fig. 2).

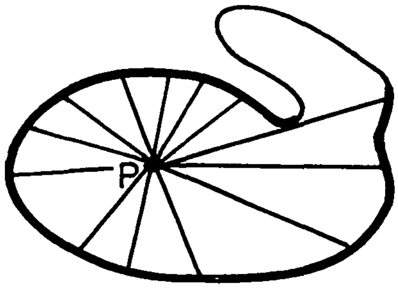

Figure 2

The absorption coefficient enters the equations in three places: in the source to determine the volume contribution, in the exponential attenuation, and in the absorption at the position where the heating is being evaluated.

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Surface Equations

The walls are treated as special cases of these equations. By virtue of the substantially isothermal surface layer of the wall, reradiation of a blackbody spectrum at the wall temperature occurs. The equations for the walls describe the disposition of the intercepted radiation as lost into the wall interior and radiated as blackbody radiation at a temperature sufficient to maintain the energy balance. The energy falling on unit area of the wall is given by $\int_{2\pi} I \cos\theta_w' \, d\Omega$, where θ_w' is the angle made by the ray with the normal to the wall element. Substituting for I from Eq. (2) as before and identifying both volume and surface sources gives

$$\int_{\text{volume}} dV \cos\theta_w' \mu_a' B \frac{e^{-\int_0^{s} \mu_a' ds'}}{s^2} + \int_{\text{walls}} d\sigma \cos\theta_w \cos\theta_w' B_w \frac{e^{-\int_0^{s_w} \mu_a' ds'}}{s_w^2} . \qquad (7)$$

Retardation of the time is required in Eq. (7) too. The loss rate per unit area of the wall and per unit frequency is denoted by L, and reradiation takes place as πB_w. When integrated in frequency these terms give the wall energy balance equation,

$$\frac{a}{4} T_w^4 = \int_0^\infty d\nu \left(\int_{\text{volume}} dV \cos\theta_w' \mu_a' B \frac{e^{-\int_0^{s} \mu_a' ds'}}{s^2} + \int_{\text{surface}} d\sigma \cos\theta_w \cos\theta_w' B_w \frac{e^{-\int_0^{s_w} \mu_a' ds'}}{s_w^2} - L \right) , \qquad (8)$$

where T_w is the wall temperature.

Equations (6) and (8) constitute integro-differential equations for determining the evolution of the system in time. To apply them to an actual problem it is necessary to consider the spatial, frequency, and time dependence of the equations. In the following paragraphs these topics are treated successively.

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Spatial Difference Equations

The system, composed of material surrounded by walls, is subdivided into cells within which the temperature and material properties are uniform, representing an average value characteristic of the cell as a whole. Two kinds of cells are distinguished: volume cells denoted by index i to which Eq. (6) applies, containing material in a thermodynamic state having density ρ_i and temperature T_i; and surface cells denoted by K which, by virtue of their blackbody behavior, are characterized by a surface temperature T_K and to which Eq. (8) applies. In order to obtain zone equations it is necessary to evaluate the integrals of Eqs. (6) and (8) in the zone approximation and to perform an average of the material energy over the cell volume or the blackbody temperature over the surface cell area.

Neglecting the work term, the energy equation, Eq. (6), becomes

$$\frac{d}{dt}\left(V_i E_i\right) = c\int_0^\infty d\nu \left(4\pi \sum_j V_j \mu_j B_j \alpha_{ij} + \pi \sum_K S_K B_K \beta_{iK} - 4\pi V_i \mu_i B_i\right) ,$$

where

$$\alpha_{ij} = \frac{1}{4\pi V_j} \int_{V_i} dV \, \mu_i \int_{V_j} dV \, \frac{e^{-\int_0^s \mu \, ds}}{s^2}$$

and

$$\beta_{iK} = \frac{1}{\pi S_K} \int_{V_i} dV \, \mu_i \int_{S_K} d\sigma \cos\theta_K \, \frac{e^{-\int_0^{s_w} \mu \, ds}}{s_w^2} \quad . \qquad (9)$$

In Eq. (9) the volume cells have volume V_i, energy density E_i, absorption coefficient μ_i, and Planck function B_i, while a second volume cell quantity is denoted by index j. Surface cells have area S_K and Planck

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function B_K. Summations in Eq. (9) range over all volume cells and surface cells, respectively. In the exponentials of α_{ij} and β_{iK} the subscript "a" and prime have been dropped, but the results are still applicable only to the pure absorption problem. The energy equation, however, is more generally applicable than to the pure absorption case. Given, for example, coefficients determined by taking account of Compton scattering, the evolution of the system can still be calculated by Eq. (9).

