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LAMS-2960

LOS ALAMOS SCIENTIFIC LABORATORY
OF THE UNIVERSITY OF CALIFORNIA ○ LOS ALAMOS NEW MEXICO

IMPLICIT RADIATION DIFFUSION

Printed in USA. Price $0.50. Available from the

Office of Technical Services
U. S. Department of Commerce
Washington 25, D. C.

LAMS-2960
UC-32, MATHEMATICS AND
COMPUTERS
TID-4500 (22nd Ed.)

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OF THE UNIVERSITY OF CALIFORNIA LOS ALAMOS NEW MEXICO

REPORT WRITTEN: August 15, 1963

REPORT DISTRIBUTED: October 21, 1963

IMPLICIT RADIATION DIFFUSION

by

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Contract W-7405-ENG. 36 with the U. S. Atomic Energy Commission

ABSTRACT

It is shown that a considerable saving in computing time can be obtained by the use of unconditionally stable, or implicit, finite difference approximations to the radiation diffusion equation. The effectiveness of implicit difference equations depends on the existence of rapidly convergent iteration procedures for solving the non linear system of equations which determines the temperature distribution at each time step. We show by application to some typical situations that Newton's method provides such a procedure. Although Newton's method can be difficult to apply when the functions appearing in the equations are tabulated, this is not the case for radiation diffusion with tabular opacity and energy; for, the flux is defined as an integral whose derivative involves only values of the opacity, and the tabulated energy can be replaced by a continuously differentiable function of temperature by the use of the spline fit. The same holds true with interfaces and various boundary conditions.

Chapter I

The distribution of temperature, T, in a diffusing slab can be described by a differential equation of the form

$$(1) \qquad \frac{\partial E}{\partial t} = - \frac{\partial F}{\partial x} + H$$

where

$$E = E(x,t,T)$$
$$F = F(x,t,T, \frac{\partial T}{\partial x})$$
$$H = H(x,t,T) \quad .$$

For our purposes we may take $H = 0$. For the moment we do not specify E and F.

We suppose the slab to be divided into cells with centers x_j and lengths Δ_j. We set $E(x_j) = E_j$, $F(x_{j+1/2}) = F_{j+1/2}$. For any function $F(t)$ we write $\overline{f} = f(t)$, $f = f(t + \Delta t)$.

A one parameter family of difference approximations to (1) is

$$(2) \quad E_j - \overline{E}_j + \frac{\alpha \Delta t}{\Delta_j} (F_{j+1/2} - F_{j-1/2}) + (1 - \alpha) \frac{\Delta t}{\Delta_j} (\overline{F}_{j+1/2} - \overline{F}_{j-1/2}) = 0 = D_j$$

where $0 \leq \alpha \leq 1$. With $\alpha = 0$ we have the ordinary explicit difference equation which has a stability condition of the form

$$\frac{\Delta t}{\Delta_j^2} \leq r(T_j) \text{ for all } j$$

for some function $r(T)$ which can be determined for E and F.

Although the explicit method is satisfactory for most problems, the following situation can occur. Suppose a wave is penetrating the slab with velocity v. Then there will be a number s such that if $\Delta t/\Delta x^2 < s$, then $v\Delta t < \Delta x$, so that one would like to take Δt not much less than $s\Delta x^2$. However, there may be a region far from the head of the wave in which $r(t)$ is much smaller than s, forcing a time interval much smaller than needed for accuracy. It is here that an unconditionally stable method is called for.

It can be shown, at least if E and F are linear, that (2) is unconditionally stable if $\frac{1}{2} \leq \alpha \leq 1$ [1]. In this case the new temperatures T_j appear in a complicated way and can only be obtained by an iteration such as Newton's method, which has the following form: to solve the system

$$D_j(T_1, \ldots T_N) = 0, \qquad j = 1, 2, \ldots, N$$

use the following algorithm.

a) Guess a first value for T_j

b) Define ΔT_j as the solution of the linear system

$$\sum G_{jk} \Delta T_k = - D_j$$

where

(3) $$G_{jk} = \frac{\partial D_j}{\partial T_k}$$

and all coefficients are evaluated at the previous iterate T_j.

(c) Replace T_j by $T_j + \Delta T_j$ and repeat (b) until convergence occurs.

Since, as we shall see, the fluxes $F_{j+1/2}$ depend only on T_j and T_{j+1}, (3) has the form

(4) $$A_j \Delta T_{j-1} + B_j \Delta T_j + C_j \Delta T_{j+1} = - D_j$$

where

$$A_j = \frac{\partial D_j}{\partial T_{j-1}} = - \frac{\alpha \Delta t}{\Delta_j} \frac{\partial F_{j-1/2}}{\partial T_{j-1}}$$

(5) $$B_j = \frac{\partial D_j}{\partial T_j} = \frac{\partial E_j}{\partial T_j} + \frac{\alpha \Delta t}{\Delta_j} \frac{\partial}{\partial T_j} [F_{j+1/2} - F_{j-1/2}]$$

$$C_j = \frac{\partial D_j}{\partial T_{j+1}} = + \frac{\alpha \Delta t}{\Delta_j} \frac{\partial F_{j+1/2}}{\partial T_{j+1}} \quad .$$

The linear system (4) is solved by the following well-known device: put

(6) $$\Delta T_j = M_j \Delta T_{j-1} + N_j \quad .$$

Substituting this into (4) we find

$$(7) \qquad M_j = \frac{-A_j}{B_j + C_j M_{j+1}} , \qquad N_j = \frac{-D_j - C_j N_{j+1}}{B_j + C_j M_{j+1}} .$$

The M's and N's are determined by (7) and the boundary condition at $x_{N+1/2}$. For example, if $F_{N+1/2} = 0$

$$M_N = \frac{-A_N}{B_N} , \qquad N_N = \frac{-D_N}{B_N} ,$$

and then (7) is used recursively. A boundary condition at the other end, say $\Delta T_0 = 0$, together with (6) then determines the ΔT_j.

