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but, in the limit of large numbers of particles and low dosage per particle, the effects are the same. This approach would seem to be desirable especially for highly soluble medications. Formulations based on this principle presently exist in crude form; however, quantitative analyses of their design and operation have not been reported.

The required distribution of inert shell thicknesses for a uniform pattern of release times may be easily determined. Because the rate of decrease of particle mass may be equated to the rate of mass transfer to the surrounding fluid, then

$$- d(4\pi r^3/3)/dt \cong k_{xmA} (4\pi r^2) (X_{A0} - X_{A\infty})/(1 - X_{A0}) \tag{7}$$

For constant X_{A0}, and k_{xm} proportional to $r^{-1/2}$

$$dr^3/dt = E\ r^{3/2} \tag{8}$$

where E is a constant. This equation indicates that the time required for complete dissolution of a shell from an outer radius R to an inner radius R_c will be

$$\text{release time} = E' (R^{3/2} - R_c^{3/2}) \tag{9}$$

Assuming that the optimum situation is one in which each capsule carries the same dose, then R_c will be the same for all capsules, and the distribution times will depend only on the distribution of the outer shell radii R, as shown in the above result. For production purposes the easiest way to achieve the desired range of bead sizes (and, therefore, of release times) would probably be to make many single batches of uniformly sized beads and blend the batches. How many different bead sizes would be needed to give a close approach to a continuous-size-distribution is a subject which requires deeper analysis and will not be explored here.

Certainly serious qualifications concerning the desirability, practicality, and feasibility of the administration of medicine by the above methods may be raised. The purpose of this paper has been to give initial insight into the nature and requirements of these approaches. Whether or not these techniques will be adjudged to have great, moderate, or little merit remains to be shown.

NOTATION

A = the medicinal compound being transferred
B = the inert carrier compound
c = total molar concentration of fluid, mole/cc.
d_p = sphere diameter at any arbitrary time, cm.
E, E' = constants
i, j = arbitrary chemical species
k_{xm} = mean mass transfer coefficient from sphere, mole/sq.cm.-sec.
K, K' = constants
n = total number of species present
r = radial coordinate, cm.
R = radius of spheres at start of dissolution, cm.
R_c = inner radius of time capsule shell, cm.
R_s = radius of sphere corresponding to $X_{A0} = X^*_{A0}$
Sc = Schmidt number, dimensionless
t = time, sec.
v = fluid velocity, cm./sec.
W = mass transfer rate, mole/cc.
X_{A0} = mole fraction of A at sphere surface at any time
X^0_{A0} = mole fraction of A at sphere surface at start of dissolution
X^*_{A0} = mole fraction of A at sphere surface corresponding to saturation
$X_{A\infty}$ = mole fraction of A in bulk of fluid stream
ϵ = void fraction in bed of particles, dimensionless
μ = fluid phase viscosity, g./cm.-sec.
ρ = fluid phase density, g./cc.

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A Stable Explicit Method for Simultaneous Quasi-Linear Differential Equations

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Differential equations that are encountered in studies of transport phenomena, such as mass transfer with a chemical reaction (1) and the transfer of heat generated by a temperature sensitive chemical reaction (2), are often of the form

$$\frac{\partial U}{\partial t} = a_0 \frac{\partial^2 U}{\partial x^2} + a_1 \frac{\partial U}{\partial x} + a_2 U \tag{1}$$

and

$$\frac{\partial V}{\partial t} = b_0 \frac{\partial^2 V}{\partial x^2} + b_1 \frac{\partial V}{\partial x} + b_2 V \tag{2}$$

where a_0, a_1, a_2, b_0, b_1, and b_2 may be functions of x, t, U, and V.

The method described for simultaneously solving sets of partial differential equations is not limited to just two differential equations or to two independent variables. For simplicity, the method is described in terms of Equations (1) and (2). Equations of the form of Equations (1) and (2) are not readily solved by analytical methods. They are best solved by finite difference methods.

Implicit, finite difference methods are cumbersome because when they are applied to nonlinear partial differen-

tial equations they usually result in a system of nonlinear algebraic equations. Also, implicit methods become progressively more complicated as the number of simultaneous differential equations are increased.

Explicit finite difference methods are not greatly complicated by the nonlinar portions of the partial differential equations but require small time steps to assure stability.

