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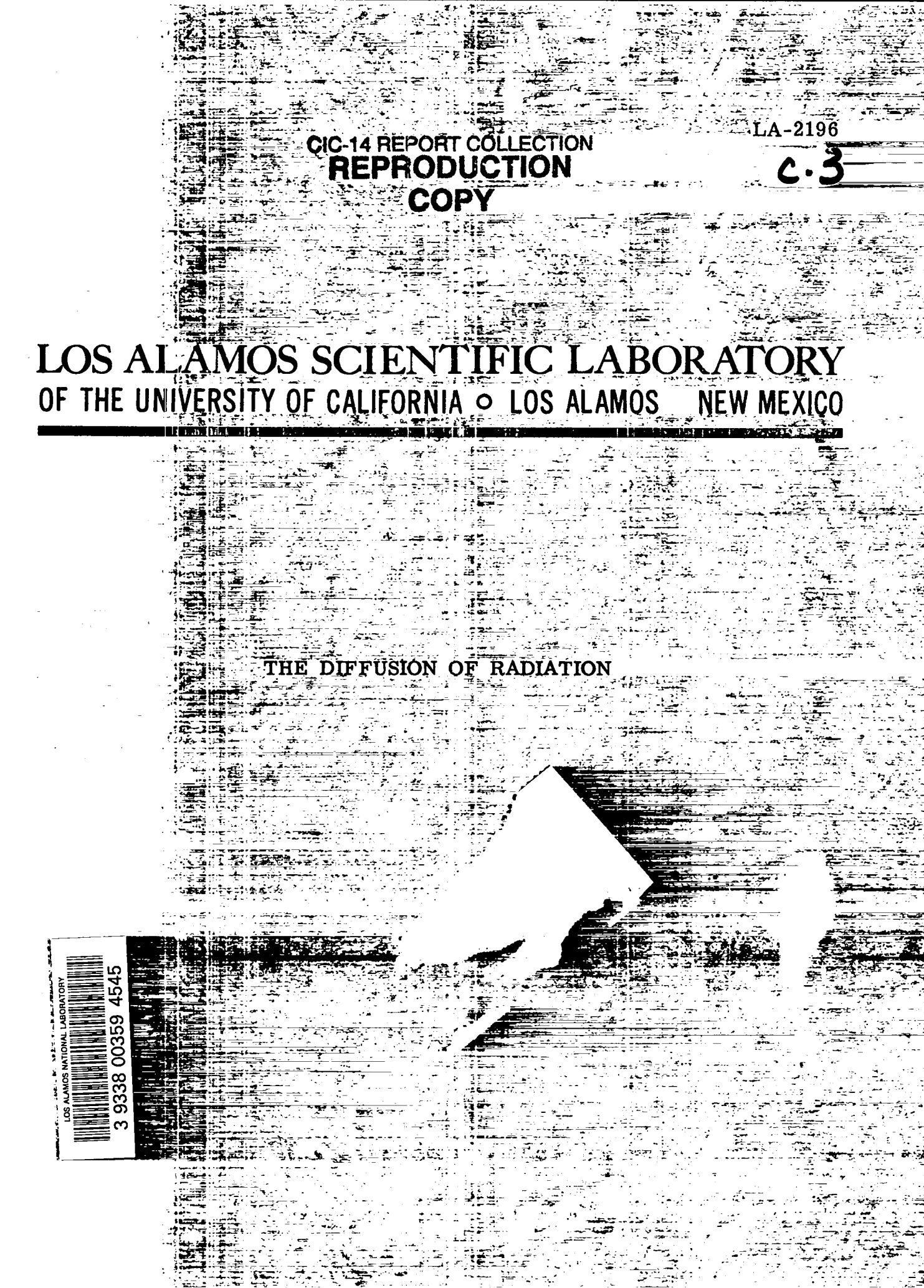
THE DIFFUSION OF RADIATION



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THE DIFFUSION OF RADIATION

by

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ABSTRACT

The diffusion approximation, a simplified formulation of the equations of radiation transport, is investigated from two points of view. First, consideration is given to derivation of the approximation, together with discussion of some of the assumptions involved and limitations of validity. Second, methods are examined for solving the diffusion equation by finite difference approximations. In this second part, particular attention is given to the problem of proper space differencing, and numerical examples are presented showing results of various procedures.

CONTENTS

INTRODUCTION

The transport of radiation through matter is accompanied by a variety of interaction phenomena whereby photons are scattered, absorbed, and emitted. A detailed description in complete generality is extremely complicated, so that various approximate treatments have been proposed for use in special situations. This paper is concerned with one of these, the "diffusion approximation," which has been used widely for the solution of problems.

In Part I, we record several of the methods by which the diffusion equation can be derived. The examples have been chosen to illustrate the nature of the assumptions and to suggest ways in which similar, but less restrictive, assumptions could be employed.

In Part II, we present results of the numerical study of this equation. This extremely nonlinear, partial differential equation has not been solved in closed form except for a small number of highly specialized situations. Application to more complicated problems of interest requires special techniques that generally result in additional errors beyond those introduced by the diffusion assumption.

Specifically, in Part II, we present results of the study of certain problems related to one of the numerical-solution techniques, that in which the differential equation is replaced by a finite difference approximation. The problem of proper space differencing is of principal concern, although some mention is given to the matter of time differencing.

All numerical solutions were obtained by use of IBM Electronic Data Processing Machines, type 704.

PART I. THE DIFFUSION APPROXIMATION

A. Basic Derivation

The fundamental entity in the transport equation is the "intensity of radiation," $I(\vec{r}, \vec{s}, \nu, t)$. This is defined so that

$$I(\vec{r}, \vec{s}, \nu, t)da_s d\omega_s d\nu dt$$

is the amount of energy of frequency ν, at position $\vec{r}$, and at time t which passes in the direction of the unit vector $\vec{s}$ through an area da_s normal to $\vec{s}$, in the solid angle $d\omega_s$, in the frequency interval $d\nu$, and in the time interval dt. As written, we have indicated no distinction as to polarization components. In the following, we neglect polarization effects (which, in certain cases, may be extremely important) by assuming that the radiation produced by any interaction is unpolarized.

Other quantities entering into the transport equation are

$c \equiv$ vacuum speed of light

$\lambda_1(\vec{r}, \nu, t) \equiv$ the scattering mean free path for radiation of frequency ν

$\lambda_2(\vec{r}, \nu, t) \equiv$ the absorption mean free path for radiation of frequency ν

$J_1(\vec{r}, \vec{s}, \nu, t) \equiv$ the rate of scattering-energy production per unit volume, per unit solid angle, per unit frequency range, per unit time

$J_2(\vec{r}, \vec{s}, \nu, t) \equiv$ the rate of emission-energy production per unit volume, per unit solid angle, per unit frequency range, per unit time

and the equation itself is

$$\left(\frac{1}{c}\frac{\partial}{\partial t} + \vec{s}\cdot\nabla\right)I = -\left(\frac{1}{\lambda_1} + \frac{1}{\lambda_2}\right)I + J_1 + J_2 \qquad (1)$$

Two useful quantities which may be derived from the radiation intensity function are the density of energy per unit volume per unit frequency range, $u(\vec{r}, \nu, t)$, and the flux of energy per unit area per unit time per unit frequency range, $\vec{F}(\vec{r}, \nu, t)$. These are*

$$u(\vec{r}, \nu, t) \equiv \frac{1}{c} \int I(\vec{r}, \vec{s}, \nu, t) d\omega_s \tag{2}$$

$$\vec{F}(\vec{r}, \nu, t) \equiv \int \vec{s} I(\vec{r}, \vec{s}, \nu, t) d\omega_s \tag{3}$$

The interpretations are made plausible by a consideration of the result of integrating Eq. (1) over solid angle:

$$\frac{\partial u}{\partial t} + \nabla \cdot \vec{F} = -\left(\frac{1}{\lambda_1} + \frac{1}{\lambda_2}\right) cu + \int \left(J_1 + J_2\right) d\omega_s \tag{4}$$

The terms on the right are the sink and source terms to the radiation energy field; if they vanish, then the equation, with the above interpretations of u and $\vec{F}$, becomes the usual expression for energy conservation.

We assume the case of conservative scattering and introduce a phase function $p(\vec{s}, \vec{s}')$ such that

$$J_1(\vec{r}, \vec{s}, \nu, t) = \frac{1}{4\pi\lambda_1} \int p(\vec{s}, \vec{s}') I(\vec{r}, \vec{s}', \nu, t) d\omega_{s'} \tag{5}$$

The following normalization of the phase function

$$\frac{1}{4\pi} \int p(\vec{s}, \vec{s}') d\omega_s = 1$$

assures that there is no net source or sink to the energy in Eq. (4).

The first drastic assumption of the diffusion approximation is that the radiation and matter fields behave at every instant as though they were in equilibrium at a temperature, $\theta(\vec{r}, t)$, so that the emission rate from the

*S. Chandrasekhar, An Introduction to the Study of Stellar Structure, Chapter V, University of Chicago Press (1939). See also S. Chandrasekhar, Radiative Transfer, pages 2-5, Oxford University Press, London (1950).

matter field can be written* in terms of an equilibrium induced emission and a spontaneous emission described by the Planck function:

$$J_2(\vec{r}, \vec{s}, \nu, t) = \frac{\exp\left(-\frac{h\nu}{k\theta}\right)}{\lambda_2} I(\vec{r}, \vec{s}, \nu, t) + \frac{1 - \exp\left(-\frac{h\nu}{k\theta}\right)}{\lambda_2} B(\nu, \theta) \tag{6}$$

where

$$B(\nu, \theta) \equiv \frac{2h\nu^3}{c^2\left[\exp\left(\frac{h\nu}{k\theta}\right) - 1\right]}$$

Thus, writing

$$\lambda_2' = \frac{\lambda_2}{1 - \exp\left(-\frac{h\nu}{k\theta}\right)} \tag{7}$$

we may put Eq. (1) into the form

$$\left(\frac{1}{c}\frac{\partial}{\partial t} + \vec{s}\cdot\nabla\right) I = -\frac{1}{\lambda_1}\left[I - \frac{1}{4\pi}\int p(\vec{s}, \vec{s}')I(\vec{r}, \vec{s}', \nu, t)d\omega_{s'}\right] - \frac{1}{\lambda_2'}\left[I - B\right] \tag{8}$$

The second drastic assumption involves the directional dependence. If the intensity function is properly behaved, then one can expand it in a double power series of the components of $\vec{s}$ along two fixed, orthogonal unit vectors. The assumption here, however, is that all the terms in this expansion vanish except those such that the intensity can be expressed as

$$I(\vec{r}, \vec{s}, \nu, t) = I_0(\vec{r}, \nu, t) + \vec{s}\cdot\vec{I}_1(\vec{r}, \nu, t) \tag{9}$$

where I_0 and $\vec{I}_1$ are to be determined by requiring the resulting equation to be an identity in $\vec{s}$.

*See S. Chandrasekhar, An Introduction to the Study of Stellar Structure, page 206, University of Chicago Press (1939).