To apply the above ideas to the diffusion equation, let

$$E(T) = E_m(T) + \frac{a}{\rho} T^4$$

$$F = - \frac{ac}{3} \frac{1}{K} \frac{\partial T^4}{\partial x}$$

where

E_m = specific material energy

a = Stefan-Boltzmann radiation constant

ρ = density

K = K(T,x) = opacity

c = speed of light

Note that x is the mass variable.

The discrete flux $F_{j+1/2}$ is defined as a mean value by the following relation,

$$(8) \qquad -\frac{\Delta_j + \Delta_{j+1}}{2} F_{j+1/2} = \int_{x_j}^{x_{j+1}} \frac{ac}{3} \frac{1}{K} \frac{dT^4}{dx} dx \quad .$$

We now make two assumptions:

a) K is a function of T only in the intervals $[x_j, x_{j+1/2}]$, $[x_{j+1/2}, x_{j+1}]$, so we write

$$K(T,x) = \begin{Bmatrix} K_L(T) & x_j \leqq x \leqq x_{j+1/2} \\ K_R(T) & x_{j+1/2} \leqq x \leqq x_{j+1} \end{Bmatrix} \quad .$$

b) $T(x)$ is monotonic in the interval (x_j, x_{j+1}).

With these assumptions the right side of (8) can be written as

$$Q = \int_{T_j}^{T_{j+1/2}} p_L(T)dT + \int_{T_{j+1/2}}^{T_{j+1}} p_R(T)dT$$

where we have introduced the function of the opacity

$$(9) \qquad p(\rho,T) = \frac{4ac}{3} \frac{T^3}{K(\rho,T)} \quad .$$

Then

$$\frac{\partial Q}{\partial T_{j+1}} = p_L(T_{j+1/2}) \frac{\partial T_{j+1/2}}{\partial T_{j+1}} + p_R(T_{j+1}) - p_R(T_{j+1/2}) \frac{\partial T_{j+1/2}}{\partial T_{j+1}} \quad .$$

The temperature $T_{j+1/2}$ can be determined from a continuity condition on the flux; namely

$$g(T_{j+1/2}) = \frac{2}{\Delta_j} \int_{T_j}^{T_{j+1/2}} p_L dT - \frac{2}{\Delta_{j+1}} \int_{T_{j+1/2}}^{T_{j+1}} p_R dT = 0 \quad .$$

The function g is monotonic and has a root between T and T_{j+1} which can readily be found by Newton's method or it can be found in the sweep defined by equations (4), (6), and (7).

We now have

$$\frac{dT_{j+1/2}}{dT_{j+1}} = \frac{p_R(T_{j+1})/\Delta_{j+1}}{p_L(T_{j+1/2})/\Delta_j + p_R(T_{j+1/2})/\Delta_{j+1}}$$

so that

(10) $$\frac{\partial F_{j+1/2}}{\partial T_{j+1}} = \frac{-2}{\Delta_j + \Delta_{j+1}} \frac{\partial Q}{\partial T_{j+1}}$$

$$= \frac{-2\; p_R(T_{j+1})\; p_L(T_{j+1/2})}{\Delta_j p_R(T_{j+1/2}) + \Delta_{j+1} p_L(T_{j+1/2})} \quad .$$

Similarly

(11) $$\frac{\partial F_{j+1/2}}{\partial T_j} = \frac{2\; p_L(T_j)\; p_R(T_{j+1/2})}{\Delta_j p_R(T_{j+1/2}) + \Delta_{j+1} p_L(T_{j+1/2})}$$

and we see that (10) and (11) are independent of $\frac{\partial p}{\partial T}$.

Let us now consider $\frac{\partial E_m}{\partial T}$. For many problems $E_m = C_v T$, C_v constant, so $\frac{\partial E_m}{\partial T} = C_v$. All our test problems are of this form. In running these problems we noticed that small errors in $\frac{\partial E}{\partial T}$ slowed down the convergence of the iteration. This leads us to believe that if $E_m(T)$ is a tabular function it is important to use an interpolation process which produces good derivatives. Such an interpolation is provided by the spline fit [2], which involves replacing $E_m(T)$ by a piecewise cubic function which has continuous first and second derivatives. This is done as follows: let the tabulated values be $E_k = E_m(T_k)$ $k = 0, 1, \ldots, I$, and let $\ell_k = T_k - T_{k-1}$. If we let

$$\left(\frac{\partial^2 E_m}{\partial T^2}\right)_{T = T_k} = M_k$$

be the second derivatives, which are to be determined, then the piecewise cubic is

$$E_m(T) = \frac{M_{k-1}(T_k - T)^3}{6\ell_k} + \frac{M_k(T - T_{k-1})^3}{6\ell_k} + \left(\frac{E_k}{\ell_k} - \frac{M_k \ell_k}{6}\right)(T - T_{k-1})$$

$$+ \left(\frac{E_{k-1}}{\ell_k} - \frac{M_{k-1}\ell_k}{6}\right)(T_k - T) \quad , \text{for } T_{k-1} \leq T \leq T_k \quad .$$

If we equate left and right values of first derivatives we get the relation

$$(12) \qquad \frac{\ell_k}{6} M_{k-1} + \frac{\ell_k + \ell_{k+1}}{3} M_k + \frac{\ell_{k+1} M_{k+1}}{6} = \frac{E_{k+1} - E_k}{\ell_{k+1}} - \frac{E_k - E_{k-1}}{\ell_k} \quad .$$

If we specify a condition at the end points T_0 and T_I such as $M_0 = M_I = 0$, or specify the first derivatives, then (12) determines M_k, from which $E_m(T)$ and $\frac{\partial E_m}{\partial T}$ can be computed. Thus, in addition to the table $[E_k]$ we need to compute (once) and store the table $[M_k]$. An example of the spline fit for a typical $E_m(T)$ is given in Chapter III.