It is the purpose of this communication to call attention to a stable explicit difference method which has been seemingly overlooked in solutions of engineering problems where it could have been most helpful. This difference method can be extended for the purpose of solving systems of simultaneous, nonlinear partial differential equations. The equations derived in this communication have a combination of simplicity and stability that is not found in previous methods.

PREVIOUS WORK

The central difference approximations for the first-order partial derivatives are, according to DuFort and Frankel (3)

$$\frac{\partial U}{\partial t} = \frac{U_{i,j+1} - U_{i,j-1}}{2\Delta t} \qquad (3)$$

$$\frac{\partial V}{\partial t} = \frac{V_{i,j+1} - V_{i,j-1}}{2\Delta t} \qquad (4)$$

$$\frac{\partial U}{\partial x} = \frac{U_{i+1,j} - U_{i-1,j}}{2\Delta x} \qquad (5)$$

$$\frac{\partial V}{\partial x} = \frac{V_{i+1,j} - V_{i-1,j}}{2\Delta x} \qquad (6)$$

In their study of the solution of one independent, partial differential equation, DuFort and Frankle found that to insure stability the second-order derivatives should be approximated by

$$\frac{\partial^2 U}{\partial x^2} = \frac{U_{i+1,j} - U_{i,j+1} - U_{i,j-1} + U_{i-1,j}}{(\Delta x)^2} \qquad (7)$$

$$\frac{\partial^2 V}{\partial x^2} = \frac{V_{i+1,j} - V_{i,j+1} - V_{i,j-1} + V_{i-1,j}}{(\Delta x)^2} \qquad (8)$$

DuFort and Frankel suggested that their method could be used to solve a single partial differential equation of the form of either Equation (1) or (2) by using the space averaged value of the dependent variable.

PURPOSE OF THIS WORK

We will show that the DuFort and Frankel method is valid for not only a single equation but also for simultaneous partial differential equations if, instead of space-averaged variables, time-averaged variables are used as follows: For Equation (1)

$$U = \frac{U_{i,j+1} + U_{i,j-1}}{2} \qquad (9a)$$

$$V = V_{i,j} \qquad (9b)$$

and in Equation (2)

$$U = U_{i,j} \qquad (10a)$$

$$V = \frac{V_{i,j+1} + V_{i,j-1}}{2} \qquad (10b)$$

Equations (9) and (10) are a combination of the finite difference approximations suggested by DuFort and Frankel and the forward difference methods. This particular combination is necessary to maintain the stability of the method and at the same time to keep the resulting algebraic equations in their simplest form.

By substituting the above relations into Equations (1) and (2), the following is obtained:

$$U_{i,j+1} = \left[\frac{1 - a_0\, s + a_2\, \Delta t}{1 + a_0\, s - a_2\, \Delta t} \right] U_{i,j-1}$$

$$+ \left[\frac{a_0\, s + a_1\, p}{1 + a_0\, s - a_2\, \Delta t} \right] U_{i+1,j}$$

$$+ \left[\frac{a_0\, s - a_1\, p}{1 + a_0\, s - a_2\, \Delta t} \right] U_{i-1,j} \qquad (11)$$

and

$$V_{i,j+1} = \left[\frac{1 - b_0\, s + b_2\, \Delta t}{1 + b_0\, s - b_2\, \Delta t} \right] V_{i,j-1}$$

$$+ \left[\frac{b_0\, s + b_1\, p}{1 + b_0\, s - b_2\, \Delta t} \right] V_{i+1,j}$$

$$+ \left[\frac{b_0\, s - b_1\, p}{1 + b_0\, s - b_2\, \Delta t} \right] V_{i-1,j} \qquad (12)$$

where

$$s = \frac{2\, \Delta t}{(\Delta x)^2} \qquad \eta = \frac{\Delta t}{\Delta x} \qquad (13)$$

In order to avoid nonlinearity in the resulting algebraic equations, a_0, a_1, and a_2 should be evaluated by using $V = V_{1,j}$ and either $U = U_{i,j}$ or $U = (U_{i+1,j} + U_{i-1,j})/2$. The terms b_0, b_1, and b_2 should be evaluated by using $U = U_{i,j}$ and either $V = V_{i,j}$ or $V = (V_{i+1,j} + V_{i-1,j})/2$.