We assume that the scattering intensity from an event is a function of the angle between the incoming and scattered beams. Then the phase function can be expanded,

$$p(\vec{s}, \vec{s}') = \sum_{n=0}^{\infty} a_n (\vec{s} \cdot \vec{s}')^n \tag{10}$$

with the normalization condition being

$$\sum_{n=0}^{\infty} \frac{a_{2n}}{2n + 1} = 1$$

For conservative Thomson scattering, for example,

$$p(\vec{s}, \vec{s}') \equiv \frac{3}{4} \left[1 + (\vec{s} \cdot \vec{s}')^2\right] \tag{11}$$

To evaluate the integral in Eq. (8), we orient the coordinate system so that $\vec{s}$ points along the z axis, and superimpose a spherical coordinate system with azimuthal angle ψ and polar angle ϕ. Then, in terms of the cartesian unit vectors,

$$\vec{s} = \hat{k}$$

$$\vec{s}' = \hat{i} \sin \psi \cos \phi + \hat{j} \sin \psi \sin \phi + \hat{k} \cos \psi$$

and

$$d\omega_{s'} = \sin \psi \, d\psi d\phi$$

After some manipulation one finds, for the more complicated of the integrals,

$$\frac{1}{4\pi} \int \vec{s}' p(\vec{s}, \vec{s}') d\omega_{s'} = \hat{k} \sum_{n=0}^{\infty} \frac{a_{2n+1}}{2n + 3}$$

and Eq. (8) becomes

$$\left(\frac{1}{c}\frac{\partial}{\partial t} + \vec{s}\cdot\nabla\right)\left(I_0 + \vec{s}\cdot\vec{I}_1\right) = -\frac{1}{\lambda_1}\left[I_0 + \vec{s}\cdot\vec{I}_1 - I_0 - \vec{s}\cdot\vec{I}_1 \sum_{n=0}^{\infty} \frac{a_{2n+1}}{2n+3}\right]$$

$$-\frac{1}{\lambda_2'}\left[I_0 + \vec{s}\cdot\vec{I}_1 - B\right]$$

Since this is to be an identity in $\vec{s}$ to first order,

$$\frac{1}{c}\frac{\partial I_0}{\partial t} = -\frac{1}{\lambda_2}\left(I_0 - B\right) \tag{12}$$

$$\frac{1}{c}\frac{\partial \vec{I}_1}{\partial t} + \nabla I_0 = -\left[\frac{1}{\lambda_1}\left(1 - \sum_{n=0}^{\infty}\frac{a_{2n+1}}{2n+3}\right) + \frac{1}{\lambda_2'}\right]\vec{I}_1 \tag{13}$$

The final drastic assumption in the derivation is that the radiation field varies so slowly that the time derivatives can be neglected in Eqs. (12) and (13). Then,

$$\left.\begin{aligned} I_0 &= B \\ \vec{I}_1 &= -\lambda\nabla I_0 = -\lambda\nabla B \end{aligned}\right\} \tag{14}$$

where

$$\frac{1}{\lambda} \equiv \frac{1}{\lambda_1}\left(1 - \sum_{n=0}^{\infty}\frac{a_{2n+1}}{2n+3}\right) + \frac{1}{\lambda_2'} \tag{15}$$

Through Eqs. (2) and (3), these results can be written

$$u = \frac{4\pi}{c} B$$

$$\vec{F} = \int \vec{s}\,[\vec{s}\cdot(-\lambda\nabla B)]\, d\omega_s$$

The integral can be evaluated by the same coordinate system as before, now with ∇B along the z axis. Then

$$\vec{F} = -\lambda \nabla B \int_0^{\pi} 2 \cos^2\psi \sin\psi d\psi$$

and the result is

$$\left.\begin{aligned} u &= \frac{4\pi}{c} B \\ \vec{F} &= -\frac{4\pi\lambda}{3} \nabla B \end{aligned}\right\} \tag{16}$$

Finally, the equation for $\theta(\vec{r}, t)$ can be found by requiring over-all conservation of energy. Let $E_m(\theta)$ be the material energy per unit volume. Then

$$\frac{\partial}{\partial t}\left[E_m(\theta) + \frac{4\pi}{c}\int_0^{\infty} B(\nu, \theta)d\nu\right] + \nabla\cdot\left[-\frac{4\pi}{3}\int_0^{\infty} \lambda(\nu, \theta)\nabla B(\nu, \theta)d\nu\right] = 0 \tag{17}$$

The first integral is the energy density of radiation:

$$\frac{4\pi}{c}\int_0^{\infty} B(\nu, \theta)d\nu = \frac{8\pi h}{c^3}\int_0^{\infty} \frac{\nu^3 d\nu}{\exp\left(\frac{h\nu}{k\theta}\right) - 1} = \frac{8\pi^5 k^4}{15 h^3 c^3}\theta^4 \equiv a\theta^4$$

where a is the radiation density constant. The flux integral is treated by introducing the Rosseland mean of the mean free path, $\bar{\lambda}(\theta)$, as follows:

$$\int_0^{\infty} \lambda(\nu, \theta)\ \nabla B(\nu, \theta)d\nu \equiv \nabla\theta \int_0^{\infty} \lambda(\nu, \theta)\ \frac{\partial B(\nu, \theta)}{\partial\theta}\, d\nu$$

$$\equiv \bar{\lambda}(\theta)\nabla\theta \int_0^{\infty} \frac{\partial B(\nu, \theta)}{\partial\theta}\, d\nu$$

Thus

$$\bar{\lambda}(\theta) \equiv \frac{\displaystyle\int_0^{\infty} \lambda(\nu, \theta)\ \frac{\partial B(\nu, \theta)}{\partial\theta}\, d\nu}{\displaystyle\int_0^{\infty} \frac{\partial B(\nu, \theta)}{\partial\theta}\, d\nu} \tag{18}$$

The denominator can be integrated to give $(ca/\pi)\theta^3$. Combining these results and inserting them into Eq. (17), we obtain

$$\frac{\partial}{\partial t}\left[E_m(\theta) + a\theta^4\right] = \nabla\cdot\left[\frac{ca}{3}\bar{\lambda}(\theta)\ \nabla\theta^4\right] \tag{19}$$

This is the diffusion equation for which the results of numerical studies are presented in Part II.

It should be noted that if the motion of the material were considered, an analogous equation could be derived in which the material energy per unit volume is the sum of internal and kinetic energy per unit volume, both of which depend on density, and the energy flux is the sum of the work flux and the radiation flux. The latter is the same as in Eq. (19) except that the value of $\bar{\lambda}$ depends also on material density, ρ. Writing $\mathscr{e}(\rho, \theta) \equiv$ material internal energy per unit mass, $\vec{v} \equiv$ fluid velocity, $\mathscr{p}(\rho, \theta) \equiv$ material plus radiation pressure, and $S \equiv$ energy source per unit volume per unit time, we have

$$\rho\frac{d}{dt}\left[\mathscr{e} + \frac{1}{2}\vec{v}\cdot\vec{v} + \frac{a\theta^4}{\rho}\right] + \nabla\cdot\left[\mathscr{p}\vec{v} - \frac{ac\bar{\lambda}}{3}\nabla\theta^4\right] = S$$

where the total time derivative means the time rate of change along the path of fluid motion ($d/dt \equiv \partial/\partial t + \vec{v}\cdot\nabla$).

B. Alternate Derivations and Discussion of Assumptions

We shall not discuss the first drastic assumption in the diffusion approximation derivation -- that of the thermodynamic equilibrium of radiation and matter fields. It is most severely violated in the vicinity of rapid space or time variations in the field, but may become valid for practical purposes far from these variations.

Some information as to the validity of applying the other two assumptions is obtained by considering certain alternate derivations of the diffusion equation. For one example, we assume the equilibrium condition and specialize to Thomson scattering only. We further assume a plane-parallel atmosphere in which the directional dependence reduces to dependence on a single angular parameter, chosen to be μ, the cosine of the angle between $\vec{s}$ and the positive x axis. Equation (8) then becomes

$$\left(\frac{1}{c}\frac{\partial}{\partial t} + \mu\frac{\partial}{\partial x}\right)I(x,\mu,\nu,t)$$

$$= -\frac{1}{\lambda_1}\left\{I(x,\mu,\nu,t) - \frac{1}{4\pi}\int\frac{3}{4}\left[1 + (\vec{s}\cdot\vec{s}')^2\right]I(x,\mu',\nu,t)d\omega_{s'}\right\}$$

$$-\frac{1}{\lambda_2'}\left\{I(x,\mu,\nu,t) - B(\nu,\theta)\right\}$$

The integration can be performed over polar angle:

$$\left(\frac{1}{c}\frac{\partial}{\partial t} + \mu\frac{\partial}{\partial x}\right)I(x,\mu,\nu,t)$$

$$= -\frac{1}{\lambda_1}\left\{I(x,\mu,\nu,t) - \frac{3}{16}\int_{-1}^{1}\left[3 - \mu^2 + \mu'^2(3\mu^2 - 1)\right]I(x,\mu',\nu,t)d\mu'\right\}$$

$$-\frac{1}{\lambda_2'}\left\{I(x,\mu,\nu,t) - B(\nu,\theta)\right\} \qquad (20)$$

Into this equation one can introduce as before the expansion

$$I(x,\mu,\nu,t) \equiv \sum_{n=0}^{\infty} I_n(x,\nu,t)\mu^n$$

and obtain an infinite set of coupled equations. The assumption that $I_n \equiv 0$ for $n \geq 2$ leads, exactly as before, to the diffusion equation.

In this alternate derivation, however, we multiply Eq. (20) by (1/2) μ^n and integrate from -1 to 1. Let

$$P_n(x,\nu,t) \equiv \frac{1}{2}\int_{-1}^{1}\mu^n I(x,\mu,\nu,t)d\mu \qquad (21)$$

and

$$\delta_{ne} \equiv \begin{cases} 1 & n \text{ even} \\ 0 & n \text{ odd} \end{cases}$$

Then

$$\frac{1}{c}\frac{\partial P_n}{\partial t} + \frac{\partial P_{n+1}}{\partial x} = -\frac{1}{\lambda_1}\left\{P_n - \frac{3\delta_{ne}}{4(n+1)(n+3)}\left[(n+4)P_0 + nP_2\right]\right\}$$

$$-\frac{1}{\lambda_2'}\left[P_n - \frac{B}{n+1}\,\delta_{ne}\right] \qquad (22)$$

Note that from Eqs. (2) and (3)

$$u(x,\nu,t) \equiv \frac{4\pi}{c}\,P_0(x,\nu,t)$$

$$F(x,\nu,t) \equiv 4\pi\,P_1(x,\nu,t)$$

Equation (22) gives an infinite set of coupled equations which can, in principle, be solved as accurately as desired. If, now, we assume $P_n \equiv 0$ for $n \geq 3$, then

$$\frac{\partial u}{\partial t} + \frac{\partial F}{\partial x} = -\frac{c}{\lambda_2'}\left(u - \frac{4\pi}{c}\,B\right) \qquad (23)$$

$$\frac{1}{c}\frac{\partial F}{\partial t} + 4\pi\frac{\partial P_2}{\partial x} = -\left(\frac{1}{\lambda_1} + \frac{1}{\lambda_2'}\right)F \qquad (24)$$

$$\frac{1}{c}\frac{\partial P_2}{\partial t} = -\frac{1}{\lambda_1}\left(\frac{9}{10}\,P_2 - \frac{3}{10}\,\frac{cu}{4\pi}\right) - \frac{1}{\lambda_2'}\left(P_2 - \frac{B}{3}\right) \qquad (25)$$