Chapter II

We have applied the method to the problem of solving for the penetration of radiation through a uniform slab with a constant driving temperature at one boundary of $T = 1.5$. The material has unit density with an opacity given by $100\ T^{-4}$. Equal mass zones of unit thickness were chosen. The differential equation to be solved is

$$(13) \qquad \frac{d}{dt}\left(.1T + .0137\ T^4\right) = + .00685\ \frac{d^2T^8}{dx^2}$$

with the boundary condition that at $x = 0$, $T = 1.5$ and $T = 0$ for $x > 0$ at $t = 0$.

For the case $\alpha = 0$ in equation (2) we have the explicit equations which are stable for

$$0.0685\ (8T^7\Delta t) < \frac{1}{2}$$

or $\Delta T < .053$.

We have solved the difference equation for $\alpha = 1/2$ and $\alpha = 1$ for $\Delta t = .0625$, $.25$, 1, and 10. In some cases we have dropped the radiation energy term, $.0137\ T^4$, so that we can compare with the similarity solution [3]. The solution compares very well for $\Delta t \leqq 1$ as can be seen by the comparison at $t = 100$ in figure 1. There was very little difference in the centered implicit ($\alpha = 1/2$) and full implicit ($\alpha = 1$) solution everywhere except at the head of the wave where the full implicit temperatures are slightly higher.

Even for $\Delta t = 10$ the solution is in good agreement with the true solution although the centered implicit is seen to have an oscillation in the first mass point. This oscillation is removed by going to the full implicit equation. A comparison at $t = 30$ is tabulated in Table I and shown in figure 2. The total number of iterations to go to $t = 30$ for various Δt's is:

Δt	.0625	.25	1	10
Iterations	960	270	104	46

The amount of calculation per iteration is roughly 2 times the calculation per time cycle in an explicit calculation. Since the number of time cycles in $t = 30$ is 600 it appears that the implicit method is faster for Δt as low as .25 and is quite accurate for $\Delta t = 1$. For $\Delta t = 10$ we gain only a factor of two in speed over $\Delta t = 1$ which doesn't appear worth while considering the inaccuracies introduced. On the other hand the results are not unreasonable for $\Delta t = 10$ so one need not worry too much if for some reason the Δt is too large in a region of some problem being considered.

The second problem consists of a slab of two materials, the first having a T^4 dependence in the mean free path and the second having a constant mean free path. The initial and boundary condition and the zoning are the same as before.

The differential equations in the two regions are:

$$(14) \qquad \frac{d}{dt}\left(.1T + .0137\ T^4\right) = + .00685\ \frac{d^2T^8}{dx^2}, \quad 0 < x < 10 ;$$

$$\frac{d}{dt}\left(.1T + .0137\ T^4\right) = + 3.425\ \frac{d^2T^4}{dx^2}, \quad 10 < x < 20 .$$

Again we have varied α and Δt, and the results are compared in figure 3 and table II for $t = 60$. We see that the full explicit solution is well behaved for large Δt as before. Although we have no similarity solution to compare with for this problem we feel that the full implicit treatment is probably better since it appears to have the same solution as the centered implicit for $\Delta t = 1$ and it doesn't have disturbing oscillations for large Δt. We have used coefficients A, B, C that are only half the right value (but the right sign!) to solve for D in equation (4). We converge to the right solution but it takes about 10 times as many iterations so we conclude that it is important that the exact derivatives be used in equation (4).

Chapter III

Thus far we have considered the equation using only simple functions of the temperature. In practice this is rarely the case, so we wish to indicate a method of attack that uses tabulated values of the energy and opacity. The known properties of these functions will be exploited to provide accurate values of the energy and its derivative, and the opacity and its integral. We first treat the energy.

In a wide variety of problems where radiation flow is important the material energy is only weakly dependent upon the density so that a linear logarithmic interpolation of the density variation will yield satisfactory values of the energy at intermediate points. The temperature interpolation will be done by the spline fit mentioned in Chapter I. We shall fit the spline fit to tabulated values of $\log E_m(T_k)$. The logarithm is used since we treat E_m over five decades in T. The derivative of E with respect to T is

$$(15) \qquad C_v = \frac{dE}{dT} = \frac{E}{T}\frac{d \log E}{d \log T} \quad .$$

We show the spline fit for a typical material in figures 4 and 5.

For most materials a table of about 150 points is sufficient to cover the full range of temperatures and densities encountered in most problems. This means, of course, that 150 values of the logarithm of the energy and 150 values of the second derivative must be tabulated.

<u>Opacity</u>

The opacity could also be treated in the same manner. However, the opacity or its related function, p, defined in equation (9), is used in an integral over a fairly small range of the temperature, so that the logarithm of p can be fitted quite well by linear interpolation and p integrated analytically. Furthermore, the density variation of the opacity is usually small so that again a logarithmic interpolation yields satisfactory results.

Since the density dependence of the opacity is small (usually varying as the one quarter power) we can simplify equation (11) for two adjacent zones of the same material. In that case $K_L = K_R$ so that

$$\text{(16)} \qquad \frac{dF_{j+1/2}}{dT_j} = \frac{+2\, p(T_j)}{\Delta_j + \Delta_{j+1}} \quad ,$$

and equation (8) for the flux becomes

$$F_{j+1/2} = \frac{-2}{\Delta_j + \Delta_{j+1}} \int_{T_j}^{T_{j+1}} p(T)dT \quad ,$$

where we use the average density of cells j and j+1. This is generally accurate except for interfaces between materials where the density and material properties are discontinuous and equations (8), (10), and (11) must be used.

