Stable Explicit Difference Approximations to Parabolic Partial Differential Equations

SHEAN-LIN LIU

Mobil Research and Development Corporation, Princeton, New Jersey

A finite-difference method is developed for numerical solution of parabolic partial differential equations. This technique is explicit and stable. It is shown that the present method is more accurate and faster, in terms of computer time, than the Crank-Nicholson method. A method of handling nonlinear problems is also presented. Two examples are given to illustrate the present technique. The first problem is a linear diffusion equation. The second problem deals with two simultaneous nonlinear parabolic partial differential equations with Neumann boundary conditions describing the steady state of a packed-bed catalytic reactor with radial mixing.

In the study of problems of mass and heat diffusion, one frequently desires to solve numerically parabolic partial differential equations. As is well known, parabolic partial differential equations can be solved by classical implicit and explicit finite-difference methods (*2, 3*). Generally, implicit methods involve less stringent stability and convergence restrictions than explicit methods. Although one can take a large time increment by implicit methods, one has to solve simultaneous algebraic equations at each time level. Therefore, implicit methods are not convenient for numerical solution of problems involving nonlinear terms of simultaneous partial differential equations. Saul'yev (*9*) developed a stable explicit method which has the best features of the implicit and explicit methods. It avoids solving simultaneous equations but retains stability for time steps. Unfortunately, with the same space and time increments, Saul'yev's method is less accurate than the classical implicit method (*4, 9*). The classical implicit method is also known as the Crank-Nicholson method.

The purpose of the present paper is to present a finite-difference scheme based upon Saul'yev's asymmetrical method. The present numerical scheme is proved to be stable using von Neumann's method (*7*). It is shown that the present method is more accurate and faster than the classical implicit method. A technique of handling nonlinear problems is presented. Two examples are given for illustration. The first problem is a linear diffusion equation. The results are compared with those obtained by analytical solution and by various numerical methods.

The second problem deals with two simultaneous nonlinear parabolic partial differential equations describing the steady state of a catalytic packed-bed reactor with radial mixing. For nonlinear problems the present method would likely be faster than the iterative implicit method used by Liu and Amundson (*10*) and the quasilinearization method used by Lee (*11*) because these latter methods require solutions of simultaneously algebraic equations several times (depending upon the number of iterations) at each time step.

DIFFERENCE SCHEMES

To demonstrate our numerical method, let us consider the following partial differential equation describing diffusion or heat conduction in a slab:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \tag{1}$$

where u is the dimensionless concentration or temperature, t is the dimensionless time and x is the distance. The boundary conditions are

$$u(0, t) = 1$$

$$u(1, t) = 1 \tag{2}$$

and the initial condition is

$$u(x, 0) = 0 \tag{3}$$

Let $u(m, n)$ denote the value of u at position $m\Delta x$ and time $n\Delta t$ (see Figure 1). Then the partial derivatives in Equation (1) can be replaced by the following finite approximations:

$$\frac{\partial u}{\partial t} = \frac{1}{\Delta t}[u(m, n+1) - u(m, n)] \tag{4a}$$

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{\Delta x}\left[\left.\frac{\partial u}{\partial x}\right|_{m+1,n} - \left.\frac{\partial u}{\partial x}\right|_{m,n+1}\right]$$

$$= \frac{1}{2\overline{\Delta x}^2}[u(m-1, n) - 4u(m, n) + 3u(m+1, n)$$

$$- u(m-2, n+1) + 4u(m-1, n+1) - 3u(m, n+1)] \tag{4b}$$

In Equation (*4b*), the backward three-point formula is used for the approximation of the first derivative $\partial u/\partial x$. If Equations (*4a*) and (*4b*) are substituted into Equation (1), the following finite difference equation can be obtained.

$$(3 + 2\beta^{-1})u(m, n+1) = u(m-1, n)$$

$$+ (2\beta^{-1} - 4)u(m, n) + 3u(m+1, n) - u(m-2, n+1)$$

$$+ 4u(m-1, n+1) \quad \text{for} \quad m = 1, \ldots, M-1 \tag{5a}$$

where

$$\beta = \frac{\Delta t}{\overline{\Delta x}^2} \tag{5b}$$

For $m = 1$ in Equation (*5a*), one must know the value of $u(-1, n+1)$, an imaginary point placed one Δx space beyond the boundary. One can use Saul'yev's difference scheme for $\partial^2 u/\partial x^2|_{0,n+1}$.