The diffusion approximation is now obtained by setting both sides to zero in Eqs. (23) and (25), and by setting $\partial F/\partial t = 0$ in Eq. (24). Then

$$\left.\begin{aligned} u &= \frac{4\pi}{c}\,B \\ P_2 &= \frac{1}{3}\,B \\ \left(\frac{1}{\lambda_1} + \frac{1}{\lambda_2'}\right)F &= -\frac{4\pi}{3}\,\frac{\partial B}{\partial x} \end{aligned}\right\} \qquad (26)$$

These are the same as the results in Eq. (16) if we define

$$\lambda \equiv \frac{1}{\frac{1}{\lambda_1} + \frac{1}{\lambda'_2}} \tag{27}$$

which, in turn, is the same as Eq. (15) for Thomson scattering. The equations as now derived, however, allow a slightly less drastic form of the assumption to be introduced. We drop the requirement that $\partial F/\partial t = 0$ in Eq. (24). Then the equations become

$$\left.\begin{aligned} &\frac{\partial u}{\partial t} + \frac{\partial F}{\partial x} = 0 \\ &\frac{\partial F}{\partial t} + \frac{c^2}{3}\frac{\partial u}{\partial x} = -\frac{cF}{\lambda} \end{aligned}\right\} \tag{28}$$

In this form we see that, as $\lambda \to \infty$ (vacuum conditions), the equations then approach the wave equations for which, however, the speed of propagation is $c/\sqrt{3}$ instead of c.

As a specific example of the further type of analysis that can be made, consider the case in which λ is a fixed constant. From Eq. (28), the flux can be eliminated giving

$$\frac{c}{\lambda}\frac{\partial u}{\partial t} = \frac{c^2}{3}\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial t^2} \tag{29}$$

Alternately, in the case that $\partial F/\partial t$ had been neglected in Eq. (28), the elimination of F would have given

$$\frac{\partial u}{\partial t} = \frac{c\lambda}{3}\frac{\partial^2 u}{\partial x^2} \tag{30}$$

There is a fundamental difference between these two equations, the first having the essential features of a wave equation and the second being a diffusion equation. [Note that Eq. (30) is identical to the one-dimensional form of Eq. (19) in which variable characteristics of the matter have been set constant.]

Considered from the point of view of an initial-condition boundary-value

problem, a difference between Eq. (29) and Eq. (30) is that one arbitrary initial profile is allowed for Eq. (30), whereas two are allowed for Eq. (29). Thus, the initial energy distribution is sufficient to "start" a solution of Eq. (30) while one can specify, in addition, the initial flux in Eq. (29).

The difference between solutions of the two equations is somewhat a measure of the error introduced by the diffusion assumptions. We consider the equation

$$\frac{c}{\lambda}\frac{\partial u}{\partial t} = \frac{c^2}{3}\frac{\partial^2 u}{\partial x^2} - \epsilon\frac{\partial^2 u}{\partial t^2} \tag{31}$$

which reduces to Eq. (29) or (30) according as $\epsilon = 1$ or $\epsilon = 0$. Assume a Fourier integral solution of Eq. (31):

$$u(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\sigma(k,\omega)e^{ikx}\,e^{i\omega t}\,d\omega dk$$

This satisfies the equation provided

$$\sigma(k,\omega) \equiv \sigma(k)\,\delta\left[\epsilon\omega^2 - \frac{c^2k^2}{3} - \frac{ic\omega}{\lambda}\right]$$

where $\delta(x)$ is the Dirac delta function. Thus, the general solution is

$$u(x,t) = \frac{1}{2\pi}\exp\left(-\frac{ct}{2\lambda\epsilon}\right)\int_{-\infty}^{\infty}e^{ikx}\left[\sigma_1(k)\exp\left(\frac{ct}{2\lambda\epsilon}\sqrt{1-\frac{4}{3}\epsilon\lambda^2k^2}\right)\right.$$
$$\left. + \sigma_2(k)\exp\left(-\frac{ct}{2\lambda\epsilon}\sqrt{1-\frac{4}{3}\epsilon\lambda^2k^2}\right)\right]dk \tag{32}$$

Suppose, now, that the initial conditions (which determine σ_1 and σ_2) are such that contributions to the integral are of importance only for $(4/3)(\lambda k)^2 \ll 1$. This means that the initial profile has important Fourier components only for wave numbers much smaller than the reciprocal of the mean free path, or that the relative change of the energy profile is initially small over a mean free path. Then the square root may be expanded and

$$u(x,t) \approx \frac{1}{2\pi}\int_{-\infty}^{\infty} \sigma_1(k)e^{ikx}\exp\left(-\frac{1}{3}\lambda k^2 ct\right)\,dk$$

$$+\frac{1}{2\pi}\exp\left(-\frac{ct}{\lambda\epsilon}\right)\int_{-\infty}^{\infty}\sigma_2(k)e^{ikx}\exp\left(\frac{1}{3}\lambda k^2 ct\right)\,dk \qquad (33)$$

The first term is exactly the solution of the equation with $\epsilon = 0$; the second term is a correction. The coefficient of t in the second term is dominantly negative for all Fourier components of importance, so that the second term decays with a half-life which is approximately equal to the time required for radiation to travel one mean free path at vacuum speed.

Thus, we have seen that the diffusion equation is nearly valid (as measured by comparison with a less drastic approximation to reality) when the mean free path is small compared with distances over which the initial energy profile changes appreciably, and, moreover, that under these circumstances, the solution of the diffusion form (30) is approached by that of the more nearly exact equation (29). That these conclusions are applicable to real problems of interest is confirmed by the work of Barfield* who demonstrated by numerical studies the approach of diffusion and transport solutions as both approached steady state.

As a second example to illustrate properties of the diffusion equation, we discuss briefly another derivation. This time, we start from an even simpler form of the transport equation, that in which there is no scattering, and the absorption mean free path is a fixed constant. We assume the equilibrium necessary for Planck emission and write the equation for a plane-parallel atmosphere:

$$\left(\frac{1}{c}\frac{\partial}{\partial t} + \mu\frac{\partial}{\partial x}\right)I(x,\mu,\nu,t) = -\frac{1}{\lambda}[I(x,\mu,\nu,t) - B(\nu,\theta)]$$

With λ independent of frequency, we can integrate over frequency and put

$$\left.\begin{aligned}\frac{4\pi}{c}\int_0^{\infty} B(\nu,\theta)d\nu &= a\theta^4 \equiv \Phi(x,t)\\ \frac{4\pi}{c}\int_0^{\infty} I(x,\mu,\nu,t)d\nu &\equiv R(x,\mu,t)\end{aligned}\right\} \qquad (34)$$

*W. D. Barfield, Los Alamos Scientific Laboratory Report LA-1709 (June, 1954).

Then

$$\left(\frac{1}{c}\frac{\partial}{\partial t} + \mu\frac{\partial}{\partial x}\right)R(x,\mu,t) = -\frac{1}{\lambda}[R(x,\mu,t) - \Phi(x,t)] \tag{35}$$

This equation can be solved for R

$$R(x,\mu,t) = f\left(\mu, t - \frac{x}{\mu c}\right)\exp\left(-\frac{x}{\mu\lambda}\right) + \int^{x} \Phi\left(x', t - \frac{x - x'}{\mu c}\right)\exp\left(-\frac{x - x'}{\mu\lambda}\right) dx' \tag{36}$$

where $f[\mu, t - (x/\mu c)]$ is an arbitrary function of its arguments. Suppose, for example, that the boundary conditions specify the functions $R(x_0,\mu,t)$ for $\mu > 0$ and $R(x_1,\mu,t)$ for $\mu < 0$, where $x_1 > x_0$. Then, for $x_0 \le x \le x_1$

$$\left.\begin{aligned} R(x,\mu,t) &= \exp\left(-\frac{x - x_0}{\mu\lambda}\right)R\left(x_0,\mu,t - \frac{x - x_0}{\mu c}\right) \\ &\quad + \int_{x_0}^{x} \Phi\left(x', t - \frac{x - x'}{\mu c}\right)\exp\left(-\frac{x - x'}{\mu\lambda}\right) dx' \qquad \text{for } \mu > 0 \\ R(x,\mu,t) &= \exp\left(-\frac{x - x_1}{\mu\lambda}\right)R\left(x_1,\mu,t - \frac{x - x_1}{\mu c}\right) \\ &\quad + \int_{x_1}^{x} \Phi\left(x', t - \frac{x - x'}{\mu c}\right)\exp\left(-\frac{x - x'}{\mu\lambda}\right) dx' \qquad \text{for } \mu < 0 \end{aligned}\right\} \tag{37}$$

The interpretation of these results is as follows. R is composed of an attenuated primary beam from the boundaries, plus the sum of the components produced by emission along a line in the direction of the beam. The contributions are "retarded" in the mathematical solution, corresponding to a finite time of travel, and have been attenuated by absorption during that travel. Thus, the effect of neglecting the time derivative in Eq. (35) (achieved by putting $c \to \infty$) is the same as neglecting the retardation. This is a valid procedure provided that the value of Φ does not change much in the time required for radiation to travel a mean free path at vacuum speed, in agreement with the previously derived condition for dropping the time derivative terms.

The diffusion equation is derived by neglecting these retardations and also by making a Taylor expansion of $\Phi(x', t)$ about the point x. The integrals can then be evaluated, higher order terms dropped, and the flux and energy density determined from the resulting expression for R. The procedure suggests ways in which higher order corrections can be added to the diffusion equation. An analogous procedure can be carried through for the more general forms of the transport equation.

PART II. NUMERICAL SOLUTION OF THE DIFFUSION EQUATION

A. Methods of Solution

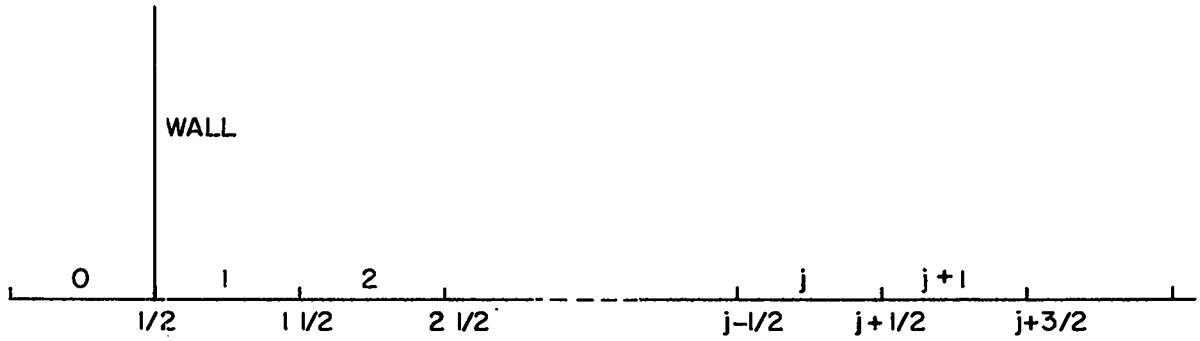
The diffusion equation, Eq. (19), has been studied in the one-dimensional form

$$\left.\begin{aligned} \frac{\partial}{\partial t}\left[E_m(x,\theta) + a\theta^4\right] &= -\frac{\partial F}{\partial x} \\ F &= -\frac{ca}{3}\,\lambda(x,\theta)\,\frac{\partial \theta^4}{\partial x} \end{aligned}\right\} \tag{38}$$

E_m and λ are explicit functions of position in some of the studies in order that the presence of two different kinds of matter can be represented. (Throughout Part II, λ without the bar represents the Rosseland mean of the mean free path.)

