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A practical method for numerical evaluation of solutions of partial differential equations of the heat-conduction type

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1. Introduction

This paper is concerned with methods of evaluating numerical solutions of the non-linear partial differential equation

$$\frac{\partial \theta}{\partial t} = \frac{\partial^2 \theta}{\partial x^2} - q\frac{\partial w}{\partial t}, \tag{1}$$

where

$$\frac{\partial w}{\partial t} = -kw\,\mathrm{e}^{-A/\theta}, \tag{2}$$

subject to the boundary conditions

$$\begin{cases} \begin{cases} \theta = f_1(x) \\ w = f_2(x) \end{cases} & \text{at } t = 0 \quad \text{for } 0 < x < 1, \\ \dfrac{\partial \theta}{\partial x} = H_1(\theta) & \text{at } x = 0 \quad \text{for } t \geqslant 0, \\ \dfrac{\partial \theta}{\partial x} = H_2(\theta) & \text{at } x = 1 \quad \text{for } t \geqslant 0, \end{cases} \tag{3}$$

A, k, q are known constants.

Equation (1) is of the type which arises in problems of heat flow when there is an internal generation of heat within the medium; if the heat is due to a chemical reaction proceeding at each point at a rate depending upon the local temperature, the rate of heat generation is often defined by an equation such as (2).

The presence of the non-linear term $q(\partial w/\partial t)$ in (1) and the empirical nature, in many cases, of the surface heat transfer function $H_1(\theta)$, render the use of formal methods unsuitable. Now Hartree [3–5] has suggested two methods (methods I and II below) of evaluating approximate solutions of partial differential equations in two

variables, of the heat-conduction type. In the first the time derivative is replaced by a finite difference ratio, and the resulting ordinary differential equation with x as independent variable is integrated numerically or mechanically. This integration is repeated for each finite step in time, and a trial and error process of solution is necessary to satisfy conditions at the two ends of the range in x. In Hartree's second method the range in x is divided into a finite number of intervals, and the second space derivative of θ at each point is expressed in terms of the values of θ at that point and at the neighbouring points on each side. In this way the partial differential equation is replaced approximately by a set of first-order equations in time, two of which express the boundary conditions at $x = 0$, $x = 1$ to the same degree of approximation. The differential analyser has been used to obtain solutions of these equations, the integration proceeding in time. In sections 2 and 3 of the present paper, the application of Hartree's methods to equations (1) and (2) with conditions (3) is discussed, and the difficulties arising in carrying out mechanical solutions are examined.

The main purpose of this paper is to discuss a numerical method, method III below, developed by the authors in which both derivatives are replaced by finite difference ratios and the solution proceeds by finite steps in time. In a method proposed by Richardson [8, 9] the steps in time are overlapping which gives rise to a rapidly increasing oscillatory error. A method recently reported by the American Applied Mathematics Panel [1] would seem liable to a similar disadvantage. In the method III below, the time steps do not overlap and an iterative process is involved at each step. In this way the oscillatory error is removed and much bigger steps in time may be used than in Richardson's treatment.

For convenience in discussion, the present paper refers to equations (1) and (2), but it is clear that the numerical method can be applied to other forms of equation (2) and is capable of extension to other types of second-order partial differential equations where there is an open boundary in one of the variables.

2. Method I: replacing the time derivative

Writing $\theta(t)$ for temperature at time t, regarded as a function of x, and considering a time interval δt, the derivative with respect to time may be written

$$\frac{\partial\theta}{\partial t}\left(t+\frac{1}{2}\delta t\right) = \frac{\theta(t+\delta t)-\theta(t)}{\delta t} + \mathrm{O}(\delta t)^2. \tag{4}$$

Hence equation (1) becomes approximately

$$(1/\delta t)\big[\theta(t+\delta t)-\theta(t)\big] = \frac{1}{2}\frac{\partial^2}{\partial x^2}\big[\theta(t+\delta t)+\theta(t)\big] - (q/\delta t)\big[w(t+\delta t)-w(t)\big]. \tag{5}$$

Similarly (2) may be written

$$(1/\delta t)\big[w(t+\delta t)-w(t)\big] = -\frac{1}{2}k\big[w(t+\delta t)+w(t)\big]\mathrm{e}^{-2A/[\theta(t+\delta t)+\theta(t)]}$$

or

$$w(t+\delta t) - w(t) = E\big[w(t+\delta t) + w(t)\big], \tag{6}$$

where

$$E = -\frac{1}{2}k\delta t\, \mathrm{e}^{-2A/[\theta(t+\delta t)+\theta(t)]}. \tag{7}$$

Therefore

$$w(t+\delta t) = \frac{1+E}{1-E}w(t). \tag{8}$$

Alternatively, on integrating with respect to time, (2) becomes

$$\log\frac{w(t+\delta t)}{w(t)} = -\int_t^{t+\delta t} k\,\mathrm{e}^{-A/\theta}\,\mathrm{d}t = k\delta t\,\mathrm{e}^{-2A/[\theta(t+\delta t)+\theta(t)]} \quad \text{(approximately)}$$

or

$$w(t+\delta t) = w(t)\,\mathrm{e}^{2E}. \tag{9}$$

It is easy to see that (8) and (9) reduce to the same for E small, for

$$\mathrm{e}^{2E} = 1 + 2E + \mathrm{O}\big(E^2\big),$$

and also

$$\frac{1+E}{1-E} = 1 + 2E + \mathrm{O}\big(E^2\big).$$

For E large, however, (9) is a better approximation to the original equation (2) than (8). The form (9) was suggested to the authors by Prof. D. R. Hartree.

Now the equations (5) and (8) or (5) and (9) are a pair of ordinary differential equations which can be solved either numerically or mechanically to determine $\theta(t+\delta t)$ and $w(t+\delta t)$ as functions of x, given $\theta(t)$ and $w(t)$ as known functions of x. The integration proceeds by a number of successive finite intervals δt, which in practice are taken to be of equal length. The approximate solution of (1) and (2) thus evaluated is a function of δt as well as of x and t, and the true solution is the limit of the approximate one as $\delta t \to 0$.

The nature of the boundary conditions for which this method can be used effectively, and for which the Richardson h^2 extrapolation process [9] can be used to remove the main part of the error in an approximate solution, has been examined by Hartree and Womersley [4].