Averaging the surface Eq. (8) over the area of zone K gives

$$\frac{a}{4} S_K T_K^4 = \int_0^\infty d\nu \left(4\pi \sum_j V_j \mu_j B_j \beta_{Kj} + \pi \sum_\ell S_\ell B_\ell \gamma_{K\ell} - I_K \right) ,$$

where

$$\beta_{Kj} = \frac{1}{4\pi V_j} \int_{S_K} d\sigma \cos \theta_K \int_{V_j} dV \, \frac{e^{-\int_0^s \mu \, ds}}{s^2}$$

and

$$\gamma_{K\ell} = \frac{1}{\pi S_\ell} \int_{S_K} d\sigma \cos \theta_K \int_{S_\ell} d\sigma \, \theta_\ell \, \frac{e^{-\int_0^{s_w} \mu \, ds}}{s_w^2} \quad . \qquad (10)$$

In addition to the remarks about notation above, the additional subscript ℓ denoting a surface cell has been introduced.

Coefficient Properties

If the temperatures of all wall and volume cells are equal, then a state of equilibrium must exist in which dE/dt = 0. This requires that

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$$\int_0^\infty B d\nu \left(4\pi \sum_j V_j \mu_j \alpha_{ij} + \pi \sum_K S_K \beta_{iK} - 4\pi V_i \mu_i\right) = 0 \quad .$$

When the loss term L_K is zero and temperatures are all equal the surface equation of Eqs. (10) become

$$\int_0^\infty d\nu\, B \left(4\pi \sum_j V_j \mu_j \beta_{Kj} + \pi \sum_{\ell} S_{\ell} \gamma_{K\ell} - \pi S_K\right) = 0 \quad .$$

Since in equilibrium a state of detailed balance must exist, the equilibrium equations can be written for each frequency as

$$\sum_j V_j \mu_j \alpha_{ij} + \frac{1}{4} \sum_K S_K \beta_{iK} = V_i \mu_i$$

and

$$\sum_j V_j \mu_j \beta_{Kj} + \frac{1}{4} \sum_{\ell} S_{\ell} \gamma_{K\ell} = \frac{1}{4} S_K \quad . \qquad (10')$$

In order for a state of thermodynamic equilibrium to be achieved and for the above equations to hold, it is necessary that for each physical process by which radiation interacts with the material the inverse process must be taken into account. Only when this is the case can the coefficients be expected to obey Eqs. (10′). For example, if the production of electron-positron pairs is included it is necessary to also take account of annihilation of pairs. These equations are considered further in connection with the reciprocity relations described below.

The normalization of the coefficients α_{ij}, β_{iK}, β_{Kj}, and $\gamma_{K\ell}$ has been chosen to simplify their calculation by Monte Carlo methods. They obey sum rules

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$$\sum_i \alpha_{ij} + \sum_K \beta_{Kj} = 1$$

and

$$\sum_i \beta_{iK} + \sum_\ell \gamma_{\ell K} = 1 \quad . \tag{11}$$

The first of these equations is equivalent to the statement that energy emitted in zone j is absorbed completely in the rest of the system, while the second equation makes the corresponding statement for energy emitted from a surface zone K. Consequently, the coefficients describe the fraction of energy emitted from the zone having the second subscript which is absorbed in the zone of the first subscript. Clearly, the sum rules of Eqs. (11) are applicable if other interactions than pure absorption (e.g., scattering) are important.

