Numerical Solution of Convective Transport Problems

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Convective transport phenomena occur in a variety of physical processes such as the flow of compressible fluids (*1*), chromatographic separation processes (*2*), or the displacement of a resident fluid from a porous medium by a second, invading fluid. This second fluid may be either miscible (*3*) or immiscible (*4*). The object of this paper is to present and apply a method of analyzing the accuracy of finite-difference analogues of the differential systems which characterize these convective transport problems.

Previous analyses of the accuracy or stability of difference approximations (*5, 6*) were limited to second-order equations which contained no first-order convection terms. These methods, therefore, considered only the accuracy of the rate of decay of the sine wave harmonics which comprise the solutions of the problems considered. The present method is general enough to treat equations containing both first- and second-order terms; it considers not only the accuracy of the rate of decay, but also the accuracy of the convective propagation of the appropriate sine-wave harmonics.

Like the previous method of analysis, the current one is limited to consideration of linear differential systems. While it is not certain that the superiority of a difference equation for solving the linear problem will extend to the case of a nonlinear one, experience with the previous methods has shown that application of this type of analysis to linearized versions of nonlinear equations often yields valuable results. At any rate, the use of the current method of analysis to indicate superior approximations for nonlinear equations is hypothesized. The validity of this hypothesis will be determined by experimental computation of cases for which the solution of the nonlinear problem can be obtained by analytic methods. The required computations are under way, and the results will be presented in a second paper.

A one-dimensional differential equation is to be analyzed in this paper, as follows:

$$\left[D\frac{\partial^2 u}{\partial x^2} - V\frac{\partial u}{\partial x} - \frac{\partial u}{\partial t} = 0 \right] \tag{1}$$

D and V are constant. The method of analysis to be described can be generalized to consider multidimensional problems, but this generalization is not within the scope of the present paper.

Equation (1) is the linear form of the more complex Equation (2):

$$\frac{\partial}{\partial x}\left[D(x,t,u)\frac{\partial u}{\partial x} \right] - \frac{\partial}{\partial x}\left[V(x,t,u)\ f(u)\right] - \frac{\partial u}{\partial t} = 0 \tag{2}$$

Many convective transport problems of interest (*1, 4*) are governed by equations of the form of Equation (2). Of special interest are the cases in which the variable D equals zero or is very small. In these cases, the physically meaningful solutions of Equation (2) usually develop discontinuities in the dependent variable u after a finite time (*7*). These discontinuities have been referred to as *shock waves*, or *shock fronts*. Von Neumann and Richtmyer (*1*) have presented an excellent discussion of the severe difficulty of obtaining numerical solutions of Equation (2) in such cases. In this reference, it is proposed that the inherent difficulties may be decreased by using an artificially large value of D in Equation (2). The effect on the numerical solution of introducing this artificially large dispersion coefficient is to smear out the discontinuities so that they are replaced by thin layers in which the dependent variable varies rapidly but continuously. Some dispersion also occurs in regions remote from the discontinuity; but this, as well as the extent of the smearing at the shock front, can be controlled by a proper selection of D and the time and distance intervals used in the numerical calculations.

Hopf (*8*) proved the convergence of the approach proposed by Von Neumann and Richtmyer for a special case, and Olenik (*9* to *11*) extended Hopf's results to the general case. A simpler proof was later found by Vvedenskaya (*12*).

In contrast to the above approach of artificially increasing the dispersion term to achieve a smoother solution, it is possible to propose difference analogues of Equation (2) which even in the complete absence of a dispersion term will smear out the shock front. An especially useful equation of this type is that of Courant, Isaacson, and Rees (*13*). This equation has been studied by Lax (*14, 15*) and applied by Sheldon et al. (*16*) and Stone and Garder (*17*). Douglas (*7*) has demonstrated the convergence of this method for a class of initial value prob-