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{\overline{\Delta x}^2}[u(1, n) - u(0, n) - u(0, n+1)$$

$$+ u(-1, n+1)] \tag{5c}$$

Substituting Equations (*4a*) and (*5c*) into Equation (1) and solving for $u(-1, n+1)$, one obtains

$$u(-1, n+1) = (1 + \beta^{-1})u(0, n+1)$$

$$+ (1 - \beta^{-1})u(0, n) - u(1, n) \tag{5d}$$

One can avoid using the imaginary point $u(-1, n+1)$ by calculating $u(1, n+1)$ with a difference equation similar to Equation (*5c*) and then using Equation (*5a*)

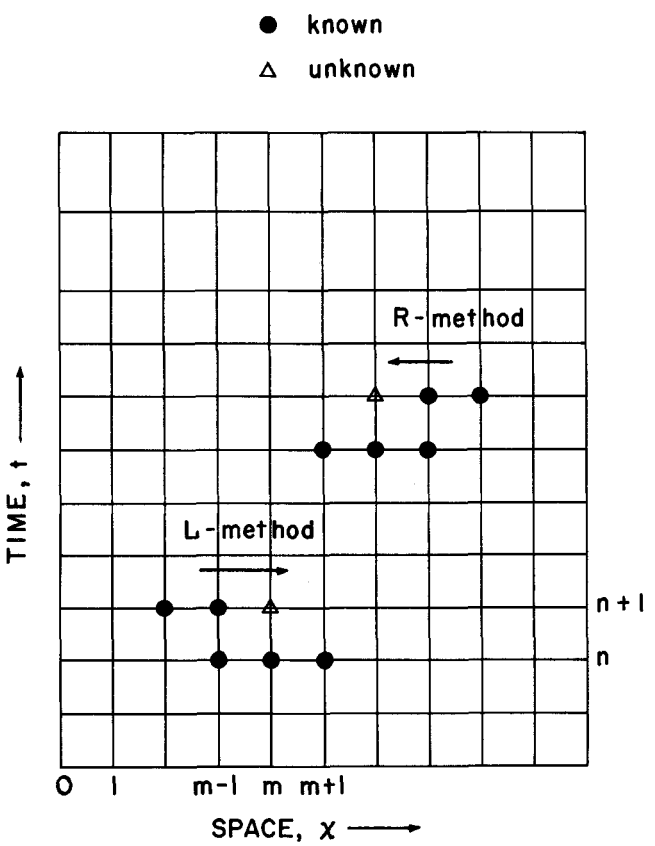

Fig. 1. Mesh spacing for parabolic partial differential equations.

starting $m = 2$. However, from actual computations on Equation (1), it was found that the method with $u(-1, n+1)$ was more accurate than the method without $u(-1, n+1)$. Therefore, Equation (5*d*) was used in this paper.

It is seen from Equation (5*a*) that, knowing all values at the nth time step, the values at the $(n+1)$ step can be calculated explicitly (that is, wthout solving simultaneous algebraic equations at each time step as required by implicit methods). Hereafter the above technique will be referred to as the *L method*, which means that integration proceeds from left to right, starting with $m = 1$. This is displayed in Figure 1.

The integration of Equation (1) can be also performed from right to left by the so-called "R-method," using the following finite approximation for $\partial^2 u/\partial x^2$.