DuFort and Frankel have shown that for the linear case the above method was stable for any value of the coefficients in Equations (11) and (12) and thus for any size of time increment. They also suggested without proof that their method could be used for single, nonlinear, partial differential equations. The stability and simplicity of their explicit method, modified to apply to systems of nonlinear, partial differential equations, are dependent upon the particular combination of substitutions given by Equations (9) and (10). An analytical proof of this stability has not been developed, but it shall be shown empirically by the following example.

Example

Consider one directional diffusion in a finite porous slab accompanied by chemical reaction. Assume that all of the resistance to mass transfer is in the slab and that one of the reactants v is soluble only in the phase of interest. If the diffusivities of the two reactants are equal and the initial concentration of the reactant soluble in only one phase (component v) is the same as the surface concentration of the reactant which is soluble in both phases (component u), then the dimensionless equations describing this process are

$$\frac{\partial U}{\partial T} = \frac{\partial^2 U}{\partial X^2} - R \qquad (14)$$

$$\frac{\partial V}{\partial T} = \frac{\partial^2 V}{\partial X^2} - R \qquad (15)$$

where R is the rate of reaction given by

$$R = kUV \qquad (16)$$

with the boundary conditions

at
$$X = 0; \quad U = 1, \quad \frac{\partial V}{\partial X} = 0 \quad (17)$$

at
$$X = 1; \quad \frac{\partial U}{\partial X} = 0, \quad \frac{\partial V}{\partial X} = 0 \quad (18)$$

and the initial conditions

at
$$T = 0; \quad U = 0, \quad V = 1 \quad (19)$$

Because the DuFort and Frankel method requires two previous values, it is necessary to calculate values for U and V at $T = \Delta T$. This was done using the forward difference method (4).

$$U_{1,1} = S'/2 \quad (20a)$$

$$U_{i,1} = 0 \qquad i > 1 \quad (20b)$$

$$V_{0,1} = 1 - K\Delta T \quad (20c)$$

$$V_{i,1} = 1, \qquad i > 0 \quad (20d)$$

and from the boundary condition (17)

$$U_{0,1} = 1 \quad (20e)$$

By substituting the finite difference approximations of Equations (3) through (8) into Equations (14) and (15), one obtains

$$(1 + S') U_{i,j+1} = (1 - S') U_{i,j-1} + S'(U_{i+1,j} + U_{i-1,j}) - 2\Delta T R_{i,j} \quad (21)$$

$$(1 + S') V_{i,j+1} = (1 - S') V_{i,j-1} + S'(V_{i+1,j} + V_{i-1,j}) - 2\Delta T R_{i,j} \quad (22)$$

By applying the finite difference approximations of Equation (5) and (6) to the boundary Equations (17) and (18)

$$V_{-1,j} = V_{+1,j} \quad (23a)$$

$$V_{N+1,j} = V_{N-1,j} \quad (23b)$$

$$U_{N+1,j} = U_{N-1,j} \quad (24a)$$

and for the remaining boundary condition, one obtains from Equation (17)

$$U_{0,j} = 1 \quad (24b)$$

The rate of reaction at each grid point $R_{i,j}$ will be approximated by different finite difference approximations to show why the substitutions of Equations (9) and (10) are preferred. The only substitutions considered for $R_{i,j}$

Fig. 1. Dimensionless surface concentration of component v, $V_{o,j}$ as a function of dimensionless time T using various methods to approximate the nonlinear term.

are those which result in linear, explicit finite difference equations.

The most straightforward approximation for Equation (16) would be

$$R_{i,j} = K U_{i,j} V_{i,j} \quad (25)$$

DuFort and Frankel suggested a space averaged approximation for nonlinear terms. This could lead to the following relation for both Equations (21) and (22)

$$R_{i,j} = \frac{K}{4} (U_{i+1,j} + U_{i-1,j}) (V_{i+1,j} + V_{i-1,j}) \quad (26)$$

Another workable approximation for Equation (21) might be

$$R_{i,j} = \frac{K}{2} (U_{i+1,j} + U_{i-1,j}) V_{i,j} \quad (27a)$$

and for Equation (22)

$$R_{i,j} = \frac{K}{2} U_{i,j} (V_{i+1,j} + V_{i-1,j}) \quad (27b)$$

The approximations in Equations (25), (26), and (27) will be compared with the approximations suggested in this article which lead to

$$R_{i,j} = \frac{K}{2} (U_{i,j+1} + U_{i,j-1}) V_{i,j} \quad (28a)$$

for Equation (21), and

$$R_{i,j} = \frac{K}{2} U_{i,j} (V_{i,j+1} + V_{i,j-1}) \quad (28b)$$

for Equation (22).