A set of solutions of (5) and (9) for given values of the constants and for simple forms of $H_1(\theta)$ and $H_2(\theta)$, namely,

$$H_1(\theta) = \alpha - \beta\theta, \qquad H_2(\theta) = 0, \tag{10}$$

has been obtained using the differential analyser. For each step δt the solution must satisfy boundary conditions at both ends of the range in x, that is, at $x = 0$ and $x = 1$. This involves evaluating a number of solutions starting at $x = 0$, with different initial values of $\theta(t+\delta t)$ and by trial and error finding a solution which

satisfies the condition $\partial\theta/\partial x = 0$ at $x = 1$. This may necessitate six or more trial solutions for each step in time; in the particular example under consideration twelve successive steps δt were used and about seventy-two solutions were needed in all. Furthermore, three operators were required to feed into the differential analyser the functions $\theta(t)$, $w(t)$ and E which is a function of $(1/2)[\theta(t+\delta t)+\theta(t)]$, so that the time and labour demanded by this method tend to be prohibitive. On the other hand, only four integrator units of the analyser are needed to handle the problem in this way. Results obtained by this method are discussed in section 10.

3. Method II: replacing the space derivative

Equation (1) may be reduced to a set of ordinary differential equations of the first order by replacing the second space derivative by a finite difference ratio. If θ_{m-1}, θ_m and θ_{m+1} are temperatures at time t, at the points $x = (m-1)\delta x$, $m\delta x$ and $(m+1)\delta x$ respectively, then

$$\theta_{m+1} - 2\theta_m + \theta_{m-1} = (\delta x)^2\left(\frac{\partial^2\theta}{\partial x^2}\right)_m + \frac{1}{12}(\delta x)^4\left(\frac{\partial^4\theta}{\partial x^4}\right)_m + \cdots .$$

Equation (1) may therefore be written approximately as

$$\frac{\partial\theta_m}{\partial t} = \frac{\theta_{m-1} - 2\theta_m + \theta_{m+1}}{(\delta x)^2} - q\frac{\partial w_m}{\partial t} . \tag{11}$$

An equation of this type holds for each point $m\delta x$ in the range $0 < m\delta x < 1$. It is convenient to take δx such that there is a whole number of steps δx in the range, i.e., $1/\delta x = p$ say, an integer. There then exist $p-1$ equations of the type (11) for $0 < m < p$. To take account of the specified conditions at $x = 0$ and 1, these points require special treatment. Consider the equation for the point $x = 0$. Assume that the range in x may be extended one step beyond $x = 0$, i.e., to the point $-\delta x$ so that the equation at $x = 0$ may be written

$$\frac{\partial\theta_0}{\partial t} = \frac{\theta_{-1} - 2\theta_0 + \theta_1}{(\delta x)^2} - q\frac{\partial w_0}{\partial t} . \tag{12}$$

To the same degree of accuracy the surface condition (3) becomes

$$\frac{\theta_{+1} - \theta_{-1}}{2\delta x} = H_1(\theta_0). \tag{13}$$

Elimination of θ_{-1} from (12) and (13) gives

$$\frac{\partial\theta_0}{\partial t} = \frac{2}{(\delta x)^2}(\theta_{+1} - \theta_0) - \frac{2}{\delta x}H_1(\theta_0) - q\frac{\partial w_0}{\partial t} . \tag{14}$$

A similar equation holds at $x = 1$.

The original partial differential equation with appropriate boundary conditions has now been replaced approximately by a set of ordinary equations. With each equation of the type (11) there is associated a second equation of type

$$\frac{\partial w_m}{\partial t} = -k w_m \, \mathrm{e}^{-A/\theta_m}. \tag{15}$$

This method has been used extensively by Hartree and co-workers to obtain approximate solutions of the simple heat-flow equation in one dimension, that is equation (1) without the term $q(\partial w/\partial t)$. In such cases adequate accuracy was obtained by taking only three or four intervals δx and it was possible to use an eight-integrator differential analyser to evaluate solutions of the resulting four or five ordinary equations. It is of interest to examine the difficulties which arise in attempting to extend such a treatment to the equations (1) and (2) of this paper.

For each point $m\delta x$ there is now a pair of equations (11), (15) and treatment of these demands three integrator units of the analyser, and also one input table from which e^{-A/θ_m} is fed in by an operator. Thus with an eight-unit machine, which is the largest machine at present available in Great Britain, only two equations of the above type can be set up simultaneously. This means taking only one step to cover the whole range in x, and so the method cannot be applied directly. It should be emphasized that this is a limitation imposed not by theoretical considerations, but by machine capacity.

Exploratory work using the method in which finite steps in time are taken, showed that for certain values of the constants A, k, q, namely those which correspond to a comparatively rapid evolution of heat at moderate temperatures, the term $q(\partial w/\partial t)$ is important only over a small part of the range in x at any given time. For the rest of the range w remains constant either at its initial value or at zero and the term does not appear. Hence not all the equations (11) contain the term $q(\partial w_m/\partial t)$, and for those which do not only one integrator is needed. In this way it is possible to use the analyser to evaluate a solution having three steps in x, the necessary condition being that only two of the four equations have the heat-generated term present and utilize simultaneously three integrators each. The interconnexions between the various units of the machine are made so that the heat-generated term can be included in successive equations of type (11) as the integration proceeds. Results discussed in section 10 show that the 3-step solution obtained in this way is not a sufficiently accurate solution of equation (1), but clearly a more accurate solution cannot be obtained without the use of a much larger machine. This method therefore, although very powerful for the simple heat-flow equation, is seriously limited by machine capacity in the case of equation (1).

4. Method III: replacing both derivatives by finite difference ratios

The authors have developed a satisfactory method of evaluating solutions of equations (1) and (2) in which derivatives with respect to both x and t are replaced in a

particular way by finite difference ratios; the solution is carried out numerically, and the only limitation on the number of intervals in x is that of time of solution.

The particular finite difference form of (1) used by the authors is given below, equation (16), and is obtained by replacing space and time derivatives at the point $[m\delta x, (n+1/2)\delta t]$ by the usual finite difference ratios:

$$\theta_m(n+1) - \theta_m(n) = \frac{\delta t}{2(\delta x)^2}\big[\theta_{m-1}(n+1) + \theta_{m+1}(n+1) + \theta_{m-1}(n) + \theta_{m+1}(n) - 2\{\theta_m(n+1) + \theta_m(n)\}\big] - q\big[w_m(n+1) - w_m(n)\big],$$

or, on rearranging,

$$\left\{1 + \frac{\delta t}{(\delta x)^2}\right\}\theta_m(n+1) = \frac{\delta t}{2(\delta x)^2}\big[\theta_{m-1}(n+1) + \theta_{m+1}(n+1) + \theta_{m-1}(n) + \theta_{m+1}(n)\big] + \left[1 - \frac{\delta t}{(\delta x)^2}\right]\theta_m(n) - q\big[w_m(n+1) - w_m(n)\big]. \tag{16}$$

Here $\theta_m(n)$ and $w_m(n)$ are the values at the point $(m\delta x, n\delta t)$, which point will in future be referred to as (m, n).