In the problems we have studied, a wall is placed at $x = 0$ across which the flux of energy is specified as a function of time. Initially, temperature and material profiles are specified to the right of the wall; in all cases, $\theta \to 0$ as $x \to \infty$.

To solve the problems numerically, we approximate the derivatives by finite differences. The space to the right of the wall is divided into "cells" of width δx, each of which has a temperature varying with time. The cells are labeled with index j and their boundaries with index $j \pm \frac{1}{2}$. A fictitious cell, #0, is introduced at the left of the wall for use in applying the input flux condition. The calculation advances time-wise in finite steps, δt. These are counted by index n in such a way that the time at the end of cycle #n is $t^n = n\delta t$.



The time advancement is by the explicit method, used throughout:

$$\left[E_m(x,\theta) + a\theta^4\right]_j^{n+1} - \left[E_m(x,\theta) + a\theta^4\right]_j^{n} = -\frac{\delta t}{\delta x}\left(F^n_{j+\frac{1}{2}} - F^n_{j-\frac{1}{2}}\right) \qquad (39)$$

Thus, the partial differential equation is reduced to a set of algebraic equations, one for each cell, from which the temperatures at the end of each time cycle can be determined in terms of known quantities at the beginning of the cycle.*

Various implicit time differencing methods have been proposed, but it is not our purpose to investigate these. In the test problems, we have required δt to be small enough so that any further decrease would produce negligible difference in results. In all cases tested, it was found that δt was small enough if the equations were stable—see Appendix I.

Our aim was to investigate the relative merit among various methods of writing $F^n_{j\pm\frac{1}{2}}$, all of which formally reduce to the differential expression as $\delta x \to 0$. Accepting the validity of the diffusion equation, we wanted to find a satisfactory method for solving it numerically in as many situations

*We have solved the equations by successively iterating with Newton's method. An alternate procedure, in which the left side of Eq. (39) is replaced by

$$\left[\frac{\partial E_m(x,\theta)}{\partial\theta} + 4a\theta^3\right]_j^n \left(\theta_j^{n+1} - \theta_j^n\right)$$

produces simpler equations to solve but can introduce fairly large inaccuracies unless δt is very small—smaller than otherwise required. The form in Eq. (39) rigorously conserves energy.

as possible. One of the methods tested, Eq. (41) below, appears to be at least as accurate in solving the diffusion equation as the diffusion equation is in representing the true radiation transport. In those circumstances where the diffusion approximation itself is most nearly valid, the method gives the best approximation to it; in certain of the circumstances in which the diffusion approximation is questionable, the method still gives a good solution; in others, the method becomes poor, but the qualitative error is rather easily estimated.

In general, any finite difference procedure used to solve Eq. (38) will yield results which differ from the true solution. Thus, our aim could be phrased as follows: Given the task of solving Eq. (38) to a particular degree of accuracy, what method of space differencing will allow one to use the largest intervals, δx ?

To answer this question, a criterion of accuracy is required. In certain circumstances, a rigorous solution of Eq. (38) can be obtained, and direct comparison of this with the numerical solutions is possible. For many problems of interest, however, no such comparative solutions have been obtained. For these, we have used as a criterion of accuracy the relative insensitivity of the various numerical solutions to variations in δx. The validity of this criterion depends upon the convergence of the numerical solution to the true solution as $\delta x \rightarrow 0$ (with δt always below the stability limit). Proof of this convergence or of the validity of the criterion has not been attempted; experience with its use, however, has shown the criterion to be acceptable in the cases tested; several examples are presented in this report.

The space differencing method which has proved most satisfactory in producing accurate solutions is based on application of the assumption that between the centers of any pair of cells, the instantaneous temperature distribution is that given by the steady state solution of Eq. (38) with the cell temperatures as boundary conditions at the two centers. Since the steady state equation is of second order, the two temperatures completely specify the solution, and in terms of them, the flux is determined. When the flow is not in local steady state, the calculation based on this assumption will be in error, but the direction of the error is usually easily estimated. Under these circumstances, however, the diffusion approximation itself is of questionable validity.

In a certain sense, this method of differencing is the "best" possible one. The criterion of "best" is that the method gives the right results in the "average" of all situations (since nonsteadiness can occur in two different directions from steadiness) and that the flux is determined by the minimum number of required data (only the two adjacent temperatures). Corrections to include the lowest order effects of unsteadiness must necessarily require the use of additional data, either in the form of temperatures in the next

adjacent cells or temperature changes in the adjacent cells.

The method is applied at a cell boundary as follows. In the steady state near this boundary, F of Eq. (38) is a constant, and we must solve the differential equation

$$F = -\frac{ca}{3}\,\lambda(x,\theta)\,\frac{d\theta^4}{dx} \tag{40}$$

subject to the conditions that $\theta = \theta_j^n$ at $x = -\delta x/2$, and $\theta = \theta_{j+1}^n$ at $x = \delta x/2$ (where we have temporarily put the origin of x at the cell boundary). The result is an expression for $F_{j+\frac{1}{2}}^n$ as a function of θ_j^n, θ_{j+1}^n, and δx.

To apply this specifically, an additional assumption is needed. This is that each cell is homogeneous within itself in such characteristics as density and material kind. If a material discontinuity is present, it should be located at a cell boundary (as is usual in the Lagrangian form of hydrodynamic calculations). If this is not possible, then a modification of this method can be carried through. General derivation of the method is given in Appendix II.

As a simple example, consider the case in which $\lambda = A_1\theta^m$ in the cell at the left and $\lambda = A_2\theta^m$ in the cell to the right. Then the solution of Eq. (40) is

$$\frac{4ac}{3(m+4)}\left[\theta^{m+4} - \left(\theta_j^n\right)^{m+4}\right] = -F\int_{-(\delta x/2)}^{x}\frac{dx}{A}$$

$$= -F\left(\frac{\delta x}{2A_1} + \frac{x}{A_1}\right) \qquad x < 0$$

$$= -F\left(\frac{\delta x}{2A_1} + \frac{x}{A_2}\right) \qquad x > 0$$

Applying the condition at $x = \delta x/2$, we get

Steady-State Method

$$F_{j+\frac{1}{2}}^n = -\frac{4ac}{3\delta x(m+4)}\left(\frac{2A_1A_2}{A_1+A_2}\right)\left[\left(\theta_{j+1}^n\right)^{m+4} - \left(\theta_j^n\right)^{m+4}\right] \tag{41}$$

For most real materials the mean-free-path formulas are considerably more complicated than the simple forms used in the example. Extension to these general forms is possible, however, because a first integral of the steady-state problem can always be obtained, and the resulting equation to solve, Eq. (40), is of first order. Further discussion is given in Appendix II.

The difference form (41) can be extended to correct for the fact that the local configuration may not be in steady state. Representing the local energy change rate by $\dot{E}$ ($\equiv 0$ in steady state), we would have

$$\dot{E} = \frac{ca}{3} \frac{d}{dx} \left[\lambda(x, \theta) \frac{d\theta^4}{dx} \right]$$

where $\dot{E}$ is now assumed to be a constant, determined for the cycle by

$$\dot{E}^n = - \frac{F^n_{j+\frac{3}{2}} - F^n_{j-\frac{1}{2}}}{2\delta x}$$

Here it is implied that the flux contributions to the correction are calculated by Eq. (41). Then, with $x = 0$ at the cell boundary in question, we have, analogous to Eq. (40),

$$x\dot{E} - F = \frac{ca}{3} \lambda(x, \theta) \frac{d\theta^4}{dx} \tag{40'}$$

This differential equation is to be solved subject to the boundary conditions of adjacent cell-center temperatures, and a new expression for flux is obtained which reduces to the form (41) if the local configuration comes to a steady state $\left(F^n_{j+\frac{3}{2}} = F^n_{j-\frac{1}{2}} \right)$.

Thus, in the example leading to Eq. (41),

Extended Steady-State Method

$$F^n_{j+\frac{1}{2}} = - \frac{4ac}{3\delta x(m+4)} \left(\frac{2A_1A_2}{A_1 + A_2} \right) \left[\left(\theta^n_{j+1} \right)^{m+4} - \left(\theta^n_j \right)^{m+4} \right] + \frac{1}{8} \left(\frac{A_2 - A_1}{A_2 + A_1} \right) \left[F^n_{j+\frac{3}{2}} - F^n_{j-\frac{1}{2}} \right] \tag{41'}$$

For comparison with results from the above differencing method, we have tried several others. In one of these, we write

λ-Average Method

$$F^n_{j+\frac{1}{2}} = -\left(\frac{ca}{3}\right)\left[\frac{\lambda_j\left(\theta^n_j\right) + \lambda_{j+1}\left(\theta^n_{j+1}\right)}{2}\right]\left[\frac{\left(\theta^n_{j+1}\right)^4 - \left(\theta^n_j\right)^4}{\delta x}\right] \tag{42}$$

where the mean free paths are calculated in terms of quantities at the adjacent cell centers and averaged.

Another method is derived, in a somewhat different manner, from the assumption of constant flux. Thus $\lambda^n_{j+\frac{1}{2}}$ is determined by

$$\lambda_j\left(\theta_j\right)\left(\theta^4_{j+\frac{1}{2}} - \theta^4_j\right) = \lambda_{j+1}\left(\theta_{j+1}\right)\left(\theta^4_{j+1} - \theta^4_{j+\frac{1}{2}}\right) = \frac{1}{2}\lambda_{j+\frac{1}{2}}\left(\theta^4_{j+1} - \theta^4_j\right)$$

from which

$$\lambda_{j+\frac{1}{2}} = \frac{2\lambda_j\left(\theta_j\right)\lambda_{j+1}\left(\theta_{j+1}\right)}{\lambda_j\left(\theta_j\right) + \lambda_{j+1}\left(\theta_{j+1}\right)}$$

and

Opacity-Average Method

$$F^n_{j+\frac{1}{2}} = -\left(\frac{ca}{3}\right)\left[\frac{2\lambda_j\left(\theta^n_j\right)\lambda_{j+1}\left(\theta^n_{j+1}\right)}{\lambda_j\left(\theta^n_j\right) + \lambda_{j+1}\left(\theta^n_{j+1}\right)}\right]\left[\frac{\left(\theta^n_{j+1}\right)^4 - \left(\theta^n_j\right)^4}{\delta x}\right] \tag{43}$$

This form is said to be reasonable, because one is adding opacities for the two cells. This is a good physical argument, but has little mathematical validity, especially when the mean free path is very small in one of the cells.