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lems. The method of Bellman, Cherry, and Wing (*18*), based on the method of characteristics, is closely related to this equation. The equation is

$$\frac{V_{j,n}\,(f_{j,n} - f_{j-1,n})}{\Delta x} + \frac{u_{j,n+1} - u_{j,n}}{\Delta t} = 0 \qquad (3)$$

where $x_j = j\Delta x$, $t_n = n\Delta t$, $u_{j,n} = u(x_j, t_n)$, $V_{j,n} \geqq 0$, Δx = length of distance interval, and Δt = length of time step. The reason that this equation smears the front is that it is only first-order correct in distance and so implicitly includes the dispersion term

$$\frac{V\Delta x}{2}\,\frac{\partial^2 f}{\partial x^2}$$

To avoid this implicit inclusion of dispersion proportional to Δx in the numerical system, it is necessary to resort to second-order correct equations. As an example of the testing of such an equation, the work of Peaceman and Rachford (*3*) is cited. The problem which they considered was a two-dimensional displacement of a fluid from a porous medium by means of a second, miscible fluid. The one-dimensional version of one of the difference analogues used by Peaceman and Rachford is

$$\frac{D}{2}\,\Delta_x^2\,(u_{j,n} + u_{j,n+1}) - \frac{V}{2}\,\Delta_x\,(f_{j,n} + f_{j,n+1}) - \frac{(u_{j,n+1} - u_{j,n})}{\Delta t} = 0 \qquad (4)$$

where

$$\Delta_x^2\, u_{j,n} = \frac{u_{j+1,n} - 2u_{j,n} + u_{j-1,n}}{\Delta x^2}$$

and

$$\Delta_x\, u_{j,n} = \frac{u_{j+1,n} - u_{j-1,n}}{2\Delta x}$$

In the miscible displacement problem, $f \equiv u$. The physical problem under consideration was characterized by a nonzero, but small, value of the dispersion coefficient D. When Peaceman and Rachford attempted to use the above analogue in conjunction with this small value of D, they found that for a practical size of Δx rather severe oscillations in u occurred, especially near the region where u changed rapidly. Of course, decreasing Δx would have decreased the magnitude of these oscillations, as would using an artificially high value of D. Since neither of these solutions was considered practical in this case, Peaceman and Rachford concluded that Equation (4) was not an entirely satisfactory approximation to Equation (2).

The method of analysis used here to evaluate finite-difference approximations will be described in the next section of this paper. In subsequent sections this method will be applied in a systematic manner to determine the better approximations to Equation (1). A comparison of the equations developed in a later section to the two described above in terms of the criteria developed in this paper will be presented. The cyclic use of a set of difference equations will be considered and compared to the more conventional use of a single difference equation at each time level, and there will be a section devoted to a comparison of numerical solutions obtained by the new equations described in this paper and by the two methods described above.

ANALYSIS OF LINEAR CONVECTIVE TRANSPORT

The differential equation to be considered in this analysis of a linear system was given as Equation (1). If u represents a concentration, the first term in Equation (1) represents transport of material by diffusion, the second term represents convective transport, and the third term represents accumulation.

It is readily shown by direct substitution that the function

$$u(x,t) = (\text{constant})\ (e^{-w^2\pi^2 Dt})\ \sin w\pi(x - Vt) \qquad (5)$$

satisfies Equation (1), and thus for appropriate boundary conditions in a finite region of x, Equation (5) represents the solution to Equation (1) for the case in which the initial condition is a sine wave of frequency proportional to w. From Equation (5) it is seen that a sinusoidal variation in u is propagated with a velocity, V, which is independent of the frequency of the sinusoidal oscillation, and the amplitude of the wave is simultaneously decayed at a rate $e^{-w^2\pi^2 Dt}$ which increases greatly as the frequency of the sinusoidal oscillation is increased. This traveling and decaying of a sinusoidal wave represent the effects of convective and diffusive transport, respectively, upon concentration variations. If the initial condition is represented by the sum of a number of sinusoidal variations of different frequencies, or by a Fourier series in the variable x, and if the boundary conditions are appropriate, superposition of terms such as that shown in Equation (5) leads to Equation (6) for the solution of Equation (1):

$$u(x,t) = \sum_{w=1}^{\infty} A_w\ e^{-w^2\pi^2 Dt}\ \sin w\pi(x - Vt) \qquad (6)$$

In this case, the various harmonics of the Fourier series are all propagated at the velocity V, but the high-frequency harmonics are decayed at a greater rate than the low-frequency harmonics.