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{\Delta x}\left[\left.\frac{\partial u}{\partial x}\right|_{m,n+1} - \left.\frac{\partial u}{\partial x}\right|_{m-1,n}\right]$$

$$= \frac{1}{2\overline{\Delta x}^2}[-u(m+2,n+1)+4u(m+1,n+1) - 3u(m,n+1)+u(m+1,n)-4u(m,n) + 3u(m-1,n)] \quad (6a)$$

In the above equation, the forward 3-point formula is used for the approximation of the first derivative $\partial u/\partial x$. The resulting finite approximation to Equation (1) becomes

$$(3+2\beta^{-1})u(m,n+1) = -u(m+2,n+1) + 4u(m+1,n+1)+(2\beta^{-1}-4)u(m,n) + u(m+1,n)+3u(m-1,n) \quad (6b)$$

$$\text{for } m = M-1,\quad M-2,\ldots,2$$

For $m = M-1$ in Equation (6*b*), one can use the following scheme to calculate the value of $u(M+1, n+1)$, an imaginary point outside the boundary.

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{\Delta x^2}[u(M+1,n+1)-u(M,n+1) - u(M,n)+u(M-1,n)] \quad (6c)$$

By substituting Equations (4*a*) for $m = M$ and (6*c*) into Equation (1) and solving for $u(M+1, n+1)$, one obtains

$$u(M+1,n+1) = (1+\beta^{-1})u(M,n+1) + (1-\beta^{-1})u(m,n) - u(M-1,n) \quad (6d)$$

As shown by Saul'yev (9) and Larkin (4), alternating and average methods can be used to reduce the truncation errors. For the average method, Equations (5*a*) and (6*b*) are used at the same time level, and the average values are taken as the desired values. For the alternating method, Equations (5*a*) and (6*b*) are used alternately. For example, one can use Equation (5*a*) at the even time levels and Equation (6*b*) at the odd ones.

STABILITY

Stability requirements imply that errors committed in the numerical solution of the difference equation do not grow exponentially. A detailed analysis of stability of finite-difference approximations for partial differential equations, known as the *von Neumann method*, was presented by O'Brien, Hyman, and Kaplan (7). Let us examine the stability of the difference equation for the L-method, Equation (5*a*). Assume that there exists an error $\epsilon_{m,n}$ at each mesh point (m, n). Following the von Neumann method, because ϵ obeys both the difference Equation (5*a*) and the boundary conditions (2), the set of errors $\epsilon_{m,n}$ at the nth time level may be expanded in a finite trigonometric series

$$\epsilon_{m,n} = \sum_{h=1}^{M-1} A_{h,n}\, e^{i\alpha_h x} \quad (7a)$$

where $\alpha_h = h\pi/M\Delta x$. Stability implies that the absolute value of the ratio $A_{h,n+1}/A_{h,n}$ must be less or equal to unity for all h. Substituting Equation (7*a*) into Equation (5*a*) and examining each term in the series separately, one obtains:

$$\frac{A_{h,n+1}}{A_{h,n}} = \frac{(\beta-4)+e^{-i\alpha_h\Delta x}+3e^{i\alpha_h\Delta x}}{(\beta+3)+e^{-2i\alpha_h\Delta x}-4e^{-i\alpha_h\Delta x}} = \frac{N}{D} \quad (7b)$$

It is clear that

$$\left|\frac{A_{h,n+1}}{A_{h,n}}\right| \leq 1$$

provided

$$|D|^2 - |N|^2 \geq 1 \quad (7c)$$

Expanding N and D in Equation (7*b*), it follows

$$|D|^2 - |N|^2 = 4\beta(4-\sin^2\alpha_h\Delta x) \quad (7d)$$

This obviously satisfies condition (7*c*) for all $\beta(=\Delta t/\overline{\Delta x}^2) > 0$. Therefore, the difference scheme for the R-method given by Equation (5*a*) is stable for positive Δt of any magnitude. By a similar analysis on Equation (6*b*), one can show that the R-method is also stable for positive Δt.