The function $p(\rho,T)$ will be given at a set of points (ρ_i, T_k). For any fixed ρ_i we assume that log p is a polygonal function of log T, that is

$$(17) \qquad p(\rho_i,T) = p_{ik}\left(\frac{T}{T_k}\right)^{\alpha_{ik}} \quad \text{for } T_k \leq T \leq T_{k+1} \quad ,$$

where

$$p_{ik} = p(\rho_i,T_k)$$

$$\alpha_{ik} = \frac{\log p_{ik} - \log p_{i,k+1}}{\log T_k - \log T_{k+1}} \quad .$$

The logarithms of p_{ik} are tabulated.

With $p(\rho,T)$ in this form we have for $T_k \leq T \leq T_{k+1}$

$$\int_{T_k}^{T} p(\rho_i,T')dT' = \frac{Tp(\rho_i,T) - T_k p_{ik}}{\alpha_{ik} + 1} \quad .$$

For any two temperatures θ_1, θ_2 with $\theta_1 < \theta_2$ we find integers j and k such that

$$T_k \leq \theta_1 < T_{k+1} < \cdot \cdot \cdot < T_j \leq \theta_2 < T_{j+1} \quad .$$

Then

$$(18) \qquad \int_{\theta_1}^{\theta_2} p(\rho_i,T)dT = \frac{T_{k+1}\, p_{i,k+1} - \theta_1\, p(\rho_i,\theta_1)}{\alpha_{i,k} + 1}$$

$$+ \sum_{r=k+2}^{j} \frac{T_r\, p_{ir} - T_{r-1}\, p_{i,r-1}}{\alpha_{i,r-1} + 1}$$

$$+ \frac{\theta_2\, p(\rho_i,\theta_2) - T_j p_{ij}}{\alpha_{ij} + 1} \quad .$$

Free Surface Boundary Condition

Let $I(\mu)$ be the intensity of radiation per unit solid angle in the angle whose cosine is μ. In the diffusion approximation

$$I = \frac{ac}{4\pi} T^4 - \mu \frac{ac}{4\pi} \frac{1}{K} \frac{dT^4}{dx}$$

for $-1 \leqq \mu \leqq 1$, except at the surface s, when

$$I = 0 \text{ for } \mu < 0$$

$$I = \frac{ac}{4\pi} T^4 - \mu \frac{ac}{4\pi} \frac{1}{K} \frac{dT^4}{dx} \quad \text{for } \mu > 0 \quad .$$

Then the flux at the surface is

$$F_s = 2\pi \int_{-1}^{1} I\, \mu d\mu = \frac{ac}{2} \int_{0}^{1} \left(T^4 - \mu \frac{1}{K} \frac{dT^4}{dx}\right) \mu d\mu$$

$$= \frac{ac}{4} T_s^4 - \frac{ac}{6} \left(\frac{1}{K} \frac{dT^4}{dx}\right)_{x = s} \quad .$$

On the other hand, at an interior point

$$F(x) = - \frac{ac}{3} \frac{1}{K} \frac{dT^4}{dx} \quad .$$

If we assume $\lim_{x \to s} F(x) = F_s$, then

$$\text{(19)} \qquad \frac{ac}{2} T_s^4 + \frac{ac}{3} \left(\frac{1}{K} \frac{dT^4}{dx} \right)_{x = s} = 0 \quad .$$

Note that if the flux is constant and equal to F, then

$$\text{(20)} \qquad F = \frac{ac}{2} T_s^4 \quad .$$

In our difference approximation we assume the flux is constant in the last half zone. Thus, (19) becomes

$$\text{(21)} \qquad \frac{ac}{2} T_s^4 + \frac{2}{\Delta_1} \int_{T_1}^{T_s} p_1 \, dT = 0 \quad .$$

Equation (21) can be solved for the surface temperature T_s by Newton's method or in the sweep defined by (4) and (6).

The flux derivatives are

$$\text{(22)} \qquad \frac{dF_1}{dT_1} = \frac{2 \, acT_s^3 \, p_1(T_1)}{\dfrac{p_1(T_s)}{\Delta_1} + acT_s^3} \quad , \qquad \frac{dF_1}{dT_0} = 0 \quad ,$$

so that $A_1 = 0$, or $M_1 = 0$ and $\Delta T_1 = N_1$.