Certain symmetries of the coefficient matrices can be recognized from the equations of definition, Eqs. (9) and (10). These reciprocity relations are

$$\alpha_{ji} = \frac{\mu_j V_j}{\mu_i V_i} \alpha_{ij} \quad ,$$

$$\beta_{Ki} = \frac{S_K}{4 \mu_i V_i} \beta_{iK} \quad , \tag{12}$$

and

$$\gamma_{\ell K} = \frac{S_\ell}{S_K} \gamma_{K\ell} \quad .$$

The relations of Eqs. (10′), (11), and (12) are not all independent. Substituting the reciprocity relations into Eqs. (10′) the normalization equations, Eqs. (11), are recovered. Consequently, the reciprocity relations are sufficient conditions for insuring that thermodynamic equilibrium be attainable by the volume and surface equations.

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The reciprocity relations of Eqs. (12) have been derived for the case of pure absorption in the material. They are more general, however, and are also valid when other interactions and their inverses are included. Such is the case for the important problem when Thomson scattering is present. When the energy loss of Compton scattering is taken into account, it is necessary to include the effect of inverse Compton collisions if the reciprocity relations are to be satisfied.

Frequency Dependence of the Equations

First, the case of absorption coefficients satisfying the grey atmosphere approximation is considered. Then it is possible to perform the indicated frequency integrations in Eqs. (9) and (10). Denoting the frequency independent absorption coefficient by $\bar{\mu}$ the equations become

$$\frac{d}{dt}\left(V_i E_i\right) = ca\left(\sum_j V_j \bar{\mu}_j T_j^4 \alpha_{ij} + \frac{1}{4}\sum_K S_K T_K^4 \beta_{iK} - V_i \bar{\mu}_i T_i^4\right) \quad ,$$

and

$$\frac{a}{4} S_K T_K^4 = a \sum_j V_j \bar{\mu}_j T_j^4 \beta_{Kj} + \frac{a}{4} \sum_\ell S_\ell T_\ell^4 \gamma_{K\ell} - \int_0^\infty d\nu \, I_K \quad . \tag{13}$$

The grey approximation is particularly applicable for (a) the surface sources which are independent of the material absorption coefficient by virtue of the optical thickness of the heated surface layer and, consequently, have a blackbody frequency dependence and (b) the Compton scattering by free electrons which is substantially frequency independent.

When the frequency dependence cannot be neglected the integrals are approximated by forming frequency groups $\nu_m \leq \nu \leq \nu_{m+1}$ in which the absorption coefficient can be considered to be approximately constant.

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Denoting quantities associated with the above frequency interval by the additional subscript m the group equations become

$$\frac{d}{dt}\left(V_iE_i\right) = ca\left(\sum_j V_jT_j^4\sum_m b_{jm}\mu_{jm}\alpha_{ijm} + \frac{1}{4}\sum_K S_KT_K^4\sum_m b_{jm}\beta_{iKm} - V_i\mu_{p_i}T_i^4\right) \quad ,$$

and

$$\frac{a}{4}S_KT_K^4 = a\sum_j V_jT_j^4\sum_m b_{jm}\mu_{jm}\beta_{Kjm} + \frac{a}{4}\sum_\ell S_\ell T_\ell^4\sum_m b_{jm}\gamma_{K\ell m} - \int_0^\infty d\nu\, I_K \quad . \qquad (14)$$

In Eqs. (14) the quantity b_m is the normalized integral of the Planck function over the frequency group given by

$$b_{jm} = \frac{15}{\pi^4}\int_{u_m}^{u_{m+1}} \frac{u^3}{e^u - 1}\,du \quad ,$$

where

$$u_m = \frac{h\nu_m}{T_j} \quad ,$$

obeying the sum rule $\sum_m b_{jm} = 1$. The partial Planck mean absorption coefficient $\mu_{p_{jm}}$ is of use in Eqs. (14) and is defined as

$$\mu_{p_{jm}} = \frac{\int_{\nu_m}^{\nu_{m+1}} d\nu\ \mu'_{a_i}B(T_i)}{\int_{\nu_m}^{\nu_{m+1}} d\nu B(T_i)} \quad .$$

In terms of these quantities the Planck mean absorption coefficient μ_{p_j}

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appearing in Eqs. (14) is $\mu_{p_j} = \sum_m b_{jm} \mu_{p_{jm}}$. The partial Planck mean absorption coefficient may also be used for μ_{jm}^{jm} in Eqs. (14). The fact that the Rosseland mean does not enter these equations is another reminder of the fact that the diffusion regime is not adequately described by the approximation of constant temperatures within zones unless each zone is optically very thin. A higher approximation taking account of variation of temperature within optically thick zones is needed for the correct limiting value in the diffusion limit.