NONLINEAR SIMULTANEOUS EQUATIONS

Let us consider a general system of N simultaneous nonlinear parabolic partial differential equations:

$$a_i \frac{\partial y_i}{\partial t} = b_i \frac{\partial^2 y_i}{\partial x^2} + c_i \frac{\partial y_i}{\partial x} + F_i \quad i = 1, 2, \ldots, N \quad (8a)$$

where a_i, b_i, c_i, and F_i may be nonlinear functions of y_i, x, and t. For nonlinear equations such as (8a), based upon our experience on actual computations, the following average method is more stable and accurate than the alternating method, because the average method has the nature of a predictor-corrector method. Two derivatives in Equation (8a), $\partial y_i/\partial t$ and $\partial^2 y_i/\partial x^2$, can be replaced by the difference approximations described in the second section, and $\partial y_i/\partial x$ by the following formulas:
For the L-method

$$\frac{\partial y_i}{\partial x} = \tfrac{1}{2}\left[\left.\frac{\partial y_i}{\partial x}\right|_{m,n+1} + \left.\frac{\partial y_i}{\partial x}\right|_{m,n}\right]$$

$$= \frac{1}{4\overline{\Delta x}}\left[y_i(m-2, n+1) - 4y_i(m-1, n+1)\right.$$

$$\left. + 3y_i(m, n+1) + y_i(m+1, n) - y_i(m-1, n)\right] \quad (8b)$$

and for the R-method

$$\frac{\partial y_i}{\partial x} = \frac{1}{4\Delta x}\left[-y_i(m+2, n+1) + 4y_i(m+1, n+1)\right.$$

$$\left. - 3y_i(m, n+1) + y_i(m+1, n) - y_i(m-1, n)\right] \quad (8c)$$

The resulting finite approximation to Equation (8a) for the L-method becomes

$$d_{i,1}y_i(m, n+1) = d_{i,2}(m, n)y_i(m-1, n)$$
$$+ d_{i,3}(m, n)y_i(m, n) + d_{i,4}(m, n)y_i(m+1, n)$$
$$+ d_{i,5}(m, n)y_i(m-2, n+1)$$
$$+ d_{i,6}(m, n)y_i(m-1, n+1) + d_{i,7}(m, n)$$
$$\text{for } i = 1, 2, \ldots, N$$
$$m = 1, \ldots, M-1 \quad (8d)$$

where

$$d_{i,1}(m, n) = 4a_i(m, n)\beta^{-1} + 6b_i(m, n) - 3c_i(m, n)\Delta x$$
$$d_{i,2}(m, n) = 2b_i(m, n) - c_i(m, n)\Delta x$$
$$d_{i,3}(m, n) = 4a_i(m, n)\beta^{-1} - 8b_i(m, n)$$
$$d_{i,4}(m, n) = 6b_i(m, n) + c_i(m, n)\Delta x$$
$$d_{i,5}(m, n) = -2b_i(m, n) + c_i(m, n)\Delta x$$
$$d_{i,6}(m, n) = 8b_i(m, n) - 4c_i(m, n)\Delta x$$
$$d_{i,7}(m, n) = 4\overline{\Delta x}^2 F_i(m, n) \quad (8e)$$

Knowing the values of y_i at the $(n+1)$ time level from Equation (8d), the values of the nonlinear terms, a_i, b_i, c_i, and F_i, at the $(n+1)$ time level can be calculated. Using these values and the following finite approximation to Equation (8a) for the R-method, one can calculate the improved values of y_i.

$$e_{i,1}(m, n+1)y_i(m, n+1)$$
$$= e_{i,2}(m, n+1)y_i(m+2, n+1)$$
$$+ e_{i,3}(m, n+1)y_i(m+1, n+1)$$
$$+ e_{i,4}(m, n+1)y_i(m+1, n) + e_{i,5}(m, n+1)y_i(m, n)$$
$$+ e_{i,6}(m, n+1)y_i(m-1, n) + e_{i,7}(m, n)$$
$$\text{for } i = 1, \ldots, N$$
$$m = 1, \ldots, M-1 \quad (8f)$$

where

$$e_{i,1} = 4a_i(m, n+1)\beta^{-1} + 6b_i(m, n+1) + 3c_i(m, n+1)\Delta x$$
$$e_{i,2} = -2b_i(m, n+1) - c_i(m, n+1)\Delta x$$
$$e_{i,3} = 8b_i(m, n+1) + 4c_i(m, n+1)\Delta x$$
$$e_{i,4} = 2b_i(m, n+1) + c_i(m, n+1)\Delta x$$
$$e_{i,5} = a_i(m, n+1)4\beta^{-1} - 8b_i(m, n+1)$$
$$e_{i,6} = 6b_i(m, n+1) - c_i(m. n+1)\Delta x$$
$$e_{i,7} = 4\overline{\Delta x}^2 F_i(m, n+1) \quad (8g)$$

As before, the average values of the results obtained by Equations (8b) and (8f) are taken as the desired values of y_i at $t = (n+1)\Delta t$.