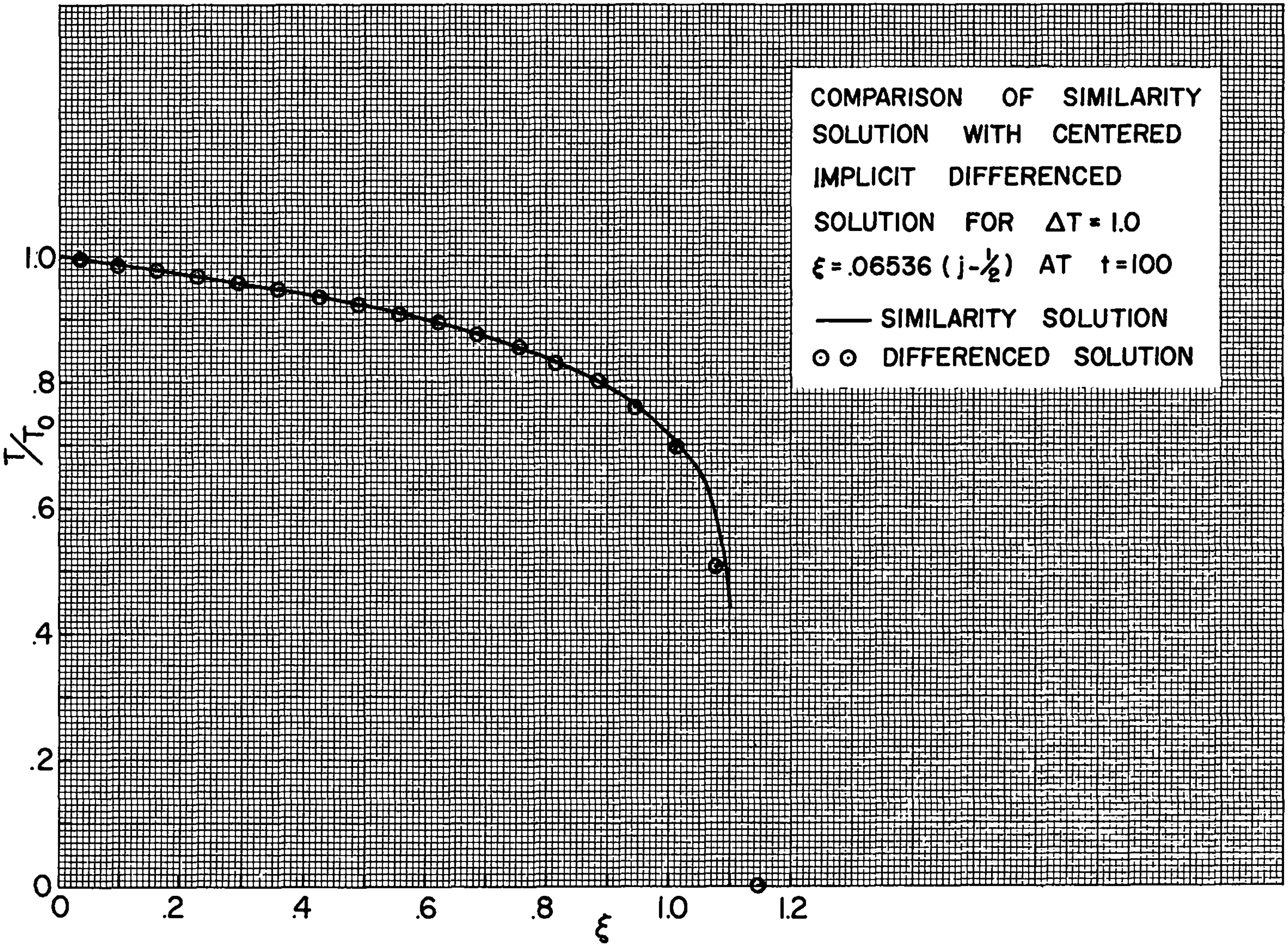

COMPARISON OF SIMILARITY SOLUTION WITH CENTERED IMPLICIT DIFFERENCED SOLUTION FOR ΔT = 1.0
ξ = .06536 (j-½) AT t = 100
SIMILARITY SOLUTION
DIFFERENCED SOLUTION
T/T₀
ξ
0
.2
.4
.6
.8
1.0
1.2

Figure 1.