Let Equation (7) represent a general form of finite-difference approximation to Equation (1):

$$-DL_x^2(u) + VL_x(u) + L_t(u) = 0 \qquad (7)$$

The quantity $L_x^2(u)$ is any finite-difference approximation to $\frac{\partial^2 u}{\partial x^2}$; $L_x(u)$, any approximation of $\frac{\partial u}{\partial x}$; and $L_t(u)$, any approximation to $\frac{\partial u}{\partial t}$. Two time levels are used in those approximations, but any number of spatial points may be involved. As a specific example, the equation tested by Peaceman and Rachford (*3*) employs

$$L_x^2(u) = \frac{\Delta_x^2(u_{j,n+1} + u_{j,n})}{2}$$

$$L_x(u) = \frac{\Delta_x(u_{j,n+1} + u_{j,n})}{2}$$

$$L_t(u) = \frac{1}{\Delta t}\,(u_{j,n+1} - u_{j,n})$$

It can be shown by direct substitution that the function

$$u_{j,n} = \xi^n\, e^{iw\pi j\Delta x} \qquad (8)$$

satisfies Equation (7) and that ξ is a complex constant; that is

$$\xi = \frac{s + ki}{q + ri}$$

where s, k, q, and r are real constants.

It can be shown that s, k, q, and r depend only upon $w\pi\Delta x$, $\frac{V\Delta t}{\Delta x}$, $\frac{D\Delta t}{\Delta x^2}$, and the definition of the finite-difference equation.

Writing ξ in the polar form yields

$$\xi = \rho e^{-iw\pi V\phi\Delta t} \qquad (9)$$

where

$$\rho^2 = \frac{s^2 + k^2}{q^2 + r^2}$$

and

$$\phi = -\frac{1}{w\pi V\Delta t}\left(\text{arc tan}\frac{k}{s} - \text{arc tan}\frac{r}{q}\right)$$

Equations (8) and (9) are combined to yield

$$u_{j,n} = (\text{const})\ \rho^n\ e^{iw\pi(j\Delta x - V\phi n\Delta t)} \qquad (10)$$

For the finite-difference equations considered here, changing the sign of w will leave ρ and ϕ unaltered. (This will be apparent later by inspection of Equations (15) and (16).) Thus, two terms of the form given in Equation (10) written for values of w which are equal in magnitude but opposite in sign will be complex conjugates. By adding such terms with appropriate values of the arbitrary constant, it is readily shown that Equation (11) is also a solution of Equation (7).

$$u_{j,n} = (\text{constant})\ \rho^n \sin w\pi\ (j\Delta x - V\phi n\ \Delta\ t) \quad (11)$$

for appropriate boundary conditions.

Initial conditions other than a single sine wave can be treated by superposition of a finite series of terms similar to Equation (11) with each term involving a different frequency. The result is

$$u_{j,n} = \sum_{w=1}^{J-1} A_w\ \rho^n \sin w\pi(j\Delta x - V\phi n\Delta t) \qquad (12)$$

in which ρ and ϕ will generally vary with w. In Equation (12), J represents the number of segments into which the x axis is divided. Any initial condition at the set of $J - 1$ interior points can be satisfied by suitable selection of the $J - 1$ constants A_w. Equation (12) is valid only for a zero initial value of u at the two extreme grid points.