$[w_m(n+1) - w_m(n)]$ is obtained by using relation (9), i.e.,

$$\frac{w_m(n+1)}{w_m(n)} = \mathrm{e}^{2E_m(n+1/2)}, \tag{16a}$$

where

$$E_m(n+1/2) = -\frac{1}{2}k\delta t\,\mathrm{e}^{-2A/[\theta_m(n+1)+\theta_m(n)]}. \tag{16b}$$

e^{2E}, being a function of the mean temperature at $m\delta x$ over the time interval δt, can be tabulated before the process of solution commences, once the interval δt has been decided.

Given $\theta_m(n)$ for all values in the interval $0 \leqslant m \leqslant p$, the equations (16), (16a) and (16b) form a set of simultaneous non-linear equations for $\theta_m(n+1)$ as a function of m. The fact that these equations are simultaneous leads to an iterative method of solution, in some ways similar to the Southwell relaxation process, applied successively at each time $n\delta t$.

Another way of replacing the derivatives by finite differences, described in detail in section 6, leads to equations which formally give each $\theta_m(n+1)$ separately from the others and so avoids the solution of a set of simultaneous equations for each time point. This method, however, suffers from the serious disadvantage that oscillatory errors are likely to arise in the process of solution, and the form (16) above is much preferable in spite of the complication of simultaneous equations. (In practice this is not a serious complication.)

The details of the method of solution of the equations (16) are best illustrated by an example.

5. Example: method III

For convenience in examining the results later in the paper, it is useful to replace the boundary conditions (3) by more definite ones, the method of solution being unaffected. Consider the solution of (1) and (2) subject to boundary conditions

$$\begin{cases} \theta = \text{constant at } t = 0 & \text{for } 0 \leqslant x \leqslant 1, \\ w = \text{constant at } t = 0 & \text{for } 0 \leqslant x \leqslant 1, \\ \dfrac{\partial \theta}{\partial x} = H_1(\theta) & \text{for } t \geqslant 0,\ x = 0, \\ \dfrac{\partial \theta}{\partial x} = 0 & \text{for } t \geqslant 0,\ x = 1. \end{cases} \tag{17}$$

Let the range $0 \leqslant x \leqslant 1$ be divided into eight intervals so that $\delta x = 1/8$, and choose the interval δt such that $\delta t/(\delta x)^2 = 1$. The equations (16) and the two boundary equations at $x = 0$, $x = 1$ then take the particularly simple forms

$$\theta_m(n+1) = \frac{1}{4}\big[\theta_{m-1}(n+1) + \theta_{m-1}(n) + \theta_{m+1}(n+1) + \theta_{m+1}(n)\big] - \frac{1}{2}q\big[w_m(n+1) - w_m(n)\big], \tag{18}$$

$$\theta_0(n+1) = \frac{1}{2}\big[\theta_1(n+1) + \theta_1(n)\big] + \frac{1}{8}H_1\big[\theta_0(n+1) + \theta_0(n)\big] - \frac{1}{2}q\big[w_0(n+1) - w_0(n)\big], \tag{19}$$

$$\theta_8(n+1) = \frac{1}{2}\big[\theta_7(n+1) + \theta_7(n)\big] - \frac{1}{2}q\big[w_8(n+1) - w_8(n)\big]. \tag{20}$$

There are seven equations of the type (18) for $1 \leqslant m \leqslant 7$. Each equation has a subsidiary equation of the form $w_m(n+1)/w_m(n) = e^{2E}$ associated with it.

Before the process of solution commences, tables of H_1, e^{2E} and $(1/2)q(1-e^{2E})$ as functions of θ, are constructed.

Table 1 shows a section of the scheme of computation adopted; it has been divided into three panels arranged vertically for ease in printing. The table is drawn up with a row for each step in t and a column for each step in x. Values of θ are recorded on the left-hand side of the columns, and those of w on the right.

Leaving until later the consideration of the problem of starting the integration from $t = 0$, assume the solution has proceeded as far as the nth step in time, i.e., $t = n\delta t$, and it is desired to evaluate the $(n+1)$th step. The following operations are performed successively:

(a) Estimate values of $\theta_0(n+1)$, $\theta_1(n+1)$, ..., $\theta_8(n+1)$ by inspection of previous differences in each column.

Table 1
Section of computation sheet.

No. of step δt	θ_0	w_0	θ_1	w_1	θ_2	w_2
28	786	0	750	0	715	0.004
29	787	0	752	0	719	0.002
30	788	0	754	0	723	0.000
31	789	0	756	0	727	0.000
No. of step δt	θ_3	w_3	θ_4	w_4	θ_5	w_5
28	684	0.132	649	0.304	618	0.360
29	691	0.094	658	0.276	628	0.350
30	697	0.062	667	0.243	638	0.336
31	703	0.037	676	0.201	647	0.322
No. of step δt	θ_6	w_6	θ_7	w_7	θ_8	w_8
28	593	0.372	578	0.374	573	0.374
29	603	0.369	588	0.373	583	0.373
30	613	0.363	598	0.371	593	0.371
31	623	0.355	608	0.369	602	0.369

(b) Evaluate $q[w_m(n+1) - w_m(n)]/2$ for each column by looking up the value of $q(1 - e^{2E})/2$ corresponding to $[\theta_m(n+1) + \theta_m(n)]/2$ in the subsidiary table, and forming the product $(1/2)w_m(n)(1 - e^{-2E})q$.

(c) Look up $H_1[\theta_0(n+1) + \theta_0(n)]/2$ in the H–θ table.

(d) Evaluate $\theta_0(n+1)$ by substituting known and estimated values in the right-hand side of equation (19).

(e) If this calculated value for $\theta_0(n+1)$ differs from the estimated, adjust H_1 and $q[w_0(n+1) - w_0(n)]/2$ and recalculate $\theta_0(n+1)$. Repeat until the calculated and estimated values agree.

(f) Solve equation (18) for $\theta_1(n+1)$ and iterate if the new $\theta_1(n+1)$ differs from the estimated value, adjusting $q[w_m(n+1) - w_m(n)]/2$ if necessary.

(g) Evaluate $\theta_2(n+1), \ldots, \theta_8(n+1)$ by solving the appropriate equations iteratively, remembering that an alteration in $\theta_m(n+1)$ may necessitate resolving the equations for $\theta_{m-1}(n+1)$ and $\theta_{m+1}(n+1)$.