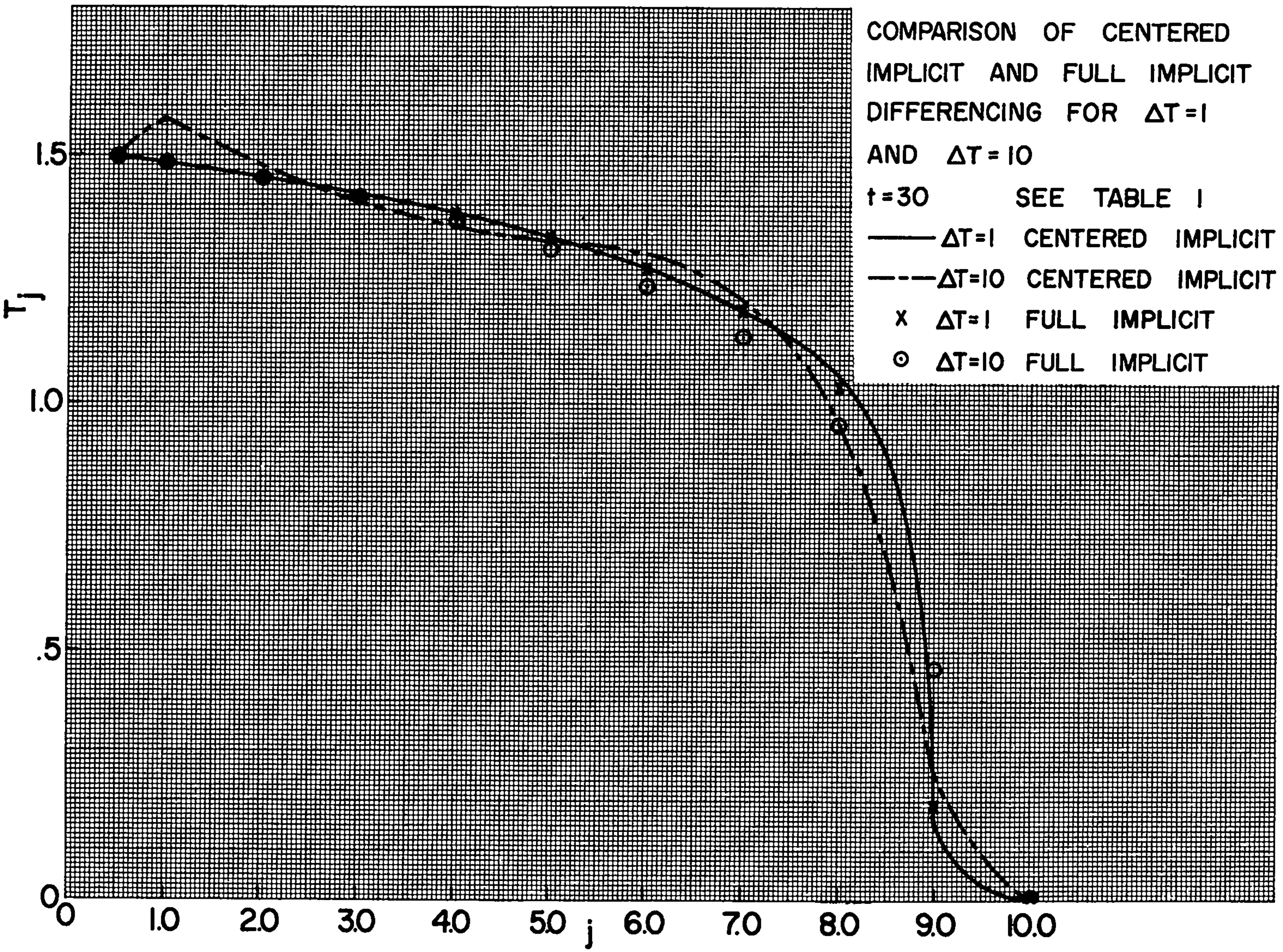

COMPARISON OF CENTERED IMPLICIT AND FULL IMPLICIT DIFFERENCING FOR ΔT = 1 AND ΔT = 10
t = 30 SEE TABLE I
ΔT = 1 CENTERED IMPLICIT
ΔT = 10 CENTERED IMPLICIT
X ΔT = 1 FULL IMPLICIT
⊙ ΔT = 10 FULL IMPLICIT
T_j
1.5
1.0
.5
0
0
1.0
2.0
3.0
4.0
5.0
j
6.0
7.0
8.0
9.0
10.0

Figure 2.

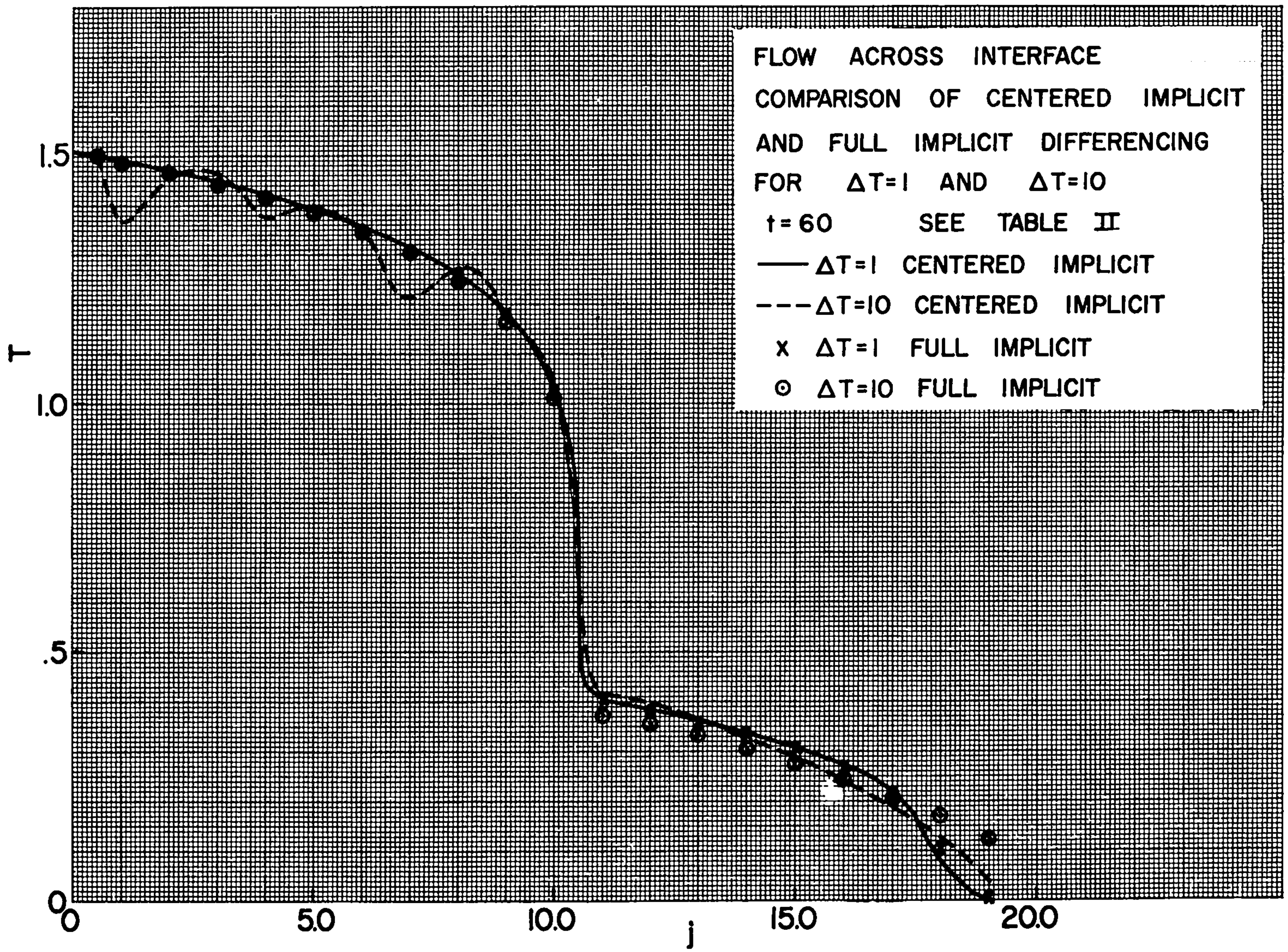

FLOW ACROSS INTERFACE
COMPARISON OF CENTERED IMPLICIT AND FULL IMPLICIT DIFFERENCING FOR ΔT=1 AND ΔT=10
t=60 SEE TABLE II
ΔT=1 CENTERED IMPLICIT
ΔT=10 CENTERED IMPLICIT
x ΔT=1 FULL IMPLICIT
⊙ ΔT=10 FULL IMPLICIT
T
1.5
1.0
.5
0
0
5.0
10.0
15.0
20.0
j

Figure 3.