The similarity of this solution of a difference approximation of Equation (1) to the true solution, Equation (6), is apparent. For a sinusoidal initial condition, both solutions result in a sinusoidal variation which travels downstream as it decays (or is amplified) at a rate dependent upon the frequency of the original variation. However, the true solution propagates any frequency of wave with the stream velocity, V, while the approximate solution propagates it with a velocity $V\phi$, and ϕ generally is not equal to unity. Furthermore, ρ in Equation (12) in general will not be identical with the decay factor, $e^{-w^2\pi^2 D\Delta t}$ of Equation (6). As stated above, both ρ and ϕ depend upon $w\pi\Delta x$, $\frac{V\Delta t}{\Delta x}$, $\frac{D\Delta t}{\Delta x^2}$, and the finite-difference approximation employed.

It is the objective in the following section to evaluate the accuracy of various finite-difference analogues of Equation (1) by comparing the velocity at which each propagates sinusoidal concentration waves of appropriate frequencies with the true convection velocity, V, and by comparing the rates of decay of the waves with the exponential rate shown in Equation (6). Toward this end, it is clear that a perfect equation would yield $\phi \equiv 1$ for all of the $(J - 1)$ frequencies involved. In the special case $D = 0$, it would yield $\rho = 1$; but for $D \geqq 0$, it is desirable that ρ be lower for the high-frequency harmonics than for low-frequency harmonics.

APPLICATION OF ANALYSIS TO A GENERAL DIFFERENCE EQUATION

In this section, the analysis described in the preceding section is used to arrive at an optimum difference analogue of Equation (1) in the sense that both velocity and decay factors are as near as possible to those of the true solution, Equation (6). The procedure used is to write a general difference equation which contains arbitrary weightings of all of the possible approximations to $\frac{\partial u}{\partial x}$ and $\frac{\partial u}{\partial t}$ which involve only three distance positions at two time levels. These weighting factors are then determined to make the velocity factor ϕ as near to unity as possible for all appropriate values of the frequencies w, and to make the decay factor ρ equal to unity when $D = 0$. For greater values of D, ρ should approximate the true decay factor, $e^{-w^2\pi^2 D\Delta t}$; hence it should decrease as w increases.

Although arbitrary weightings of various approximations for $\frac{\partial u}{\partial x}$ and $\frac{\partial u}{\partial t}$ are used in the general equation, a similar approach is not employed for $\frac{\partial^2 u}{\partial x^2}$. Instead, a Crank-Nicholson (*19*) type of approximation is used. There are two reasons for this approach. First, the Crank-Nicholson approximation for second derivatives is of high-order accuracy and has been demonstrated to result in a superior approximation in many problems. Second, in the present study, emphasis is upon problems in which the diffusion term is small relative to the convection term.

The Crank-Nicholson approximation involves three spatial positions at two time levels. The approximations of $\frac{\partial u}{\partial x}$ and $\frac{\partial u}{\partial t}$ appearing in the general difference equation involve these same six points.*

The general finite-difference analogue of Equation (1) to be considered is given as Equation (13):

$$-D\left[\Delta_x^2\frac{(u_{j,n} + u_{j,n+1})}{2}\right] + \frac{V}{\Delta x}\Big[a\ (u_{j+1,n} - u_{j,n}) + \frac{\epsilon}{2}\ (u_{j,n} - u_{j-1,n}) + c\ (u_{j+1,\,n+1} - u_{j,n+1}) + d\ (u_{j,n+1} - u_{j-1,\,n+1})\Big] + \frac{1}{\Delta t}\Big[g\ (u_{j,n+1} - u_{j,n}) + \frac{\theta}{2}\ (u_{j-1,n+1} - u_{j-1,n}) + m\ (u_{j+1,n+1} - u_{j+1,n})\Big] = 0 \qquad (13)$$

The coefficients a, $\frac{\epsilon}{2}$, c, and d are the weighting coefficients used in formulating the finite-difference analogue of the convective transport term in Equation (1). The coefficients g, $\frac{\theta}{2}$ and m are the weighting coefficients used in the finite-difference analogue of the time derivative. These coefficients are subject to the restrictions

$$a + \frac{\epsilon}{2} + c + d = 1$$

$$g + \frac{\theta}{2} + m = 1 \qquad (14)$$

Following the procedure outlined in the foregoing section, it is found that ρ and ϕ are given by Equations (15) and (16):

$$\left\{ g + \beta\left(a - \frac{\epsilon}{2}\right) + \left[\left(\frac{\theta}{2} + m\right) - \beta\left(a - \frac{\epsilon}{2}\right)\right] \cos w\pi\Delta x - \alpha \sin^2\left(\frac{w\pi\Delta x}{2}\right)\right\}^2$$