(h) Calculate $w(n+1)$ for each column by looking up the value of e^{2E} corresponding to $[\theta(n+1) + \theta(n)]/2$ and multiplying it by $w(n)$.

The iteration of a whole line may appear prohibitive, but in practice very little labour is involved and the method has proved quite easy to carry out. In parts of the range where the term involving q is negligible the differences in the θ column are so smooth that it is rarely necessary to solve an equation more than once. Also since a change Δ in $\theta_m(n+1)$ produces a change $(1/4)\Delta$ in $\theta_{m-1}(n+1)$ which affects $\theta_m(n+1)$ itself by only $(1/16)\Delta$, these adjustments are readily made without repeating the full solution of an equation. Even for the δx steps in which there is a contribution from the heat-generated term, it is rarely necessary to iterate more than twice.

It is to be noted that for the δt defined above, i.e., $\delta t/(\delta x)^2 = 1$, a change of 4 in $\theta_m(n+1)$ produces only a change of 1 in $\theta_{m-1}(n+1)$, and so the iterative process converges rapidly. It is clear that the convergence is more rapid for a smaller value of $\delta t/(\delta x)^2$. It is interesting to note that a value of $\delta t/(\delta x)^2$ as large as 4 has been found quite satisfactory in cases where the rate of evolution of heat is fairly slow; with this value a change of 5 in $\theta_m(n+1)$ produces a change of 2 in $\theta_{m-1}(n+1)$ and $\theta_{m+1}(n+1)$.

6. Richardson's "overlapping steps" method

It is useful to state briefly Richardson's method of overlapping time steps and to see what difficulties arise in the use of it.

Consider the solution of the simple heat-conduction equation

$$\frac{\partial \theta}{\partial t} = \frac{\partial^2 \theta}{\partial x^2}. \tag{21}$$

Richardson constructs a table similar to table 1 of the present paper in which there is a line for each step in t and a column for each step in x. Let table 2 be a sample of the main table, taken well away from the boundaries.

Let the entries in the lines $t = (n-1)\delta t$ and $n\delta t$ be known. At the point (m, n), $\partial^2\theta/\partial x^2$ is approximately $[\theta_{m+1}(n) - 2\theta_m(n) + \theta_{m-1}(n)]/(\delta x)^2$, and by equation (21) this is the value of $\partial\theta/\partial t$ at the same point. Richardson replaces the latter by

$$\big[\theta_m(n+1) - \theta_m(n-1)\big]/2\delta t,$$

and obtains

$$\theta_m(n+1) = \theta_m(n-1) + \gamma\big[\theta_{m-1}(n) - 2\theta_m(n) + \theta_{m+1}(n)\big], \tag{22}$$

where

$$\gamma = 2\delta t/(\delta x)^2. \tag{22a}$$

In this way $\theta_m(n+1)$ is obtained without any estimation or iteration, which at first sight is a great advantage.

An obvious disadvantage of the method, as compared with method III above, is that, although it only advances by steps δt, the effective interval for the integration is $2\delta t$ and hence the second-order error term of equation (4) is increased by a factor 4.

A much more serious objection to the method is that rounding-off errors tend to build up and may produce rapidly increasing oscillatory errors as the solution

Table 2

	$(m-1)\delta x$	$m\delta x$	$(m+1)\delta x$
$(n-1)\delta t$	$\theta_{m-1}(n-1)$	$\theta_m(n-1)$	$\theta_{m+1}(n-1)$
$n\delta t$	$\theta_{m-1}(n)$	$\theta_m(n)$	$\theta_{m+1}(n)$
$(n+1)\delta t$	$\theta_{m-1}(n+1)$	$\theta_m(n+1)$	$\theta_{m+1}(n+1)$

Table 3
Error/Δ is shown. As the table is symmetrical about $m\delta x$ only half is shown.

	$(m-5)\delta x$	$(m-4)\delta x$	$(m-3)\delta x$	$(m-2)\delta x$	$(m-1)\delta x$	$m\delta x$
$n\delta t$	–	–	–	–	–	1
$(n+1)\delta t$	–	–	–	–	$+\gamma$	-2γ
$(n+2)\delta t$	–	–	–	γ^2	$-4\gamma^2$	$1+6\gamma^2$
$(n+3)\delta t$	–	–	γ^3	$-6\gamma^3$	$[2\gamma+15\gamma^3]$	$-[4\gamma+20\gamma^3]$
$(n+4)\delta t$	–	γ^4	$-8\gamma^4$	$[3\gamma^2+28\gamma^4]$	$-[12\gamma^2+56\gamma^4]$	$[1+18\gamma^2+70\gamma^4]$
$(n+5)\delta t$	γ^5	$-10\gamma^5$	$[4\gamma^3+45\gamma^5]$	$-[24\gamma^3+12\gamma^5]$	$[3\gamma+60\gamma^3+210\gamma^5]$	$-[6\gamma+80\gamma^3+252\gamma^5]$

progresses. The cause of this is clear. Suppose a small positive error Δ arises in $\theta_m(n)$, i.e., $\theta_m(n)$ is too large by an amount Δ. Then from equation (22) $\theta_m(n+1)$ will be too small by an amount $2\gamma\Delta$ and $\theta_m(n+2)$ will be too large by an amount $(1+6\gamma^2)\Delta$. The way in which errors build up is illustrated in table 3, in which an error Δ is supposed to arise in $\theta_m(n)$. It is clear that the error in $\theta_m(n+s)$ builds up as s increases, however small γ is. (It is significant to note here that method III was satisfactorily used with a value of γ as large as 8.)

The error after a given number of steps clearly decreases with γ decreasing, but the error in a definite total time T may not do so; for if the reduction in γ is due to a decrease in δt more steps will be required to cover the range T, and the increase in error due to this may more than counteract the decrease due to a smaller γ. If, on the other hand, the reduction in γ is effected by an increase in δx, i.e., fewer steps in x, the error in the solution of equation (22) will be less, but this equation will be a poorer approximation to the exact equation (21).

An alternative way of examining the accumulation of errors in the case of Richardson's process was proposed to the authors by Prof. D. R. Hartree, following a suggestion by Prof. J. von Neumann. As this treatment can also be applied to method III it will now be outlined.