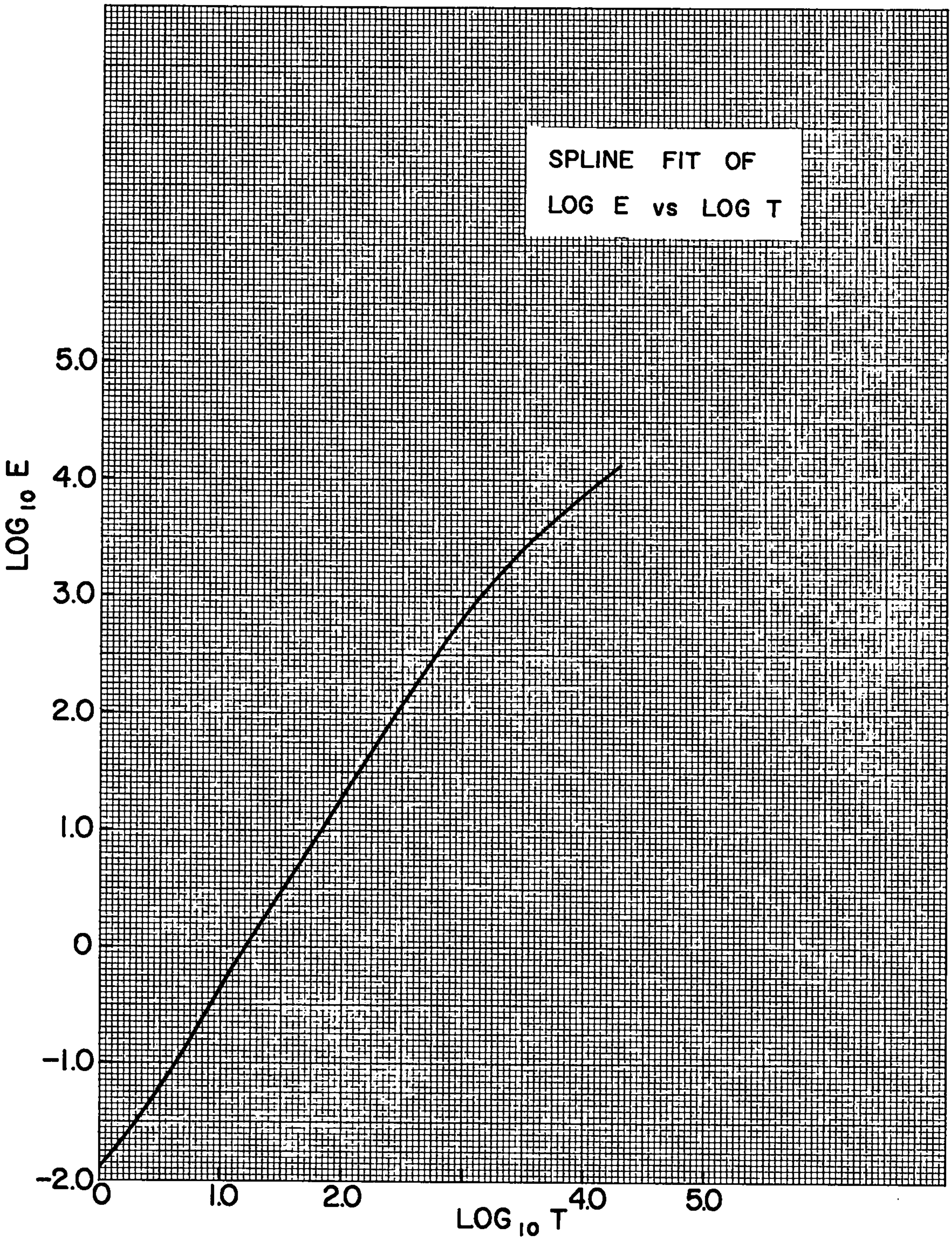
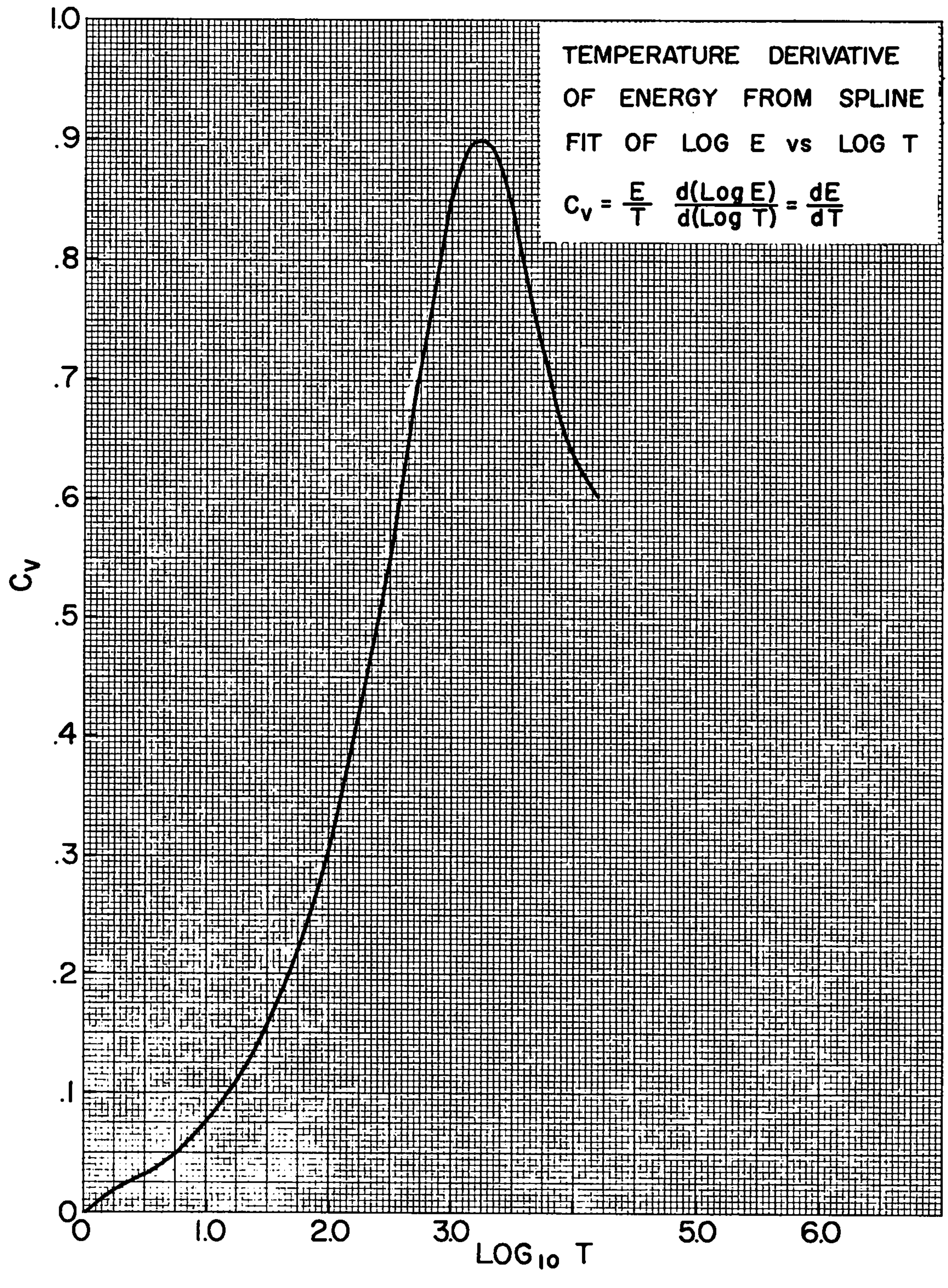