Difference Equations in Time

In the equations as discussed above the time dependence has been omitted. Both the retardation of the source terms and the difference approximation to the energy derivative must be formulated in a way which gives adequate accuracy.

The treatment of retardation has two related aspects: first, the heating rate is modified by sampling the source at distant positions at an earlier time when the temperature was different; and second, the energy stored in the radiation field is a consequence of the finite speed of light and vanishes when this speed is made infinite. Consequently, in order to include the effect of the specific heat of the radiation in the material energy equations it is essential to take account of retardation. This consideration is illustrated by the equations derived above. The rate of change of the material energy of the entire system E_T is obtained by summing Eq. (9) over all material cells,

$$\frac{dE_T}{dt} = c\int_0^\infty d\nu \left(4\pi \sum_j V_j \mu_j B_j \sum_i \alpha_{ij} + \pi \sum_K S_K B_K \sum_i \beta_{iK} - 4\pi \sum_i V_i \mu_i B_i \right) .$$

Equation (10) in which the wall loss has been set to zero is summed over all surface cells and then added to and subtracted from the above equation.

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Provided the sources are <u>not</u> retarded the terms can be grouped as follows:

$$\frac{dE_T}{dt} = c\int_0^\infty d\nu \left[4\pi\sum_j V_j\mu_j B_j\left(\sum_i \alpha_{ij} + \sum_K \beta_{Kj} - 1\right) + \pi\sum_K S_K B_K\left(\sum_i \beta_{iK} + \sum_\ell \gamma_{\ell K} - 1\right)\right].$$

Comparing with the sum rules of Eqs. (11) the result $dE_T/dt = 0$ is obtained. It is clear in the derivation, however, that the sources must be taken at the same time as in the calculation omitting retardation, for the necessary factorization of the equation to occur.

The differential equation in time of Eq. (9) is approximated by a first order difference equation. The calculation is to proceed forward in time by evaluation of quantities at a finite number of instants t^n separated by time intervals Δt^n: $t^{n+1} - t^n = \Delta t^n$. Denoting quantities evaluated at the instant t^n by the corresponding superscript (e.g., T^n) the energy equation is approximated by

$$(V_iE_i)^{n+1} = (V_iE_i)^n + \frac{\Delta t^n}{2}\left\{\left[\frac{d(V_iE_i)}{dt}\right]^{n+1} + \left[\frac{d(V_iE_i)}{dt}\right]^n\right\} , \qquad (15)$$

which is a time-centered difference approximation accurate through terms of order $(\Delta t^n)^2$. Equation (10), being an algebraic equation to be evaluated at a particular time offers no difficulties other than the treatment of the retardation. Both of the equations may be implicit in the unknown quantities requiring the solution of simultaneous nonlinear equations. The method of solution will be indicated in the following paragraphs after the retardation is considered.

Evaluation of Retardation

The degree to which the above equations are implicit depends on how information about the retarded source functions in remote zones is retained in the calculation. In this paragraph the form of the retarded source functions appearing in Eqs. (9) and (10) or Eqs. (14) is specified. In each type of equation the expression is to be evaluated at a particular time, t^{n+1}, to which the retarded sources are referred. For each pair of zones an additional coefficient having dimensions of time is introduced. The coefficient τ_{ij} between volume cells i and j is the average time interval required for energy to be absorbed in cell i after emission from cell j. Coefficients having the same interpretation are introduced from a volume cell to a surface cell, τ_{Ki}, from a surface cell to a volume cell, τ_{iK}, and from a surface cell to a surface cell, $\tau_{K\ell}$. These time interval coefficients, in simple problems, may be calculated analytically or, more generally, may be calculated by the Monte Carlo method. In terms of these quantities the retarded time t'_{ij} when the source in cell j emits radiation arriving in cell i at time t^{n+1} is $t'_{ij} = t^{n+1} - \tau_{ij}$. The retarded sources are to be approximated by interpolation in time between quantities tabulated at times bracketing the retarded time. To make the interpolation possible for all zones it is necessary to provide tabulated data at a time earlier than $t^{n+1} - \tau_{max}$, where τ_{max} is the greatest of all time intervals between cells. To provide these data a number $Q(\sim 10)$ of arrays of the temperature are stored. The times corresponding to adjacent arrays need not be sequential cycles but are adjusted to cover the time interval τ_{max} approximately uniformly. These temperatures are denoted by T_j^g and correspond to the time t^g. Using linear interpolation between adjacent values the temperature for zone j at the time t'_{ij} is