NUMERICAL EXAMPLES

Linear Equations

In order to compare the accuracy and computing time of the present scheme with other schemes, let us consider the following diffusion equation.

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \quad (9a)$$

$$u(1, t) = 1, t > 0$$
$$u(x, 0) = 0, 0 \leq x \leq 1 \quad (9b)$$
$$\frac{\partial u}{\partial x} = 0, x = 0$$

Table 1 shows the exact solution and numerical solution by various methods for the points $x = 0.2$, 0.6, and 0.8 at $t = 0.1$. The numerical results are shown by their errors, that is, the difference between the exact solution and the numerical solution. Computing time was recorded from the internal clock of the IBM 7040. The exact solution was obtained from Crank (*1*). The implicit method formulation and the Thomas algorism for solving the resulting simultaneous algebraic equations are described by Lapidus (*3*). Table 2 shows the results at $t = 0.5$. It is seen from Tables 1 and 2 that the present technique is more accurate and faster than the implicit method. Although the present method is a little slower than Saul'yev's method, the former method is more accurate than the latter method.

Figures 2 and 3 are plots of error vs. computing time

TABLE 1.

$t = 0.1$, $\Delta x = 0.05$, $\Delta t = 0.002$

Method	$x =$ 0.2	0.6	0.8	Computing time (sec.)
Analytical	0.080929	0.371439	0.654747	
Implicit	$+1.565 \times 10^{-3}$	-2.268×10^{-3}	-1.689×10^{-3}	1.93
Saul'yev's average	$+6.465 \times 10^{-3}$	-1.779×10^{-3}	-1.892×10^{-3}	0.66
Saul'yev's alternate	$+7.075 \times 10^{-3}$	-2.25×10^{-4}	-4.75×10^{-4}	0.38
Present: average	-1.907×10^{-3}	-2.17×10^{-4}	$+1.44 \times 10^{-4}$	1.00
Present: alternate	-1.729×10^{-3}	$+2.7 \times 10^{-5}$	$+3.45 \times 10^{-4}$	0.50

for various numerical methods using different increments. The results for the method of lines are obtained by Hicks and Wei (5). The error is calculated as 10^8 times the sum of squared deviations from the true solution at $x = 0.2$, 0.4, 0.6, and 0.8. From Figures 2 and 3, it is seen that the results of the present technique are about the same as those of the method of lines with noncentral finite difference approximations.

Nonadiabatic Catalytic Reactor with Radial Mixing

Let us consider a catalytic reactor packed with relatively large catalyst particles in which significant intraparticle mass concentration and temperature gradients may exist. Fluid is introduced into the bed at $x = 0$ and a first-order irreversible chemical reaction, $A \rightarrow B$, takes place on the porous surface of the particle. Then the mass and heat conservation equations for the reactor with radial mixing can be written as (in dimensionless form)

$$\frac{\partial f}{\partial s} = c_1\left[\frac{\partial f}{\partial z^2} + \frac{1}{z}\frac{\partial f}{\partial z}\right] - c_2\eta f \exp\left[-q/y\right] \quad (10a)$$

$$\frac{\partial y}{\partial s} = c_3\left[\frac{\partial^2 y}{\partial z^2} + \frac{1}{z}\frac{\partial y}{\partial z}\right] - c_4\eta f \exp\left[-q/y\right] \quad (10b)$$