A variation of this last procedure is derived by setting

$$\lambda_j\left(\theta_{j+\frac{1}{2}}\right)\left[\theta^4_{j+\frac{1}{2}} - \theta^4_j\right] = \lambda_{j+1}\left(\theta_{j+\frac{1}{2}}\right)\left[\theta^4_{j+1} - \theta^4_{j+\frac{1}{2}}\right] = \frac{1}{2}\lambda_{j+\frac{1}{2}}\left[\theta^4_{j+1} - \theta^4_j\right]$$

Here the solution is, in general, somewhat more difficult to obtain; we exhibit it for a special case, that in which $\lambda = A_1\theta^m$ to the left and $\lambda = A_2\theta^m$ to the right. In this case,

$$\lambda_{j+\frac{1}{2}} = \frac{2A_1A_2}{A_1 + A_2}\left[\frac{A_1\theta_j^4 + A_2\theta_{j+1}^4}{A_1 + A_2}\right]^{m/4}$$

and

Modified Opacity-Average Method

$$F_{j+\frac{1}{2}}^n = -\frac{ca}{3}\left\{\frac{2A_1A_2}{A_1 + A_2}\left[\frac{A_1\left(\theta_j^n\right)^4 + A_2\left(\theta_{j+1}^n\right)^4}{A_1 + A_2}\right]^{m/4}\right\}\left\{\frac{\left(\theta_{j+1}^n\right)^4 - \left(\theta_j^n\right)^4}{\delta x}\right\} \qquad (44)$$

In the case that $A_1 = A_2$, λ at the boundary is simply calculated as a function, for that material, of the fourth root of the average of the fourth powers of the adjacent cell-center temperatures. This is true in this method for any form of the mean-free-path formula, as long as it is the same for the two adjacent cells. The results suggest a variety of other ways in which boundary mean free paths could be calculated from various sorts of temperature averages when the two cells are of the same material; we have investigated none of these.

A final method which we have investigated is obtained from the (differentially) equivalent flux expression

$$F = -\frac{4ca}{3}\,\theta^3\lambda(x,\theta)\,\frac{\partial\theta}{\partial x}$$

This form is often convenient in implicit time differencing schemes because the resulting equations are linear in the unknown temperatures. A wide variety of forms could be used for the average of $\theta^3\lambda$ at cell boundaries; we have investigated only that which leads to the expression

Linear-Difference Method

$$F_{j+\frac{1}{2}}^n = -\frac{ca}{3}\left\{\frac{1}{2}\left[\left(\lambda\theta^3\right)_j^n + \left(\lambda\theta^3\right)_{j+1}^n\right]\right\}\left[\frac{\left(\theta_{j+1}^n\right) - \left(\theta_j^n\right)}{\delta x}\right] \qquad (45)$$

B. The Test Problems

We choose particular forms for $E_m(x, \theta)$ and $\lambda(x, \theta)$ which show the qualitative features of real materials but are relatively simple for calculation. Thus

$$\left.\begin{aligned} E_m(x, \theta) &\equiv K(x)\theta \\ \lambda(x, \theta) &\equiv A(x)\theta^3 \end{aligned}\right\} \tag{46}$$

where A(x) and K(x) are constants for one-material problems and step functions for two-material problems.

It is convenient to introduce dimensionless variables for all quantities as follows:

$$\left.\begin{aligned} \theta &\rightarrow \alpha T \\ A(x) &\rightarrow \beta L(y) \\ K(x) &\rightarrow \gamma Q(y) \\ t &\rightarrow \tau z \\ x &\rightarrow \xi y \end{aligned}\right\} \tag{47}$$

where the Greek symbols on the right are constants which carry the dimensions of the quantities on the left. Then Eq. (38), with Eqs. (46) and (47) inserted, can be written

$$\left.\begin{aligned} &\frac{\partial}{\partial z}\left(QT + \eta T^4\right) = \zeta \frac{\partial}{\partial y}\left(LT^3 \frac{\partial T^4}{\partial y}\right) \\ &\text{where} \\ &\eta \equiv \frac{a\alpha^3}{\gamma} \\ &\zeta \equiv \frac{ca\beta\alpha^6\tau}{3\gamma\xi^2} \end{aligned}\right\} \tag{48}$$

The value of η is chosen according to the range of values of Q and T, which in turn are arbitrarily chosen to be numbers in the range 0-10. This

means that a value of $\eta \approx 0.1$ allows a study of situations where either radiation or material specific heat dominates. Since the radiation density constant, in units appropriate to many situations, is

$$a = 137 \frac{\text{ergs}}{\text{cm}^3 \ \text{volt}^4}$$

we have chosen $\eta = 0.137$ throughout the problems.

In a sense, the value of ζ is immaterial; as long as δy and δz are small enough, the results of a calculation at the completion of a certain relative change of configuration are independent of ζ. This follows from the fact that, having picked the relevant physical parameters of the system (which determine the nature of the configuration changes), a time or space scale can be chosen to produce any arbitrary desired value of ζ. To interpret the results in terms of specific physical parameters, however, ζ must be specified. We have chosen $\zeta = \eta = 0.137$ throughout the problems.

The results of the test problems are arranged according to the type of problem studied as follows.

1. A Rigorous Comparison Solution

The flux-difference form (41)* has been tested with a rigorous solution of Eq. (48). We introduce a similarity variable $r \equiv y - vz$ and assume that T is a function of r alone. Q and L are taken to be fixed constants (one material only). The corresponding solution is

$$\Gamma(T) \equiv \frac{\eta T^3}{Q} - \ln\left(1 + \frac{\eta T^3}{Q}\right) = \frac{3\eta^2 v}{4\zeta LQ}(vz - y) \tag{49}$$

To solve the problem numerically, it is necessary to devise a way of developing the proper input at the wall. This is accomplished by using the condition

$$\frac{\partial \Gamma(T)}{\partial y} = -\frac{3\eta^2 v}{4\zeta LQ}$$

and approximating this by

*Names of the flux-difference forms are summarized on page 40 for reference.

$$\Gamma\left(T_0^n\right) = \Gamma\left(T_1^n\right) + \frac{3\eta^2 v\delta y}{4\xi LQ}$$

In this manner we solve numerically (iterating with Newton's method) for T_0^n each cycle and, in terms of it and T_1^n, calculate a wall flux according to the form in Eq. (41), assuming that cell #0 has the same value of A (or L) as #1. The value chosen for v is v = 2.6.

The result is shown in Fig. 1 for a time by which the radiation wave had traveled a little over 30 cells. At this time, the total energy was about 1.5 per cent higher than the correct amount.

A similar test was made using flux-difference form (42). The results were equally good, showing that this form is also useful when the material is homogeneous.

2. A Set of One-Material Problems

In this set of problems, we have but one material for which $L(x) \equiv Q(x) \equiv 1$. The wall flux is identically zero, and the temperature is put in initially as a step function, having the value T = 10 from y = 0 to y = 50, and T = 0 thereafter.

The first series of tests used a weighted average of the flux-difference forms (42) and (43), the weight for (42) being α and that for (43) being $(1 - \alpha)$. Tests were performed for various values of α from zero to one. For $\alpha = 0$, the configuration never changes. In the first cell for which T = 0, λ also is zero and (43) gives zero flux at its left boundary.

A series of temperature profiles for $\delta y = 10$ at a time z = 100 is shown in Fig. 2 for various values of α. The most noticeable effect of decreasing α is that the radiation wave front becomes more and more abruptly truncated. Since the system is rigorously conservative of energy, the temperature behind the front becomes slowly larger, but the change in that region is relatively small.

Some of the problems of the series were repeated with smaller or larger cell sizes to see if the calculation results could be invariant for any particular value of α. A measure of the change of configuration with cell size is given by the change of radiation front position. These variations are shown in Fig. 3. It is seen that for $0.7 \lesssim \alpha \lesssim 1$, there is near invariance with δy, and the results are given with fairly good accuracy in that range. On this basis, the temperature profile in Fig. 2 for $\alpha = 1$ is considered to be close to the correct form. The convergence of other methods to give this profile as δy became small was further verification of the validity of the criterion that based the validity of a solution on its invariance with δy.

This same calculation was also performed with flux-difference form (45). The result was in close agreement with the previous results for $\alpha = 1$, and so this form also seems acceptable for one-material problems. If the method is in error, it is in the direction of calculating the radiation flow to be slightly too fast.

Likewise, flux-difference forms (41) and (44) were applied to the same problems, and the results appear equally good. In all cases, the results were good at all times.

The conclusion from this series of tests is that there is a wide variety of methods for performing the flux space differencing that lead to very nearly the correct numerical solution in this rather extreme one-material problem. The applicability to two-material problems, however, is by no means universal as the following tests show.

3. A Set of Two-Material Problems

The wall is opaque; extending from it to $y = 100$ is a material for which $L(x) \equiv 0.001$, $Q(x) \equiv 10$; beyond that material is a second one for which $L(x) \equiv Q(x) \equiv 1$. Initially, the first material is at a temperature $T = 10$; the second one has $T = 0$.

In the first series of tests, we used flux-difference form (42) everywhere except at the material interface (which always lay on a cell boundary). There we used a weighted average of forms (42) and (43) with weights α': $(1 - \alpha')$, respectively. The results show that the boundary flux becomes smaller as α' decreases. Several of the profiles are shown in Fig. 4.

To determine which value of α' gives best results, we performed some of the calculations again with larger or smaller values of δy. Cutting δy to half its value, for example, resulted in a greater flux at the boundary for the case $\alpha' = 0.001$ and a smaller flux for the case $\alpha' = 1.0$. Doubling δy produced just the opposite effects. Thus, it seemed possible to determine a value of α' which would give the correct result. This proved not to be the case.

The criterion of invariance with δy was applied to the total energy that had flowed into the second material by a given time. Thus, we could find a value of α' such that the energy would be nearly independent of δy at, say, time $z = 100$. Using this value of α' throughout the problem, however, we discovered that before the time at which the energy was correct, there was too little, and afterwards there was too much. In other words, for any fixed α', there was an initial delay in flux passage, but this was gradually overcome by too great a flux, and, eventually, the amount of energy which was calculated to pass the interface surpassed the correct value and continued to

climb beyond it. These results are shown in Fig. 5, where we have plotted the fixed value of α' required to ensure that the proper energy had gone into the second material by a given time z, as a function of z. On the basis of these results, it was concluded that no fixed combination of forms (42) and (43) was adequate. Attempts at devising a variable weighting of them were abandoned in favor of other more promising methods.

The same tests were performed using flux-difference form (44), and these gave extremely poor results. The radiation does not flow nearly fast enough across the interface.

Likewise, we obtained results for the same problem using flux-difference form (41) everywhere. The results of the tests showed that for any finite value of δy, there is an initial delay in getting the flow started, but once started, the flow thereafter proceeds at the proper rate. The incorrect flow occurs during the time when conditions near the interface are far from steady. In many problems of interest, flow at an interface differs from steadiness for only a small part of the total time of interest.

In Fig. 6 is shown the total energy which has passed across the interface as a function of time for two different values of δy.