The results obtained using the four methods of treating the nonlinear portion of Equations (14) and (15) are shown in Figure 1. The surface concentration of component v seemed to be the point concentration most sensitive to instability and error. The surface concentration of component v, $V_{0,j}$ is plotted as a function of dimensionless time T.

Curve (1) represents the solution of Equations (21) and (22) in which the nonlinear term is approximated by Equation (25). As time increases, this solution oscillates with increasing amplitude about the true solution. This is due to the fact that one of the coefficients in the finite difference equation is negative when the approximation in Equation (25) is used. This causes the solution to be alternately too large and then too small.

Curves (2) and (3) are both based on space-averaged approximations to eliminate the problem of a negative coefficient discussed above. However, curves (2) and (3) both show values of the surface concentration of component v which are too low—and even become negative at the larger dimensionless times shown. This is due to the fact that when the boundary condition $(23a)$ is applied to either Equation (26) or Equation $(27b)$ at the boundary $(i = 0)$, the V value in the reaction term is actually the V value for one space increment away from the boundary. This value of V is always larger than should be used in approximating the reaction term. Thus, too large a number is subtracted in calculating the new value of V at the surface, and so the value of V at the surface is always too small. A secondary effect causes curve (2) to be higher than curve (3). This error is also due to the space-averaging approximation for the nonlinear term. Equations (26) and $(27a)$ are good approximations only if the concentration profile of component u at any given time is nearly linear. However, at small dimensionless times, the concentration profile of component u near the
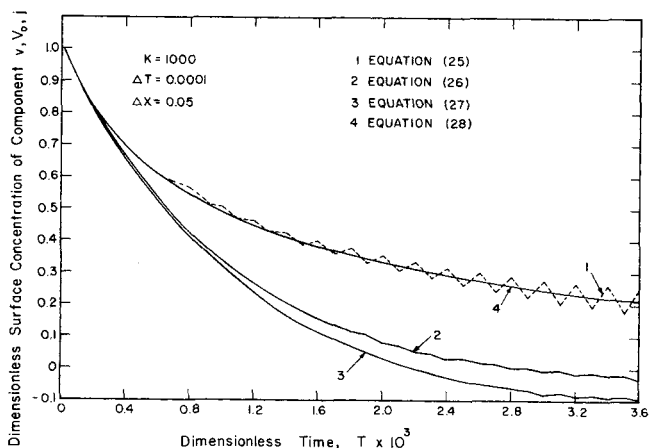
TABLE 1. DIMENSIONLESS CONCENTRATION PROFILE
OF COMPONENT U

(For $K = 1,000$ at $T = 0.01$)

Equation/X	0.05	0.10	0.15	0.20
(25)	−0.2612	0.2952	−0.6836	0.3629
	(0.4870)	(0.1802)	(0.0510)	(0.0118)
(26)	0.4802	0.1508	0.0246	0.0012
	(0.4855)	(0.1778)	(0.0486)	(0.0105)
(27)	0.4332	0.0863	0.0038	−0.0001
	(0.4817)	(0.1738)	(0.0468)	(0.0100)
(28)	0.4900	0.1830	0.0536	0.0134
	(0.4854)	(0.1790)	(0.0502)	(0.0114)

surface is very curved and is concave upward. Thus at any given time step, Equation (26) uses too large a value for the reaction term causing the value of V at one space increment from the boundary to be smaller than it should be. This then partially offsets the error discussed above in calculating the surface value of V for the next time step by using the value of V one space increment from the surface.

Evidence of the inaccuracy of both curve (2) and curve (3) is the fact that both curves predict surface concentrations less than zero. Also the fact that curves (2) and (3) both become broken lines at large dimensionless times indicates slight instability; however, it is not the type of instability which grows as was the case with curve (1). The inaccuracy of the use of either Equation (26) or Equation (27) was less apparent far away from the boundaries. The errors discussed above in using either Equation (26) or Equation (27) could be reduced by reducing the size of the space increments, but very large reductions would be necessary before the solution would become accurate and the additional computing time required makes this impractical. Alternatively, the approximation given by Equation (25) could be imposed at the surface and either Equation (26) or (27) could be used away from the surface. However, this would result in the same type of instability as shown in curve (1). In addition, the concept of space-averaging becomes more complex if there is more than one distance coordinate.