7. Analytical treatment of the building up of errors

This treatment is simplest in the case of equation (21), where the term containing q is absent. As equation (21) is linear, the error $\Delta\theta$, to which θ is subject, must satisfy the same finite difference form of (21) as does θ. For simplicity the surface boundary condition, θ a specified function of t, is taken, so that the boundary conditions for $\Delta\theta$ may be written

$$\begin{cases} \Delta\theta = 0 & \text{at } x = 0,\ x = 2, \\ \Delta\theta \text{ symmetrical} & \text{about } x = 1. \end{cases}$$

Taking $2P$ intervals across the block, the equation (22) for $\Delta\theta$ has an exact solution of the form

$$\Delta\theta_m(n) = \sum_{j=1}^{P} f_j(n\delta t) \sin\left[(2j-1)\pi m\delta x/2\right], \tag{23}$$

where $f_j(n\delta t)$ is independent of x. The form of this function f_j depends upon the particular finite difference form of (21) used.

(*a*) *Richardson's method*

From (23)

$$\Delta\theta_{m+1}(n) - 2\Delta\theta_m(n) + \Delta\theta_{m-1}(n) = -2\sum f_j(n\delta t)\sin\frac{(2j-1)\pi m\delta x}{2}\left(1-\cos\frac{(2j-1)\pi\delta x}{2}\right).$$

Substituting this in (22), taking a single component of the sum, and dividing through by the factor $\sin(2j-1)\pi m\delta x/2$ gives

$$f_j\big[(n+1)\delta t\big] - f_j\big[(n-1)\delta t\big] = -2\gamma f_j(n\delta t)\left(1-\cos\frac{(2j-1)\pi\delta x}{2}\right). \tag{24}$$

The general solution of (24) is

$$f_j(n\delta t) = A_j\,\mathrm{e}^{nk_1\delta t} + B_j(-1)^n\,\mathrm{e}^{-nk_1\delta t}, \tag{25}$$

where k_1 is given by

$$\sinh(k_1\delta t) = -\gamma\left(1-\cos\frac{\pi j\delta x}{2}\right). \tag{26}$$

From (26) k_1 is real and negative, and so the term in the expression for f_j which alternates in sign in successive t steps, increases exponentially in magnitude. This is true for each j. The rate of increase in amplitude of the oscillating term is different for different modes (k_1 being a function of j); however these modes are superimposed to give $\Delta\theta$, that is, whatever the coefficients A_j, B_j, the resulting $\Delta\theta$ must oscillate with increasing amplitude for large enough n. This is true however small γ is. Furthermore, the aggregate error over a given time range T is roughly independent of δt for, from (26)

$$nk_1\delta t = (T/\delta t)\sinh^{-1}\big[\{2\delta t/(\delta x)^2\}\big(1-\cos\big[(2j-1)\pi\delta x/2\big]\big)\big]$$

which, for small γ, is independent of δt.

(*b*) *Method III*

$\Delta\theta$ now satisfies equation (16) with $q = 0$, that is

$$(1+\gamma/2)\Delta\theta_m(n+1) = (\gamma/4)\big[\Delta\theta_{m-1}(n+1) + \Delta\theta_{m+1}(n+1) + \Delta\theta_{m-1}(n) + \Delta\theta_{m+1}(n)\big] + (1-\gamma/2)\Delta\theta_m(n).$$

Each component of $\Delta\theta$ therefore satisfies

$$\left(1+\frac{\gamma}{2}\right)f_j(n+1)\sin\frac{j\pi m\delta x}{2} = \frac{\gamma}{4}\big[f_j(n+1)+f_j(n)\big]\left[2\sin\frac{j\pi m\delta x}{2}\cos\frac{j\pi\delta x}{2}\right] + f_j(n)\left(1-\frac{\gamma}{2}\right)\sin\frac{j\pi m\delta x}{2},$$

Table 4

	$(m-2)\delta x$	$(m-1)\delta x$	$m\delta x$	$(m+1)\delta x$	$(m+2)\delta x$
$(n-3)\delta t$	–	–	×	–	–
$(n-2)\delta t$	–	–	×	–	–
$(n-1)\delta t$	–	–	×	–	–
$n\delta t$	×	×	×	×	×
$(n+1)\delta t$	–	–	×(P)	–	–

from which it follows that

$$f_j(n+1)/f_j(n) < 1 \quad \text{for all } \gamma \text{ and } j.$$

Since this is true for all j, $\Delta\theta$ must decrease as n increases, i.e., any error tends to disappear. If γ is very large an oscillatory error which only disappears very slowly may arise.

This treatment thus confirms the conclusion arrived at empirically, that errors tend to be damped out when method III is used.

8. Methods reported by the American Applied Mathematics Panel [1]

The main method of section II of the A.M.P. report is similar to the above using finite differences in both directions; terms up to the fourth order are taken into account in the differentiation formulae by using sets of points as indicated by × in table 4 to derive the value of θ at the point P, $[m\delta x, (n+1)\delta t]$.

This makes the formula giving θ at P very cumbersome; also the method would seem liable to the same defect as Richardson's in that errors may tend to build up.

An alternative scheme for the solution of the finite difference equations, analogous to the Adams–Bashforth method [6] is outlined in the A.M.P. report. It involves an iterative process at every step, but is not used by the A.M.P., since not only are the formulae to be evaluated very elaborate but also many iterations are required.

The other main method described in this report (section I) is completely different and does not use finite difference approximations. The method is based upon the formal expression of the solution of (1) as an integral equation [7]; this integral equation is then solved by a method of successive approximations. In the case of boundary conditions (3) above, where surface temperature is not constant, the method is impracticable on account of the extreme complexity of the formal expression for the solution. Its use would seem to be restricted to the special case in which the surface temperature is held constant.

9. Formal solutions in special cases

To avoid starting numerical integration at $t = 0$ and for the purposes of testing the accuracy of the step by step solutions, formal solutions of the equation $\partial^2\theta/\partial x^2 =$

$\partial\theta/\partial t$ subject to appropriate boundary conditions have been developed for (1) a semi-infinite slab, (2) a finite slab, heated symmetrically.

The boundary conditions for these two cases are tabulated below, (27) and (29). The solutions were obtained by the method of Laplace transforms and only the results need be quoted here.