We also used the flux-difference form (41') which allows for a correction if the situation is nonsteady. The correction did, indeed, give an improvement, having an effect during the early nonsteady phase only, as expected. It raised the later flux function to a slightly higher value parallel to its former self. Even, so, there is still a small lag in getting the flow started.

C. Conclusions from the Numerical Tests

The results of the tests indicate that in a one-material problem, or one for which the material is nearly homogeneous, several methods of calculating give good results. The method of opacity averaging (43) is, perhaps, poorest.

For problems in which there is a strong and persistent material discontinuity, several of the methods give consistently poor results. The method which has most nearly universal applicability is (41) [or (41') for persistently nonsteady situations], since the energy flux asymptotically approaches the correct local value as local conditions approach steady state. The often-used methods (42) and (43) or a fixed combination thereof are of questionable validity, as the interface fluxes may be in error even as steady state is approached.

APPENDIX I

MATTERS RELATED TO TIME DIFFERENCING

The replacement of a differential equation by a finite-difference approximation thereto results in solutions that differ from the exact solutions. The errors may be small and roughly proportional to the time and space intervals. An analysis of such errors is called an accuracy study. The errors can, in certain circumstances, become suddenly very large—indeed, grow without bound—even under circumstances such that an accuracy study would predict decreasing errors. An analysis of these errors is called a stability study.

1. Stability

A solution of the diffusion equation (19) is $\theta \equiv \theta_0 \equiv$ const. Likewise, one can find a solution $\theta = \theta_0(1 + \epsilon)$, where $\epsilon(x, t)$ is a function whose magnitude is everywhere small compared with 1. By keeping lowest order terms in an expansion in ϵ, we obtain in place of Eq. (19)

$$\frac{\partial \epsilon}{\partial t} = D\nabla^2 \epsilon$$

where

$$D \equiv \frac{4ca\ \theta_0^3\ \lambda(\theta_0)}{3\ \frac{\partial}{\partial \theta_0}\left[E_m(\theta_0) + a\theta_0^4\right]}$$

Since the equation for ϵ is now linear, its general solution will be a sum of

all special solutions. In particular, it can be a sum of terms of the sort

$$\epsilon = e^{i\vec{k}\cdot\vec{r}}\, e^{\omega t}$$

which is a solution provided $\omega = -Dk^2$. Thus, since $D > 0$, the disturbance, ϵ, will damp for any wave number k.

This same analysis can be applied to the difference equation which is (in one-dimension for simplicity)

$$\epsilon_j^{n+1} - \epsilon_j^n = \frac{D\delta t}{\delta x^2}\left(\epsilon_{j+1}^n + \epsilon_{j-1}^n - 2\epsilon_j^n\right)$$

The trial function

$$\epsilon_j^n = e^{ikj}\, e^{\omega n}$$

is a solution provided

$$e^{\omega} = 1 - \frac{2D\delta t}{\delta x^2}(1 - \cos k)$$

The most extreme case is that for which $\cos k = -1$, in which case, $e^{\omega} > -1$ only if

$$\frac{2D\delta t}{\delta x^2} < 1$$

This condition, then, must be satisfied for stability, for if it is violated and $e^{\omega} < -1$, then the perturbation oscillates with increasing amplitude rather than damping as it should.

We have tested this well-known stability requirement on many of the problems reported here, and found that its prediction is, in all cases, highly accurate.

Various implicit differencing methods have been proposed for the time advancement. Some of these are unconditionally stable. The methods studied in this paper for space differencing can be incorporated into several of these implicit time-differencing procedures. The incorporation is more convenient in some cases than in others.

2. Accuracy

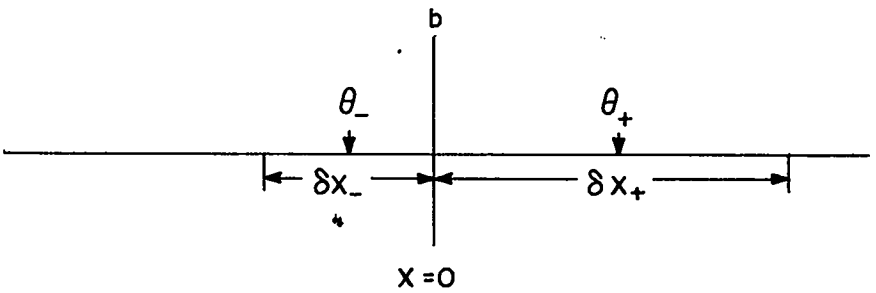
Repeatedly, tests were made to ensure that δt was small enough in the numerical computations so that any further decrease in its size made a negligible difference in the results. The result of all these tests is that whenever δt is small enough for stability, it is also small enough for the desired accuracy. This fact is of value in applying explicit differencing methods, because the resulting solution is either accurate (relative to time advancement), or else the computation cannot proceed at all owing to instability. The stability of implicit methods removes this automatic warning system of error.

APPENDIX II

FURTHER DISCUSSION OF THE STEADY-STATE DIFFERENCING METHOD

The principle by which flux-difference form (41) was derived may be difficult to apply when expressions for mean free path as a function of temperature are complicated or are of different form for two adjacent materials. In some circumstances, the mean-free-path function is used in the form of a table of numbers, in which case the situation is even more complicated. The discussion in this appendix is meant to indicate how some of these difficulties may be overcome.

Consider the general application of the principle to the problem of determining the instantaneous energy flux at a cell boundary which lies between two materials.



The boundary, b is placed at x = 0. For generality, we assume two different cell sizes with the known temperatures, θ_- and θ_+, located at the centers. The mean-free-path formula is assumed to be of the form

$$\lambda\ (\theta, x) = \begin{cases} \lambda_+(\theta) & \text{for } x > 0 \\ \lambda_-(\theta) & \text{for } x < 0 \end{cases}$$

It is further assumed that F is a fixed constant and that θ is continuous in the range $-\delta x_-/2 \le x \le \delta x_+/2$. Then Eq. (40) can be integrated,

$$\int_{-(\delta x_-/2)}^{0} F dx = \int_{\theta_-}^{\theta_b} \left(-\frac{4}{3} ca\right) \theta^3 \lambda_-(\theta) d\theta$$

or

$$F = -\frac{8ca}{3\delta x_-} \int_{\theta_-}^{\theta_b} \theta^3 \lambda_-(\theta) d\theta$$

Similarly,

$$F = -\frac{8ca}{3\delta x_+} \int_{\theta_b}^{\theta_+} \theta^3 \lambda_+(\theta) d\theta$$

This is a pair of simultaneous equations from which the boundary temperature, θ_b, is to be eliminated, giving an expression for the boundary flux. In those cases where the algebraic manipulations are simple, the procedure is straightforward to apply. In the more complicated cases, the following approximation procedure may be useful.

In each of the simultaneous equations, F, considered to be a function of θ_b, can be expanded in a Taylor's series about some temperature θ_0, as yet not specified:

$$F = -\frac{8ca}{3\delta x_-} \left[\int_{\theta_-}^{\theta_0} \theta^3 \lambda_-(\theta) d\theta + (\theta_b - \theta_0)\theta_0^3 \lambda_-(\theta_0) + \ldots \right]$$

$$F = -\frac{8ca}{3\delta x_+} \left[\int_{\theta_0}^{\theta_+} \theta^3 \lambda_+(\theta) d\theta - (\theta_b - \theta_0)\theta_0^3 \lambda_+(\theta_0) + \ldots \right]$$

If θ_0 is chosen sufficiently close to θ_b, then one can achieve sufficient accuracy even though the series be truncated beyond those terms explicitly shown. Then θ_b can be eliminated, and we obtain

$$F = -\left(\frac{8ca}{3}\right)\frac{\lambda_+(\theta_0)\int_{\theta_-}^{\theta_0}\theta^3\lambda_-(\theta)d\theta + \lambda_-(\theta_0)\int_{\theta_0}^{\theta_+}\theta^3\lambda_+(\theta)d\theta}{\lambda_+(\theta_0)\delta x_- + \lambda_-(\theta_0)\delta x_+}$$

Note that if $\lambda_\pm(\theta) \equiv A_\pm f(\theta)$ where $f(\theta)$ is the same function for both materials, then this approximate expression yields the exact solution. In such a case, the result is, of course, independent of θ_0, and we could put $\theta_0 = \theta_+$. In general, if there is a large discontinuity in transparency at the interface, then θ_b will be close to the temperature on the side with greater transparency. For illustration, let that side be the + side. Then it seems reasonable to approximate $\theta_0 = \theta_+$, in which case

$$F = -\left(\frac{8ca}{3}\right)\left[\frac{\lambda_+(\theta_+)}{\lambda_+(\theta_+)\delta x_- + \lambda_-(\theta_+)\delta x_+}\right]\int_{\theta_-}^{\theta_+}\theta^3\lambda_-(\theta)d\theta$$

This form is relatively easy to work with, and will be valid in many situations of interest. The integral can be evaluated numerically if necessary, and if one is working with tables of numbers to represent the mean-free-path formula, then one could also form values of $\int_0^\theta \theta^3\lambda_-(\theta)d\theta$ and work with differences of these.

Tests of these approximation forms with the simple functions used in this report for mean free path would not be useful, since these approximation forms become exact with the functions used. This fact is encouraging when one considers that there is generally a qualitative similarity in mean-free-path behavior among many materials, the differences being capable of representation, approximately, by various multiplicative constants.

NOTE

In the following figures, all quantities are plotted in their dimensionless forms as shown at the coordinate axes and on the graphs:

$T \equiv$ dimensionless temperature
$y \equiv$ dimensionless distance
$z \equiv$ dimensionless time

Tick marks on distance axes show cell size.