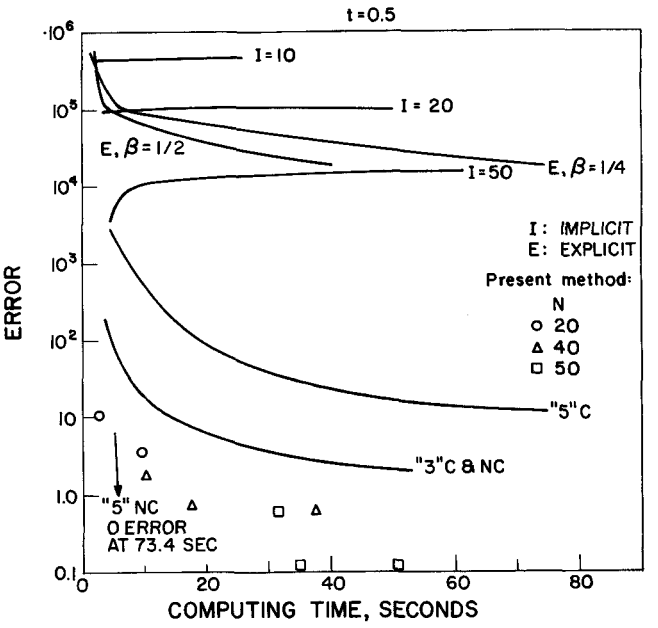

Fig. 3. Error vs. computing time for various numerical methods at $t = 0.5$.

TABLE 2.

$t = 0.5$

Analytical	0.647367	0.782053	0.885416	
Implicit	$+1.767 \times 10^{-2}$	$+8.446 \times 10^{-3}$	$+4.14 \times 10^{-3}$	8.45
Saul'yev's average	$+1.745 \times 10^{-2}$	$+8.35 \times 10^{-3}$	$+4.14 \times 10^{-3}$	4.11
Saul'yev's alternate	$+1.818 \times 10^{-2}$	$+8.81 \times 10^{-3}$	$+4.46 \times 10^{-3}$	2.50
Present: average	$+6.9 \times 10^{-5}$	$+3.3 \times 10^{-5}$	$+1.0 \times 10^{-6}$	5.61
Present: alternative	$+1.52 \times 10^{-4}$	$+9.4 \times 10^{-5}$	$+3.9 \times 10^{-5}$	3.15

The boundary conditions are

$$s = 0;\ f = f_e(z),\ y = y_e(z)$$

$$z = 0;\ \frac{\partial f}{\partial z} = 0,\ \frac{\partial y}{\partial z} = 0 \quad (10c)$$

$$z = 1;\ \frac{\partial f}{\partial z} = 0,\ \overline{u}(y - y_w) = -\frac{k_r}{R_b}\left(\frac{\partial y}{\partial z}\right)_{z=1}$$

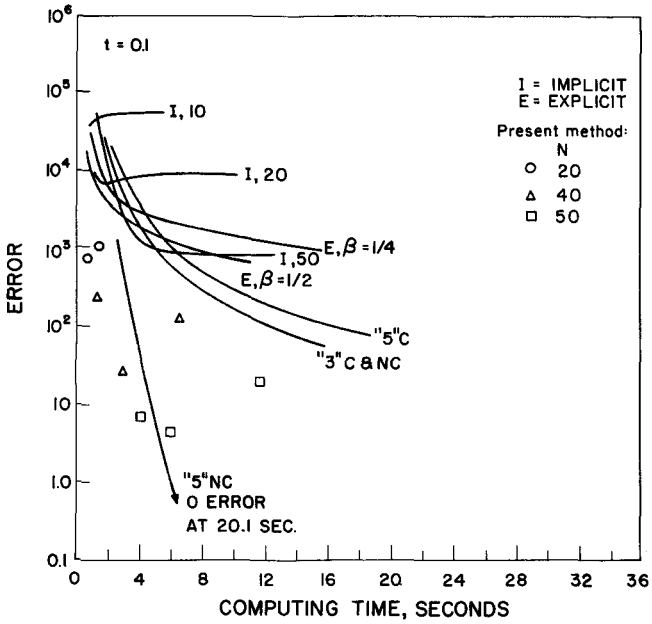

Fig. 2. Error vs. computing time for various numerical methods at $t = 0.1$.

with the following expression for catalyst effectiveness factor η, (6).