When Equations (28a) and (28b) are substituted into Equations (21) and (22), respectively, the results are analogous to Equations (11) and (12) where $a_0 = b_0 = 1$, $a_1 = b_1 = 0$, $a_2 = -KV_{i,j}$ and $b_2 = -KU_{i,j}$. The results of this finite difference equation are represented by curve (4) in Figure 1. Although curve (1) and curves (2) and (3) can be made to approach curve (4) by reducing the size of the time increments [for curve (1)] and the space increments [for curves (2) and (3)], the factor of considerably increased computing time makes further increment size reduction unacceptable.

By reducing the time increments used for calculating curve (1) to $\Delta T = 0.00001$, the new curve would differ from curve (4) by < 1%. However, this would increase the necessary computing time by a factor of 10.

When the size of the space increment was decreased to $\Delta X = 0.01$, the results corresponding to curve (3) oscillated more than the original curve (3), but the oscillation was within a band of values between the original curve (4) and 25% greater than curve (4). For this example, this reduction of the size of the space increment increased the necessary computing time by a factor of 5. However, for a two-dimensional problem the computing time would be increased by a factor of 25.

To simplify Figure 1, these two revised curves were not shown.

The concentration profile of the component U being

transferred is shown in Table 1 for the dimensionless time equal to 0.01. The first value shown in each case was calculated using the same increment sizes as were used in preparing Figure 1 ($\Delta T = 0.0001$ and $\Delta X = 0.05$).

The second value in Table 1, shown in parentheses, was calculated by reducing the size of both the time and space increments. For Equations (26), (27), and (28), the size of the increments was reduced to $\Delta X = 0.0125$ and $\Delta T = 0.00002$. However, the substitution of Equation (25) did not lead to a stable solution for $\Delta X = 0.0125$ even when the time increment was reduced to $\Delta T = 5 \times 10^{-6}$. Therefore the increment sizes used for the term in parentheses for Equation (25) were $\Delta X = 0.025$ and $\Delta T = 5 \times 10^{-6}$. Even at this reduced time increment size, the value of the concentration of component u oscillated with a range of as much as 0.01. Because of this oscillation, the values given in parentheses in Table 1 for Equation (25) were averaged as

$$(U_{i,j}) = (U_{i,j-1} + 2 U_{i,j} + U_{i,j+1})/4$$

Table 1 confirms the conclusions drawn from Figure 1, and the numbers in parentheses show that the approximations given by Equations (25), (26), and (27) approach the approximation of Equation (28), as the size of the time and space increments is reduced.

In conclusion, the method developed and resulting in Equations (11) and (12) is the only one recommended as an explicit method for simultaneous quasi-linear differential equations. Other methods appear to require much greater computer time.

NOTATION

a_0, a_1, a_2 = arbitrary functions of x, t
b_0, b_1, b_2 = arbitrary functions of x, t, U, and V
C_u = concentration of component u, moles/l.
C_{us} = surface concentration of component u, moles/l.
C_v = concentration of component v, moles/l.
C_{v0} = initial concentration of component v, moles/l.
D = diffusivity of u, cm.^{2}/sec.
i = index of grid point in distance direction, $X/\Delta X$
j = index of grid point in time direction, $T/\Delta T$
K = reaction rate constant, $K_2 L^2 C_{v0}/D$
K_2 = second-order reaction rate constant, liter/moles-sec.
L = length of diffusion path, cm.
n = number of distance grid points, $L/\Delta x$
p = $\Delta t/\Delta x$
R = dimensionless rate of reaction, KUV
s = $2 \Delta t/(\Delta x)^2$
S' = $2 \Delta T/(\Delta X)^2$
t = time, sec.
T = dimensionless time, Dt/L^2
U = any dependent variable, for example, C_u/C_{us}
u = reactant being transferred into reaction phase
V = any dependent variable, for example, C_v/C_{v0}
v = reactant soluble only in the reaction phase
x = distance variable, cm.
X = dimensionless distance, x/L

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