The difference forms are summarized for reference:

(41) Steady-State Method
(41') Extended Steady-State Method
(42) λ-Average Method
(43) Opacity-Average Method
(44) Modified Opacity-Average Method
(45) Linear-Difference Method

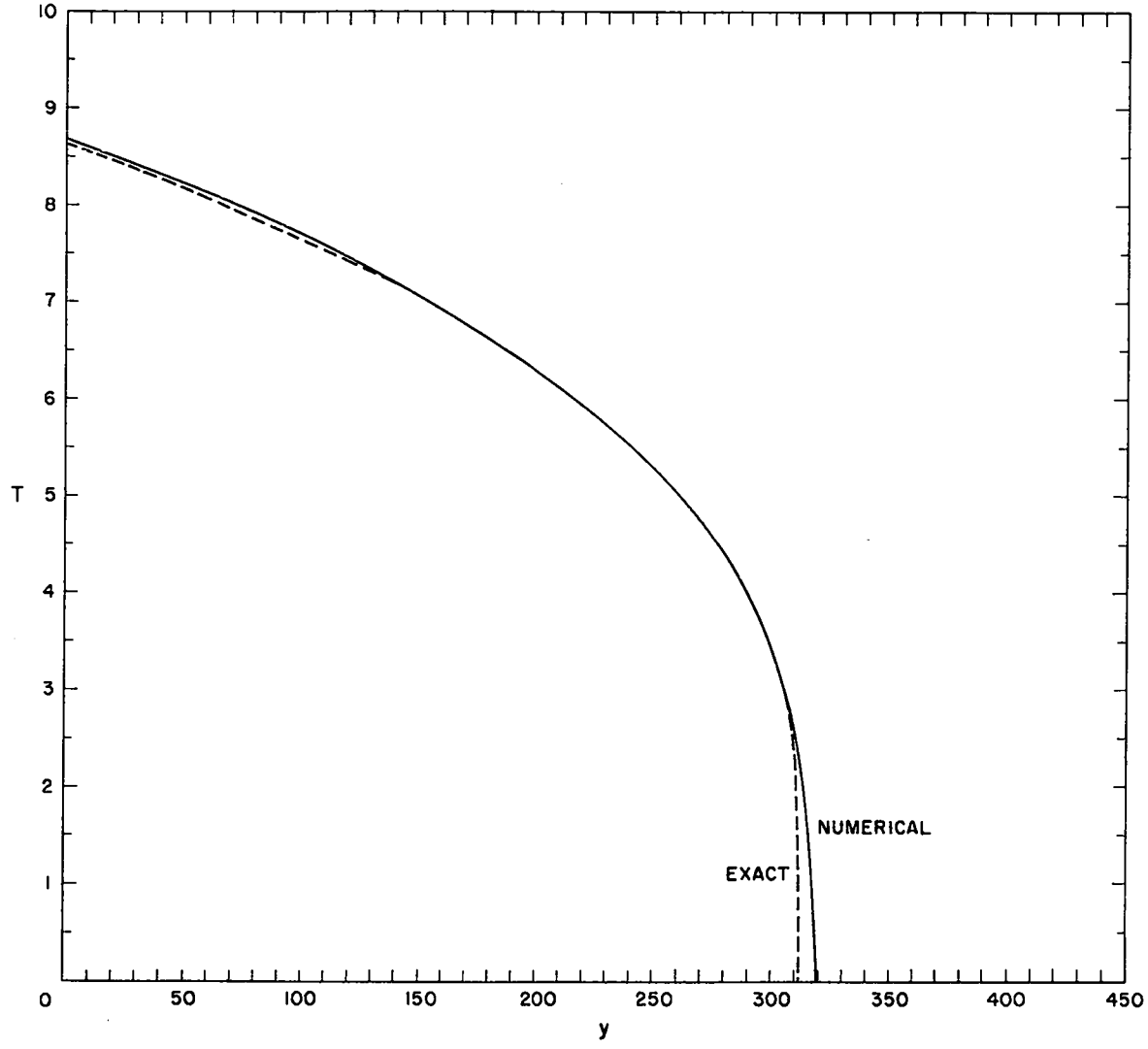


Fig. 1 Temperature profiles for the similarity problem at time z = 120. Flux-difference form is Eq. (41).

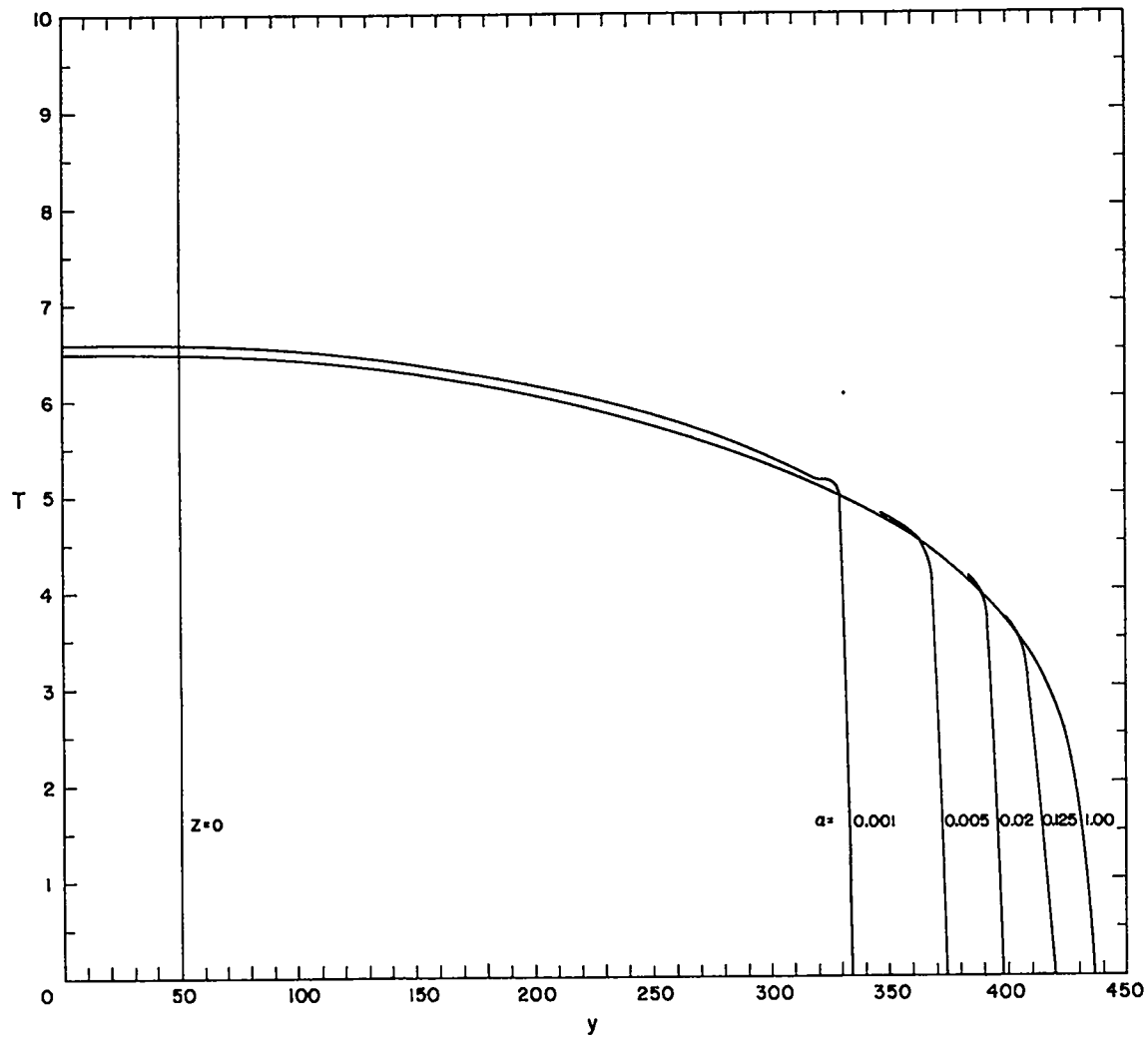


Fig. 2 Temperature profiles at time z = 100 for the one-material problem with initial temperature profile as shown for z = 0. Wall flux is zero. The relative weighting of flux-difference forms of Eqs. (42) and (43) is $\alpha:(1-\alpha)$. $\delta y = 10$.

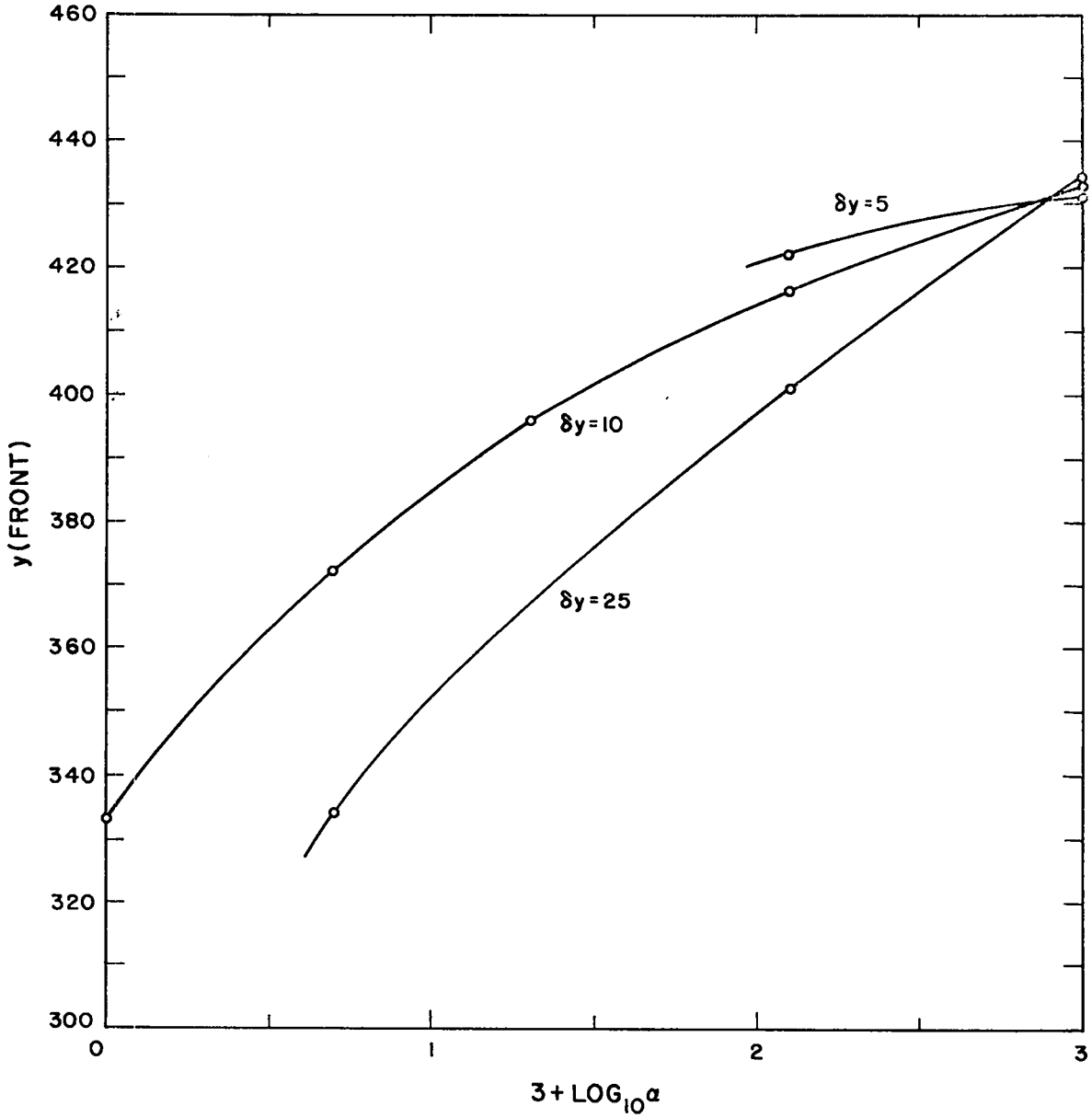


Fig. 3 Position of the radiation front (at T = 1) as a function of $3 + \log_{10} \alpha$, derived from data shown in Fig. 2 and analogous data for $\delta y = 5$ and 25.