(1) Semi-infinite slab

Boundary conditions:

$$\begin{cases} \theta = 0 \text{ at } t = 0 & \text{for } x > 0, \\ \dfrac{\partial\theta}{\partial x} = -\alpha + \beta\theta \text{ at } x = 0 & \text{for } t \geqslant 0, \\ \dfrac{\partial\theta}{\partial x} \to 0 \text{ as } x \to \infty & \text{for } t \geqslant 0. \end{cases} \tag{27}$$

Solution

$$\theta = \frac{\alpha}{\beta}\left[1 - \mathrm{e}^{\beta x + \beta^2 t}\,\mathrm{erfc}\left(\frac{x}{2\sqrt{t}} + \beta\sqrt{t}\right) - \mathrm{erf}\frac{x}{2\sqrt{t}}\right]. \tag{28}$$

(2) *Finite slab*

Boundary conditions:

$$\begin{cases} \theta = 0 \text{ at } t = 0 & \text{for } -1 < x < +1, \\ \dfrac{\partial\theta}{\partial x} = -\alpha + \beta\theta \text{ at } x = -1 & \text{for } t \geqslant 0, \\ \dfrac{\partial\theta}{\partial x} = \alpha - \beta\theta \text{ at } x = +1 & \text{for } t \geqslant 0. \end{cases} \tag{29}$$

(Here the solution was developed in the form of a series suitable for use at small values of t; only the first two terms of this series will be given.)

Solution:

$$\theta = \frac{\alpha}{\beta}\left[\left\{1 - \mathrm{e}^{\beta(1-x)+\beta^2 t}\mathrm{erfc}\left(\frac{1-x}{2\sqrt{t}} + \beta\sqrt{t}\right) - \mathrm{erf}\frac{1-x}{2\sqrt{t}}\right\}\right.$$
$$\left. + \left\{1 - \mathrm{e}^{\beta(1+x)+\beta^2 t}\mathrm{erfc}\left(\frac{1+x}{2\sqrt{t}} + \beta\sqrt{t}\right) - \mathrm{erf}\frac{1+x}{2\sqrt{t}}\right\}\right]. \tag{30}$$

The first term gives the main contribution to the heat flow from the surface $x = +1$ and the second from $x = -1$. For t and $(1 - |x|)$ small, this solution is for practical purposes the same as solution (28) referring to a semi-infinite slab; physically this means that at small t no appreciable amount of heat flowing from one surface has reached a point in the vicinity of the second surface.

Table 5
Comparison of results obtained by method III with formal solution.

$1+x$	$t = 5\delta t$		$t = 20\delta t$	
	θ (method III)	θ (formal)	θ (method III)	θ (formal)
0	459	458	587	586
0.125	283	281	468	466
0.25	156	156	361	359
0.375	76	75	269	269
0.500	33	32	194	196
0.625	12	11	138	137
0.750	4	3	98	98
0.875	1	1	75	77
1.000	0	0	66	68

From (28) it will be seen that $\partial\theta/\partial t$ at $x = 0$ is infinite at $t = 0$ (for small t, $\theta_0 \sim \beta\sqrt{t}$). Consequently it is inadvisable to start any method, in which $\partial\theta/\partial t$ is replaced by a finite difference ratio, from $t = 0$. In the physical problem actually treated, the term due to evolution of heat is negligible until the temperature has risen considerably from its initial value, so that in the neighbourhood of $t = 0$, the equation to be solved is simply $\partial^2\theta/\partial x^2 = \partial\theta/\partial t$; the solution of the full equation may therefore be started at some convenient value of $t > 0$ with values calculated from solution (28).

(3) Accuracy of the numerical method III

To examine the accuracy of the step by step process described in section 5, it was used to evaluate a solution of equation (21) subject to conditions (29); this was then compared with the formal solution of equation (21) for the same values of α and β, namely $\alpha = 3618$, $\beta = 4.44$. In the numerical solution 8 steps were taken between $x = 0$ and 1, so that $\delta x = 1/8$ and the time interval was such that $\delta t/(\delta x)^2 = 1/2$. In table 5 comparison between the two solutions at two values of t is shown.

Although only three figures were carried in the computation, the largest difference between the finite step solution and the formal solution is two in the last figure. This accuracy is quite adequate for most practical purposes. It is interesting to note that using method III, the computation of a single line with $\delta x = 1/8$ takes under 10 min which is considerably quicker than evaluation of the formal solution, for the same number of points.

(Using Richardson's method with the above values of δx and δt, and error of order $(2\gamma)^{20}$, i.e., 2^{20} or say 10^6 in the last figure kept, could be expected after 20 steps in time.)

10. Discussion of results in two particular cases

This paper is concerned with methods of evaluating solutions rather than with physical applications of the methods. However, the number of steps needed in x and t is so

Table 6
θ_0 = surface temperature of block.

	Example I (2 cm block)	Example II (1 cm block)
A	22,500	16,580
q	532	261
k	7.23×10^{17}	1.62×10^{11}
$H_1(\theta)$	$0.90(\theta_0 - 1400)$	$1.1(\theta_0 - 1400) + 0.253\{(\theta_0/100)^4 - 1920\}$

closely related to the nature of each particular problem that it is most convenient to discuss the effect of interval size on solutions by reference to a specific example.

The equations relating to a parallel-faced slab of wood, heated symmetrically on each face by a flame, reduce to (1) and (2) with suitable choice of variables. Equation (2) describes the rate at which the wood decomposes into charcoal and volatile substances; this decomposition is an exothermic reaction and gives rise to the second term on the right-hand side of (1). A reaction zone is established at the wood surface and moves inwards leaving charcoal behind it. (The physical aspects of this problem are discussed in detail in a separate paper [2].)

It is to be expected that the high derivatives of θ will be most important near the wood surface at the start of the heating, i.e., when the flame is applied, and later in that part of the wood which is then decomposing. For a given external supply of heat, the behaviour of the solution near the wood surface ($x = 0$) for small t, is independent of the slab thickness and clearly a given number of steps in the whole thickness will give a better representation of surface behaviour in a thin block than in a thick one. Furthermore, a slow rate of decomposition in the reaction zone will have less local effect on the temperature gradient than a rapid decomposition. These general considerations suggest that a thin block with comparatively slow chemical reaction will present a more favourable case for finite step methods (i.e., fewer steps will be required for a given accuracy) than a thick block with rapid reaction. Solutions for these two extreme types of conditions have been evaluated for various sizes of steps in x and t and the results are described below. The values of the various constants and the form adopted for $H_1(\theta)$ in the two examples are shown in table 6.

In example I, $H_1(\theta)$, the surface heat transfer function, is based upon Newton's law of heating; in all the early work on this problem this law was assumed to give an adequate representation of the transfer of heat from the flame to the surface. Later, as a result of more serious consideration of the surface transfer combined with new experimental data [2], the form of $H_1(\theta)$ was modified to that used in example II. With this new law, heat is transferred more rapidly at the beginning and more slowly later; transfer ceases when the surface temperature is about 800° K as $H_1(\theta)$ vanishes at about this value.