* Difference equations involving more than these six points have been investigated, and the results have been deposited as document 7652 with the American Documentation Institute, Photoduplication Service, Library of Congress, Washington 25, D. C., and may be obtained for $1.25 for photoprints or for 35-mm. microfilm.

$$\rho^2 = \frac{+\left\{\left[\beta\left(a+\frac{\epsilon}{2}\right)+\left(\frac{\theta}{2}-m\right)\right]\sin(w\pi\Delta x)\right\}^2}{\left\{g+\beta(d-c)+\left[\left(\frac{\theta}{2}+m\right)-\beta(d-c)\right]\cos w\pi\Delta x+\alpha\sin^2\left(\frac{w\pi\Delta x}{2}\right)\right\}^2 + \left\{\left[\beta(c+d)-\left(\frac{\theta}{2}-m\right)\right]\sin(w\pi\Delta x)\right\}^2} \tag{15}$$

$$\phi = \left\{\frac{1}{\beta w\pi\Delta x}\right\}\left\{\text{arc tan}\left[\frac{\left[\beta\left(a+\frac{\epsilon}{2}\right)+\left(\frac{\theta}{2}-m\right)\right]\sin w\pi\Delta x}{g+\beta\left(a-\frac{\epsilon}{2}\right)+\left[\left(\frac{\theta}{2}+m\right)-\beta\left(a-\frac{\epsilon}{2}\right)\right]\cos w\pi\Delta x-\alpha\sin^2\left(\frac{w\pi\Delta x}{2}\right)}\right] + \text{arc tan}\left[\frac{\left[\beta(c+d)-\left(\frac{\theta}{2}-m\right)\right]\sin w\pi\Delta x}{g+\beta(d-c)+\left[\left(\frac{\theta}{2}+m\right)-\beta(d-c)\right]\cos w\pi\Delta x+\alpha\sin^2\left(\frac{w\pi\Delta x}{2}\right)}\right]\right\}$$

where

$$\beta = \frac{V\Delta t}{\Delta x} \text{ and } \alpha = \frac{2D\Delta t}{\Delta x^2} \tag{16}$$

From Equation (15) it is seen that the criterion that ρ approaches unity as D approaches zero can be satisfied for all values of β and $w\pi\Delta x$ by making $c = \frac{\epsilon}{2}$, $a = d$, and $m = \frac{\theta}{2}$. These three restrictions are applied in the remainder of this paper. When they and the restrictions of Equation (14) are imposed, and D is set equal to zero, Equation (16) becomes Equation (17):

$$\phi = \left[\frac{2}{\beta w\pi\Delta x}\right]\left[\text{arc tan}\left\{\frac{\frac{\beta}{2}\sin(w\pi\Delta x)}{1+\left[\beta\left(\frac{1}{2}-\epsilon\right)-\theta\right][1-\cos w\pi\Delta x]}\right\}\right] \tag{17}$$

The two remaining degrees of freedom, represented by ϵ and θ in Equation (17), will be chosen so that the velocity factor, ϕ, is as near as possible to unity over a wide range of the variables β and $w\pi\Delta x$. Unlike the criterion that ρ should approach unity at small values of D, this second criterion cannot be satisfied unconditionally. It will be seen in the discussion to follow that appropriate choices of θ and ϵ can result in a finite-difference analogue which travels the low-frequency harmonics at velocities very close to the true convection velocity, V, but the highest frequency harmonics ($w\pi\Delta x$ approaching π) cannot be given perfect velocities. Furthermore, a small departure of ϕ from unity for the higher frequency harmonics will cause these harmonics to shift completely from the proper phase in a relatively short length of time. Thus, it is the authors' opinion that the most fruitful approach is to concentrate upon making ϕ near unity for as many of the low-frequency harmonics as is possible, and to decay out the high-frequency harmonics by inclusion of a minimal amount of diffusion or by use of a fractional weighting of a difference equation like the Courant-Isaacson-Rees equation. This concept guides the analysis to follow.