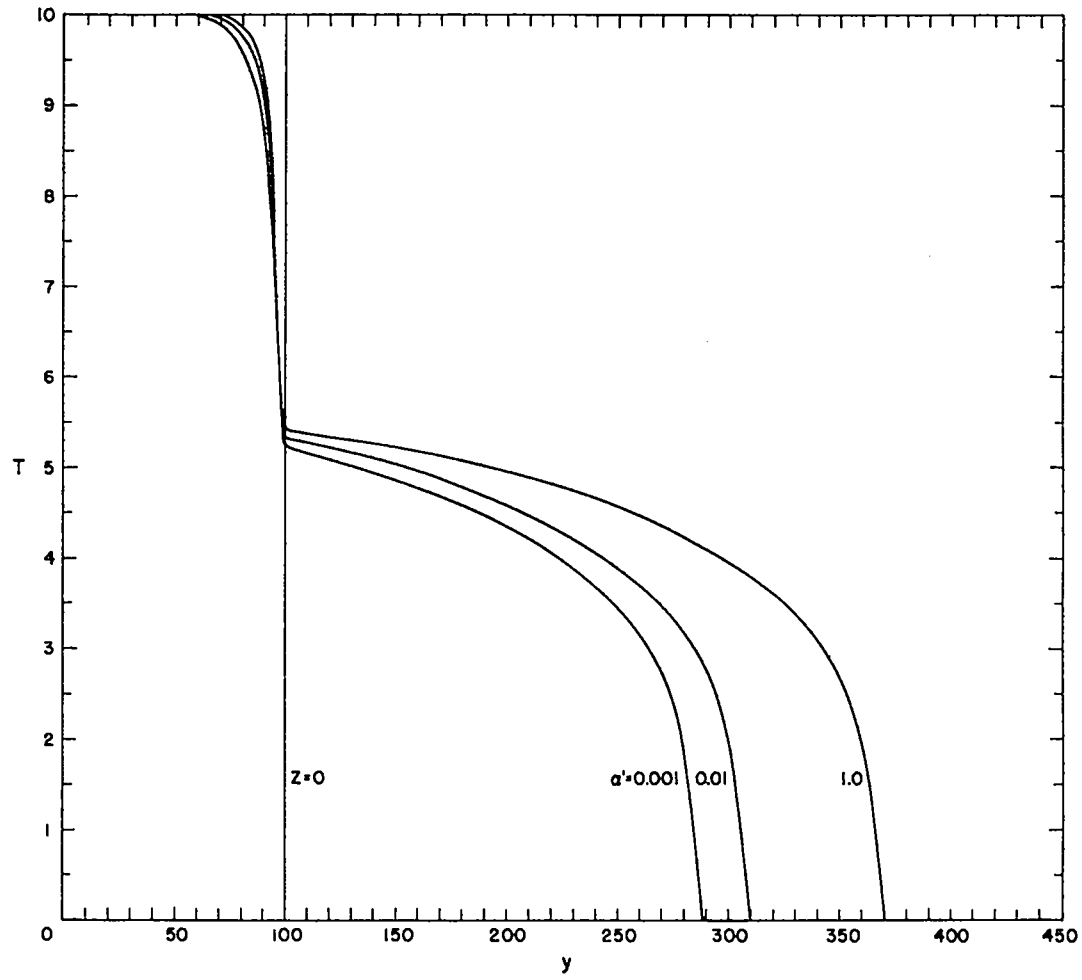


Fig. 4 Temperature profiles at time z = 100 for the two-material problem with initial temperature profile as shown for z = 0. Material discontinuity is at y = 100. Wall flux is zero. The relative weighting of flux-difference forms of Eqs. (42) and (43) is 1:0 everywhere except at the material discontinuity where it is $\alpha' : (1 - \alpha')$. $\delta y = 10$.

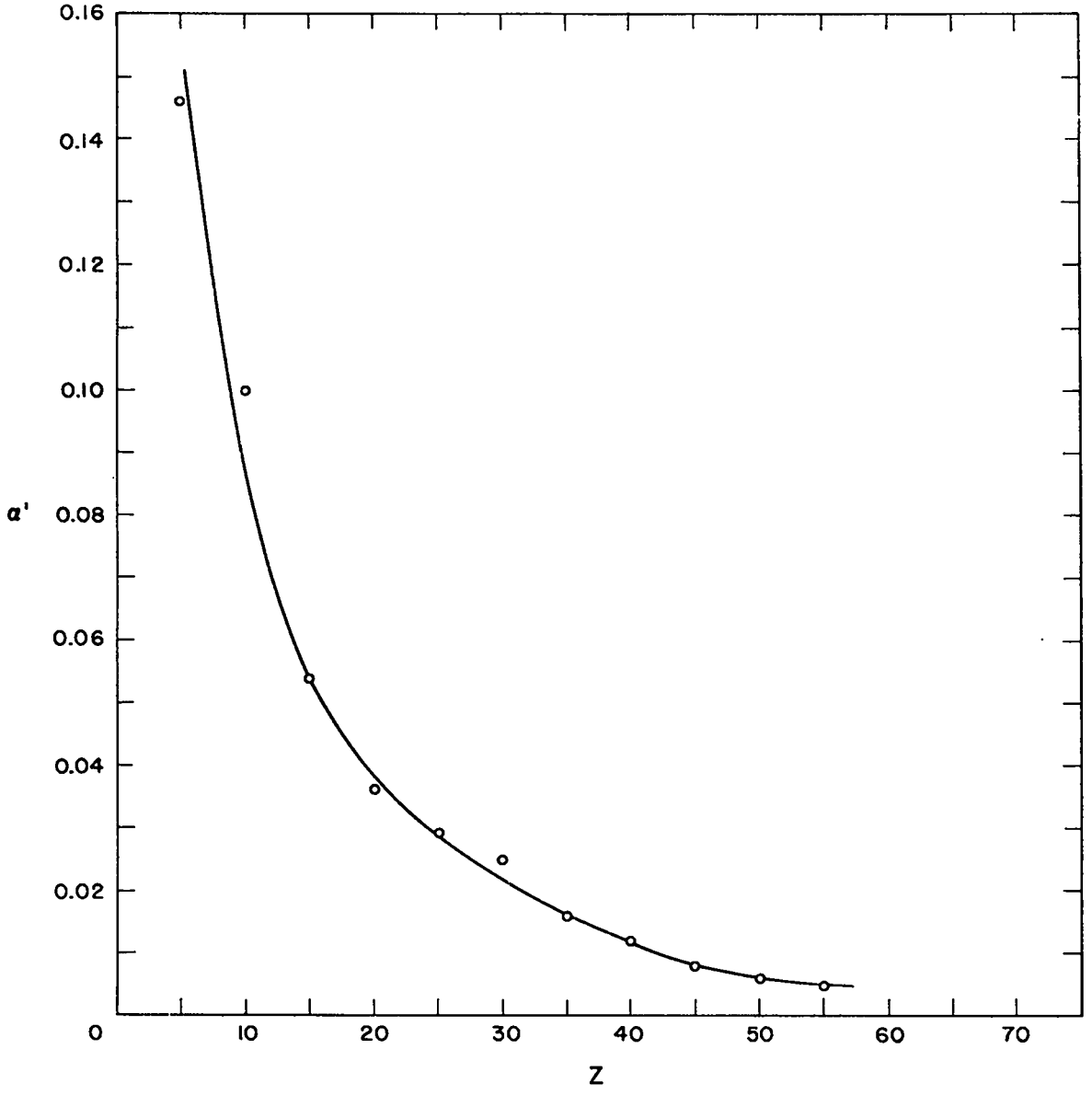


Fig. 5 The fixed value of α' required in order to ensure that the proper total energy would cross the material interface by time z, as a function of z.

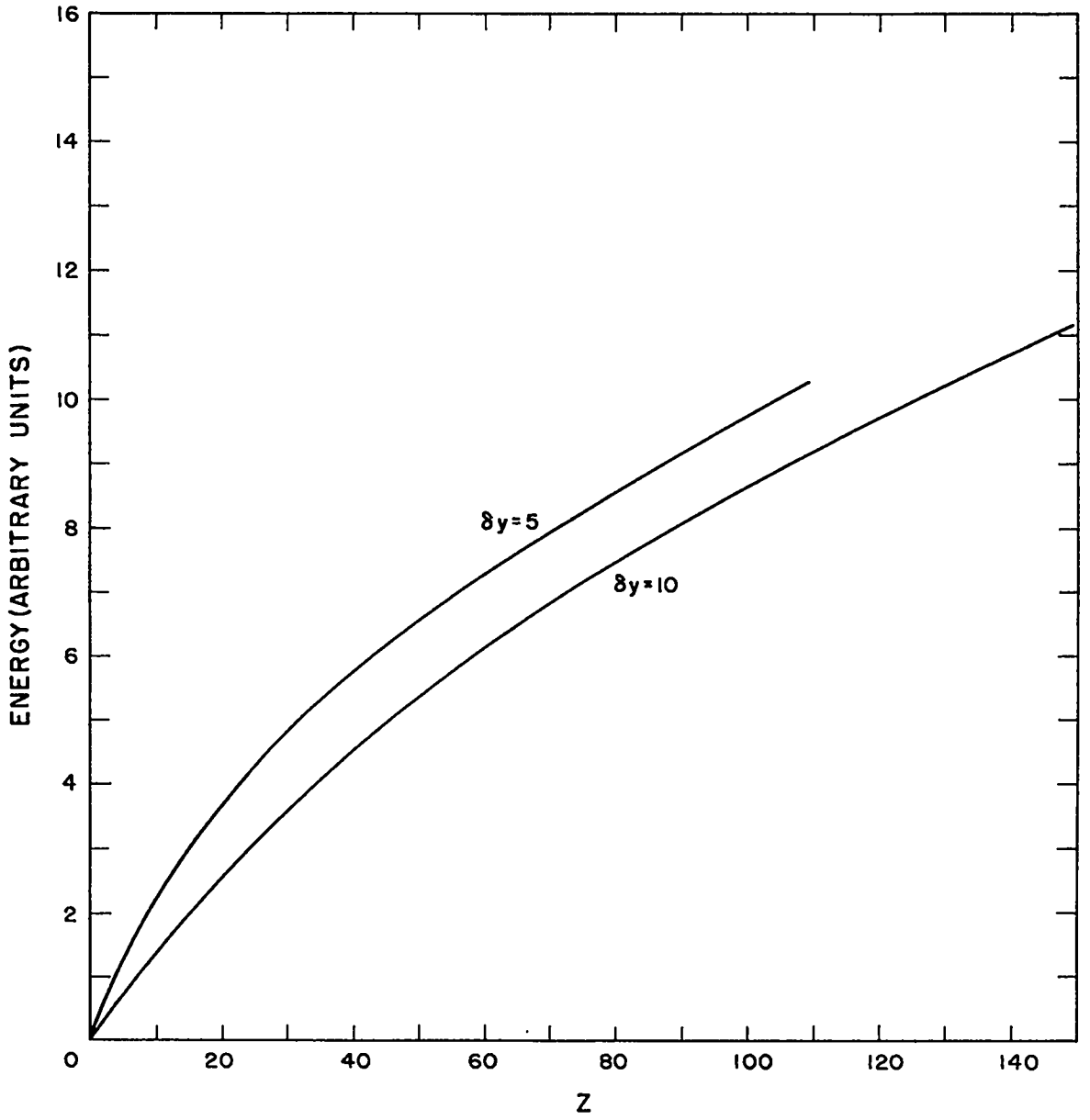


Fig. 6 Energy as a function of time passing the material interface for two different cell sizes. Flux-difference form is Eq. (41).