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$$T_j^4(t'_{ij}) = \frac{\left(T_j^n\right)^4\left(t^{n+1} - t'_{ij}\right) + \left(T_j^{n+1}\right)^4\left(t'_{ij} - t^n\right)}{\Delta t^n}, \text{ if } t'_{ij} > t^n \quad ,$$

$$T_j^4(t'_{ij}) = \frac{\left(T_j^{g_{max}}\right)^4\left(t^n - t'_{ij}\right) + \left(T_j^n\right)^4\left(t'_{ij} - t^{g_{max}}\right)}{\left(t^n - t^{g_{max}}\right)}, \text{ if } t^{g_{max}} \le t'_{ij} \le t^n ,$$

$$T_j^4(t'_{ij}) = \frac{\left(T_j^g\right)^4\left(t^{g+1} - t'_{ij}\right) + \left(T_j^{g+1}\right)^4\left(t'_{ij} - t^g\right)}{t^{g+1} - t^g}, \text{ if } t^g \le t'_{ij} \le t^{g+1} . \quad (16)$$

As the calculation proceeds the earliest interval $(t^{g=1}, t^{g=2})$ eventually will become of no use because even the earliest retarded time will no longer fall in it. Thus, if $t^{n+1} - \tau_{max} \ge t^{g=2}$ the first array may be replaced by the second, the second by the third, etc., and the last by T_j^{n+1}. In this way the interpolation arrays are maintained with temperatures always spanning the required time interval for retardation.

Substituting the retarded temperatures from Eq. (16) in the expressions for

$$\left[\frac{d(V_i E_i)}{dt}\right]^{n+1}$$

and the surface temperature equation, Eq. (10), gives expressions which contain some terms which are known in terms of temperatures at t^n and t^g, and other terms depending on T_j^{n+1}. The latter terms are the ones which may couple the equations together to form a system of implicit equations. Symbolically, these equations are of the form

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$$\left[\frac{d}{dt}\,(V_iE_i)\right]^{n+1} = \sum_j A_{ij}\left(T_j^{n+1}\right)^4 + \sum_K B_{iK}\left(T_K^{n+1}\right)^4 - a_i\left(T_i^{n+1}\right)^4 + b_i$$

and

$$\frac{a}{4}\,S_K\left(T_K^{n+1}\right)^4 = \sum_j B_{Kj}\left(T_j^{n+1}\right)^4 + \sum_\ell C_{K\ell}\left(T_\ell^{n+1}\right)^4 + c_K \quad , \qquad (17)$$

where A_{ij}, B_{iK}, B_{Kj}, and $C_{K\ell}$ are matrices which may depend on T_j^{n+1}, but a_i, b_i, and c_K do not. If the time step is small compared to the τ_{ij}'s, then many of the elements of A_{ij}, B_{iK}, B_{Kj}, and $C_{K\ell}$ will be zero, since those terms will occur instead in b_i and c_K.