SPLINE FIT OF
LOG E vs LOG T
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
LOG_{10} E
0
1.0
2.0
4.0
5.0
LOG_{10} T

Figure 4.



TEMPERATURE DERIVATIVE OF ENERGY FROM SPLINE FIT OF LOG E vs LOG T
$C_v = \frac{E}{T} \frac{d(\text{Log } E)}{d(\text{Log } T)} = \frac{dE}{dT}$
C_v
1.0
.9
.8
.7
.6
.5
.4
.3
.2
.1
0
0
1.0
2.0
3.0
5.0
6.0
LOG_{10} T

Figure 5.

TABLE I

$t = 30$

	Centered Implicit			Full Implicit	
j	$\Delta t = 1/6$	$\Delta t = 1$	$\Delta t = 10$	$\Delta t = 1$	$\Delta t = 10$
1/2	1.5000	1.5000	1.5000	1.5000	1.5000
1	1.4868	1.4868	1.5761	1.4866	1.4850
2	1.4576	1.4576	1.4804	1.4572	1.4520
3	1.4239	1.4240	0.4037	1.4232	1.4131
4	1.3842	1.3842	1.3536	1.3831	1.3670
5	1.3359	1.3359	1.3278	1.3343	1.3107
6	1.2741	1.2741	1.3021	1.2718	1.2366
7	1.1889	1.1886	1.2051	1.1844	1.1344
8	1.0510	1.0507	0.9586	1.0350	0.9545
9	0.1518	0.1527	0.2438	0.1882	0.4630
10	0	0	0	0	0.0014

TABLE II

t = 60

	Centered Implicit		Full Implicit	
j	Δt = 1	Δt = 10	Δt = 1	Δt = 10
1/2	1.5000	1.5000	1.5000	1.5000
1	1.4903	1.3696	1.4903	1.4898
2	1.4694	1.4595	1.4693	1.4680
3	1.4463	1.4635	1.4461	1.4436
4	1.4203	1.4375	1.4200	1.4163
5	1.3906	1.3946	1.3901	1.3849
6	1.3557	1.3429	1.3552	1.3482
7	1.3134	1.3114	1.3127	1.3038
8	1.2589	1.2733	1.2580	1.2470
9	1.1806	1.1694	1.1797	1.1663
10	1.0288	1.0374	1.0278	1.0118
11	0.4040	0.4140	0.4010	0.3750
12	0.3843	0.3911	0.3811	0.3540
13	0.3623	0.3623	0.3589	0.3311
14	0.3370	0.3266	0.3334	0.3057
15	0.3071	0.2835	0.3032	0.2773
16	0.2702	0.2359	0.2656	0.2451
17	0.2204	0.1829	0.2135	0.2093
18	0.0760	0.1202	0.1079	0.1700
19	0	0.0353	0.0048	0.1257

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