If $\alpha > 2.5$ and $\phi < 1.235 - 0.094\,\alpha$

or $\alpha \leq 2.5$ and $\phi < 1.82 - 0.328\,\alpha$

then

$$\eta = \exp\left(0.14\,\phi\,\alpha^{1.6}\right) - 1.0 + \frac{\tanh\phi}{\phi} \quad (10d)$$

For other values of α and ϕ

$$\eta = \exp\left(\alpha/5.0\right)/\phi \quad (10e)$$

In the above equations

$$y = \frac{T}{T_e},\ s = \frac{x}{l},\ f = \frac{c}{c_e},\ z = \frac{r}{R_b}$$

$$\phi = \frac{R}{3}\sqrt{\frac{k_v}{D_s}}$$

$$\alpha = \left[\frac{c(-\Delta H)D_s}{TK_s}\right]\left[\frac{E}{R_J T}\right]$$

$$c_1 = \frac{lD_r}{u_f\delta R_b{}^2},\ c_2 = \frac{(1-\delta)lk_0}{u_f\delta}$$

$$c_3 = \frac{lK_r}{u_f\delta\rho_f c_f R_b{}^2},\ c_4 = \frac{(1-\delta)lc_e(\Delta H)K_r}{u_f\delta c_f\rho_f T_e}$$

where c is the concentration of component A, T is the interstitial fluid temperature, x is the axial variable, r is the radial variable, and y, f, s, and z are the corresponding dimensionless variables. The other variables are de-

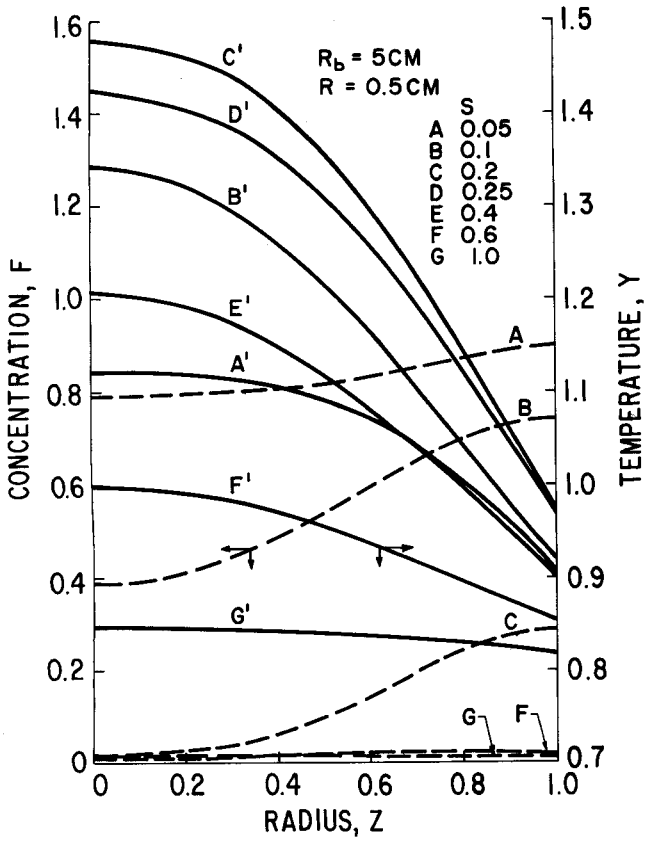

Fig. 4. Radial temperature and concentration profiles in different tube sections for the case of nonadiabatic with radial mixing.

fined in the nomenclature. Equations (10*a*) to (10*b*) are solved by the average method described in the section on nonlinear simultaneous equations. Figure 4 shows radial profiles of temperatures and concentrations in different tube sections, obtained from a calculation using the following numerical values:

$\rho_f = 2.5 \times 10^{-3}$ g./cc.
$c_f = 0.4$ cal./g.
$E = 2.5 \times 10^4$ cal./g. mole
$A_0 = 3 \times 10^7$
$\delta = 0.4$
$(-\Delta H) = 2.0 \times 10^4$ cal./g. mole
$D_s = 4.0 \times 10^{-3}$ sq.cm./sec.
$K_s = 6.0 \times 10^{-4}$ cal./cm. sec. °K.
$u_f = 20$ cm./sec.
$c_e = 2.0 \times 10^{-5}$ g. mole/c.
$T_e = 600$°K.
$R = 0.5$ cm.
$l = 200$ cm.
$R_b = 5$ cm.
$\overline{u} = 10^{-3}$ cal./min.sq.cm. °K.
$T_w = 550$°K.
$N_{pe} = \dfrac{Ru_f}{D_r} = 10$

The calculations showed that $\Delta z = 0.05$ and $\Delta s = 5 \times 10^{-3}$ were satisfactory and the computing time was about 1 min./run on the IBM 7040. Smaller increments showed little improvement in the temperature and concentration profiles. If one uses Liu and Amundson's iterative implicit method (*10*) or Lee's quasilinearization method (*11*) to solve Equations (10*a*) through (11*e*), the computing time will be undoubtedly much longer than 1 min. because at each s level one has to solve iteratively two sets of simultaneous algebraic equations, one for y and the other for f.

NOTATION

A,B = chemical species
A_0 = frequency factor
c = concentration of species A
c_e = influent gas concentration of component A
c_f = specific heat of gas mixtures
D_r = reactor effective radial diffusivity
D_s = particle effective diffusivity
E = activation energy
f = c/c_e, dimensionless concentration of component A
$(-\Delta H)$ = heat of reaction
k_s = intrinsic reaction-rate constant for surface reaction
k_v = $k_s S_v = A_0 \exp(-E/R_g T)$, intrinsic first-order rate coefficient
K_r = reactor effective thermal conductivity
l = reactor length
N_{pe} = Ru_f/D_r, radial Peclet number
R = particle radius
R_b = reactor radius
R_g = gas constant
s = x/l = dimensionless reactor length
S_v = total area of catalyst per unit volume
t = time variable
Δt = time increment
T = gas temperature
T_e = influent gas temperature
T_w = ambient temperature
u = dimensionless temperature or dimensionless concentration in Equation (1)
u_f = average interstitial velocity
$\overline{U}$ = reactor overall heat transfer coefficient
x = space variable
Δx = space increment
y = T/T_e, dimensionless temperature
y_w = T_w/T_e, dimensionless ambient temperature
z = r/R_b, dimensionless reactor radius

Greek Letters

α = $[c(-\Delta H)D_s/TK_s][E/R_g T]$
α_h = $h\pi/M\Delta x$
β = $\Delta t/\overline{\Delta x}^2$
δ = bed void fraction
$\epsilon_{m,n}$ = error at mesh point (m, n)
η = effectiveness factor
ρ_f = density of gas mixture
ϕ = $R/3\sqrt{k_v/D_s}$: Thiele Modulus

LITERATURE CITED

1. Crank, J., "The Mathematics of Diffusion," Oxford Univ. Press, London (1956).
2. Forsythe, G. C., and W. E. Wasow, "Finite Difference Methods for Partial Differential Equations," John Wiley, New York (1960).
3. Lapidus, L., "Digital Computation for Chemical Engineers," McGraw-Hill, New York (1962).
4. Larkin, B. K., *Math. Computation*, 18, 196 (1964).
5. Hicks, J. S., and J. Wei, *J. Assoc. Comput. Machinery*, 14, 549 (July, 1967).
6. Liu, S. L., unpublished work.
7. O'Brien, G. G., M. A. Hyman, and K. Kaplan, *J. Math. Phys.*, 29, 223 (1951).
8. Richmyer, R. D., "Difference Methods for Initial-Value Problems," Interscience, New York (1957).
9. Saul'yev, V. K., "Integration of Equations of Parabolic Type by the Method of Nets," MacMillan, New York, (1964).
10. Liu, S. L., and N. R. Amundson, *Ind. Eng. Chem. Fundamentals*, 1, 200 (1962).
11. Lee, E. S., *Chem. Eng. Sci.*, 21, 143 (1966).

Manuscript received February 1, 1968; revision received April 9, 1968; paper accepted April 11, 1968. Paper presented at AIChE St. Louis meeting.