Iteration Equations

The equations for the material and surface temperatures at t^{n+1} are nonlinear and may be implicit. An iteration method has been devised to solve them based directly on Eqs. (15) and (17) and which contains a series of steps which are detailed below. The iteration starts with the energy equation and provides first an estimate of material temperatures based on an explicit method. Surface temperatures are next brought into conformity with the estimated material temperatures. Both sets of temperatures are then used to find a new set of material temperatures and surface temperatures as before. As many cycles of this iteration are performed as necessary to obtain an accurate solution. More specifically, the steps are as follows:

1. The energy difference equation, Eq. (15), is solved for $E^{n+1}_{i,k+1}$,

$$V_iE^{n+1}_{i,k+1} = V_iE^n_i + \frac{\Delta t^n}{2}\left\{\left[\frac{d}{dt}\,(V_iE_i)\right]^n + \left[\frac{d}{dt}\,(V_iE_i)\right]^{n+1}_k\right\} \quad , \qquad (18)$$

[redacted]

where k is an index denoting the iteration. In Eq. (15) $[d/dt\,(V_iE_i)]^n$ is known, and $[d/dt\,(V_iE_i)]^{n+1}_k$ is the value of the term in Eqs. (17) evaluated with $T^{n+1}_{j,k}$. For each zone the temperature $T^{n+1}_{j,k+1}$ is obtained from the equation of state and immediately placed in T-storage. Its value is subsequently used for the remaining zones of the energy equation. Consequently the notation of Eq. (18) is not precise in that the k + 1 terms on the left side are not indicated. The iteration resembles the the Seidel method[4] for linear equations. The sequence of calculations of new material temperatures indicated above constitutes the volume cell part of one iteration.

2. With the new material temperatures the surface cell equations of Eqs. (17) are next solved as follows:

$$\frac{a}{4} S_K \left(T^{n+1}_{K,k+1}\right)^4 = \sum_j B_{Kj}\left(T^{n+1}_{j,k+1}\right)^4 + \sum_{\ell} C_{K\ell}\left(T^{n+1}_{\ell,k}\right)^4 + c_K \quad . \tag{19}$$

As in the material equations, the newly calculated temperature $T^{n+1}_{K,k+1}$ is placed in storage for use in the remaining equations. Upon completion of the calculation of Eq. (19) for all surface cells, the current iteration is complete.

3. Tests are performed to determine whether the iterations may be terminated. Separate tests are performed for the volume cells and surface cells,

$$\sum_i \left| V_iE^{n+1}_{i,k+1} - V_iE^{n+1}_{i,k} \right| \le \delta_1 \sum_i V_iE^{n+1}_{i,k} \quad ,$$

and

$$\sum_K \left| S_K\left(T^{n+1}_{K,k+1}\right)^4 - S_K\left(T^{n+1}_{K,k}\right)^4 \right| \le \delta_2 \sum_K S_K\left(T^{n+1}_{K,k}\right)^4 \quad . \tag{20}$$

[redacted]

[redacted]

Values of $\delta_1 = \delta_2 \simeq 10^{-2}$ are suggested. When either of the tests is not satisfied steps 1 and 2 are repeated. When both are satisfied the cycle calculation is considered complete.

4. The initial values for the iteration are based on $T^{n+1}_{i,k=0} = T^n_i$. Accelerated convergence doubtless could be achieved through use of a method based on estimation of the first eigenvalue. Preliminary calculations indicate, however, that rapid convergence is attained without the acceleration method.

Time Step Calculation

A variable time step Δt^n is desirable to balance the accuracy of the integration throughout the problem. At early times more rapid changes are expected than at later times so Δt^n can increase as the problem progresses without incurring any large error. A prescription for choosing Δt^n based on the rate of change of the material energy has the desired properties. In preparation for the first iteration of a time cycle the quantities $[d/dt\ (V_i E_i)]^n$ are formed for use in Eq. (18). Using them immediately before the iteration is started, Δt^n is calculated,

$$\Delta t^n = \min \left[\Delta t_0, \frac{\delta_3 \sum_i (V_i E_i^n)}{I \max_i \left| \frac{d}{dt} V_i E_i \right|^n} \right] , \qquad (21)$$

where Δt_0 is the input number determining the maximum permissible time step throughout the problem, I is the total number of volume cells, $\max_i$ selects the maximum absolute value of the energy change in each volume cell, and δ_3 is an input test number ($\sim$0.1) determining the fraction of the average zone energy which the largest energy change is permitted to attain in one cycle.

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