Example I. 2 cm block with very rapid reaction rate

Figure 1 shows the variation of the surface, central and halfway to the centre ($x = 0,\ 1/2,\ 1$) temperatures with time as calculated by method I, i.e., by taking finite steps in time and integrating with respect to x by the differential analyser.

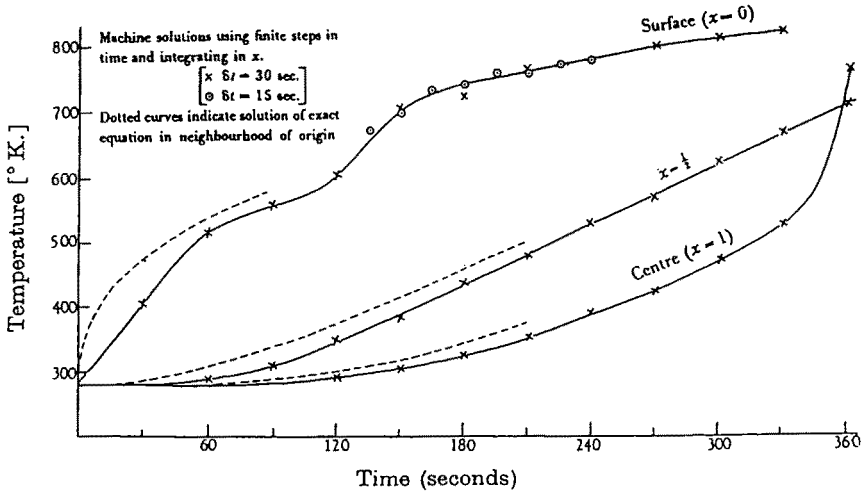

Figure 1. Example I: temperature–time curves for $x = 0,\ 1/2,\ 1$.

For the main evaluation, steps of 30 sec were used. In the region 120–240 sec, the surface temperature oscillates, suggesting that 30 sec steps are too big in this region. Values using $\delta t = 15$ sec are also shown in this diagram; the oscillation although reduced is still present, and it is clear that even smaller steps are required to define the curve accurately when the surface layers are decomposing. No further solutions were obtained in this way mainly because the time taken was prohibitive (see table 7).

It is to be noted that the machine solutions start at $t = 0$ and so the infinite time gradient at this point is replaced by a finite difference ratio. The effect of this is seen by comparing the full and dotted curves. The latter are thought to be a fairly accurate solution of the exact equation; they are started by numerical evaluation of the formal solution (28) and then continued by method III; they end at the point where 8- and 12-step solutions (see figures 2 and 3) begin to diverge significantly. The error introduced at $t = 0$ appears to cause the machine solutions using finite steps in t to lag behind the true solution over almost the whole range in x and t.

Figure 2 shows the surface temperature–time relation, calculated by dividing the range $0 < x < 1$ into 3, 8 and 12 steps respectively and for part of the time range a solution for 48 steps is given. In the case of the 3-step solution the integration was carried out by the differential analyser (method II). The other solutions were obtained by method III.

It will be seen that the general shape of the surface temperature curve as defined by the 3-step solution is quite different from the corresponding curve of figure 1. These were the first two solutions obtained and at that stage of the work, their lack of agreement was very puzzling. It was not obvious whether the peaks of figure 2 were a direct result of taking finite steps in x and would disappear in the true solution of equation (1) or whether the peaks were real but were smoothed out in figure 1 by taking finite steps in t. It was this difficulty that led to the development of method III. It will be seen that the peaks become less prominent as more steps in x are taken and

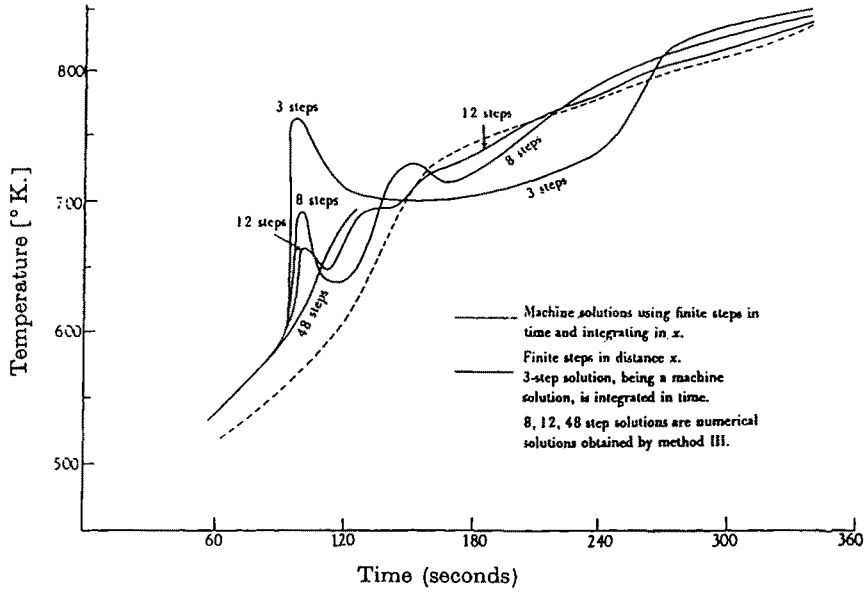

Figure 2. Example I: surface temperature–time curves obtained by various methods.

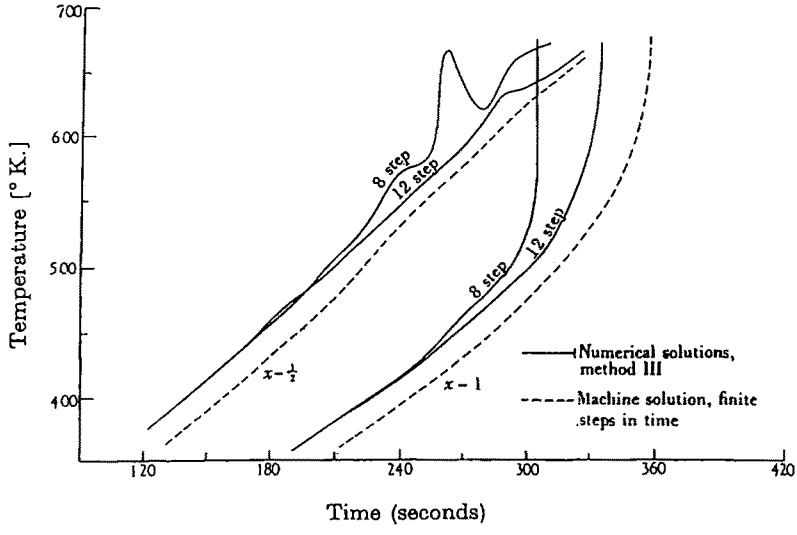

Figure 3. Example I: temperature–time curves for $x = 1/2$ and $x = 1$.

have entirely disappeared in the 48-step solution. It is clear therefore that the peaks are spurious, being a result of taking too few steps in x.

In the critical region $90 < t < 120$ sec, the surface temperature for the 48-step solution is in fairly good agreement with that obtained by method I (shown in figure 1) when allowance is made for the lag of the latter behind the true solution. This 48-step solution is taken to define the true solution in this region. For $t > 4.5$ min all

solutions, even including the 3-step, tend to the same curve which suggests that this is the true surface temperature.

In figure 3 temperature–time curves are shown for $x = 1/2$ and $x = 1$ derived by 8- and 12-step solutions respectively. The solution obtained by taking finite steps in time is also shown. There is a spurious peak in the 8-step solution when the wood in the region of $x = 1/2$ is decomposing and subsidiary peaks when decomposition is occurring in the steps centred on $x = 3/8$ and $5/8$. In the 12-step solution the peaks have almost disappeared and this solution is in good agreement with the solution using finite steps in time when allowance for the time lag of the latter is made.

The 8- and 12-step central temperatures are in good agreement until the centre of the block begins to decompose, then the 12-step lags behind the 8-step solution. The discrepancy in this region is not surprising as the temperature is very difficult to determine precisely once the exothermic reaction has started, on account of the rapidity with which this reaction proceeds.

Example II. 1 cm block with moderate rate of reaction

Figure 4 shows the corresponding 8- and 12-step solutions for a case where the block is thinner and the reaction slower. The two solutions are now in good agreement throughout the range in x and t; there is no trace of the spurious peaks which were so conspicuous in the surface temperature curves for both 8 and 12 steps in x, in example I. The variation of w with time was almost identical in the two solutions as is illustrated in figure 5 for the surface layer.

In the particular problem for which the methods described above were investigated, a quantity whose behaviour was ultimately required was

$$\frac{\mathrm{d}W}{\mathrm{d}t} = \int_0^1 \frac{\partial w}{\partial t}\,\mathrm{d}x.$$

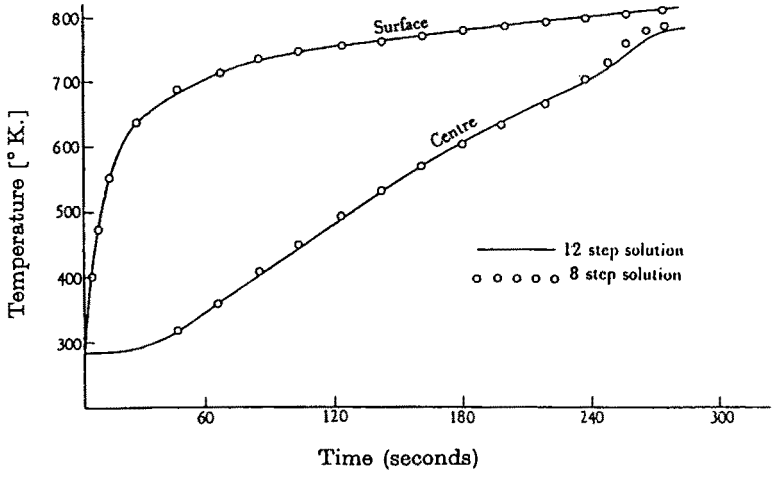

Figure 4. Example II: comparison of 8- and 12-step numerical solutions.

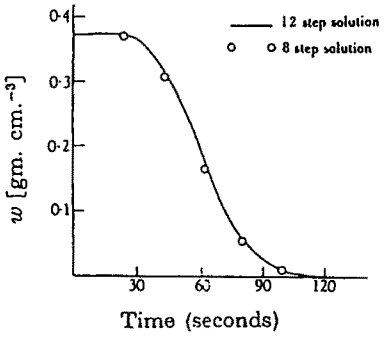

Figure 5. Example II: w-t at surface.

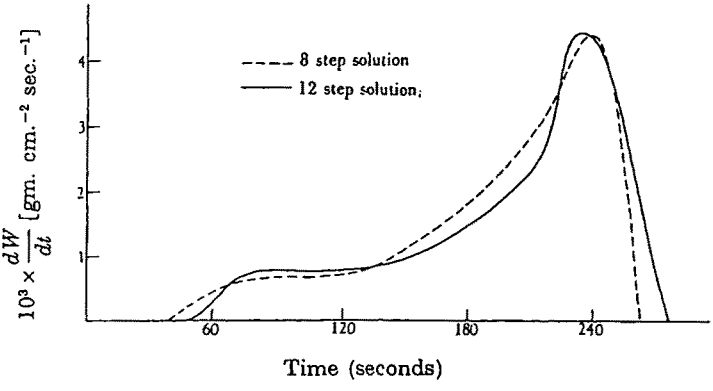

Figure 6. Example II: dW/dt for 8- and 12-step solutions.

The reasons for the importance of this quantity are not relevant here, but it is of interest to note that satisfactory agreement in dW/dt was obtained from the 8- and 12-step solutions in example II (see figure 6). In example I, on account of the rapidity of the reaction and the consequent narrowness of the reaction zone, fewer than 12 steps in the range $0 < x < 1$ were insufficient to define dW/dt.

11. Conclusion

From the comparison of θ, w and dW/dt for 8- and 12-step solutions, it is evident that an 8-step solution defines these quantities adequately throughout the range in x and t, in the case of example II.

For example I, where the reaction is much more rapid, more steps are needed to define θ and w at any point of the slab in the time range during which the reaction is occurring there; outside this time range an 8-step solution gives a fairly good approximation to the temperature.

A great deal of exploratory work has been undertaken on the effect of variations in the function $H_1(\theta)$ and the constants A, k and q, intermediate between those corresponding to examples I and II above. For this purpose method III, using 8 steps

Table 7

Method		No. of operators required	Approximate time for 1 complete solution
I. Finite steps in t; Integrate in x	Differential analyser	3	2 weeks
II. 3 steps in x; Integrate in t	Differential analyser	2	3–4 h
III. Finite steps in x and t			
(a) 8 steps in x	Numerical	1	7–8 h
(b) 12 steps in x	Numerical	1	10–12 h

in x, has proved a most valuable tool. In this context it is significant to compare the approximate time of evaluation of a single solution by the three main methods described in this report (table 7).

These times refer to the actual process of solution only. They do not include time spent in preliminaries such as setting up the machine and constructing input curves in the case of methods I and II, and constructing the table of e^{2E} as a function of θ in the case of method III.

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