While both ϵ and θ affect the value of ϕ in general, only θ is effective in the limit as β approaches zero. When the limit of Equation (17) is taken as β approaches zero, Equation (18) results:

$$\lim_{\beta\to 0} \phi \equiv \phi^* = \frac{\frac{\sin(w\pi\Delta x)}{(w\pi\Delta x)}}{1-\theta[1-\cos(w\pi\Delta x)]} = \frac{1-\frac{(w\pi\Delta x)^2}{3!}+\frac{(w\pi\Delta x)^4}{5!}-\frac{(w\pi\Delta x)^6}{7!}\ldots}{1-\theta\left[\frac{(w\pi\Delta x)^2}{2!}-\frac{(w\pi\Delta x)^4}{4!}+\frac{(w\pi\Delta x)^6}{6!}\ldots\right]} \tag{18}$$

From Equation (18) it is clear that no choice of θ can produce a value of ϕ^* near unity for all harmonics, but the best choice of θ for the low-frequency harmonics is one-third. This choice results in matching the second terms in the Taylor's series expansions in the numerator and in the denominator of the right-hand side of Equation (18).

With $\theta = 1/3$, Equation (17) becomes

$$\phi = \left\{\frac{2}{\beta w\pi\Delta x}\right\}\text{arc tan}\left\{\frac{\frac{\beta}{2}\sin(w\pi\Delta x)}{1+\left[\beta\left(\frac{1}{2}-\epsilon\right)-1/3\right][1-\cos w\pi\Delta x]}\right\} \tag{19}$$

The best value of the one remaining degree of freedom, ϵ, probably is one-half. It can be shown that this choice results in $\frac{\partial\phi}{\partial\beta} = 0$ for $\beta \to 0$ for all values of $w\pi\Delta x$. Thus, the choice of $\theta = 1/3$ insures good values of ϕ for the low-frequency harmonics for $\beta \to 0$, and the choice of $\epsilon = 1/2$ insures that these values of ϕ do not change rapidly for a range of β just above zero. Another value for ϵ which has merit is two-thirds. This choice results in ϕ being identically equal to unity for all values of $w\pi\Delta x$ in the special case when β is equal to unity. Thus, the corresponding finite-difference equation yields a perfect answer even for $D = 0$ when β is equal to unity. Although the objective here is to obtain an equation which is optimum without being restricted to a particular value of β, the choice of $\epsilon = 2/3$ and $\theta = 1/3$ insures that ϕ will be near unity both for values of β near unity and for very small values of β.

In the next two sections the two equations corresponding to $\epsilon = 1/2$, $\theta = 1/3$, and $\epsilon = 2/3$, $\theta = 1/3$ will be compared to each other and to those of the true solution, Equation (6). Similar comparisons will be made for the second-order correct equation tested by Peaceman-Rachford, for which $\theta = 0$ and $\epsilon = 1/2$, and for the first-order correct equation proposed by Courant, Isaacson, and Rees.

DATA ON VELOCITY AND DECAY FACTORS OF SELECTED DIFFERENCE EQUATIONS

In Figures 1 and 2, the velocity factors of four equations are presented. These factors correspond to a zero value of the diffusion coefficient. The four equations are the two derived in the previous section for $\epsilon = 2/3$ and $\epsilon = 1/2$ ($\theta = 1/3$), one for $\epsilon = 1/2$ with $\theta = 0$, and the Courant-Isaacson-Rees equation. Hereafter, the first two equations will be referred to solely by the ϵ value and the third by its θ value in the interest of brevity. In each figure the velocity factor, which ideally should be unity, is shown as a function of the frequency angle $w\pi\Delta x$. This angle varies from zero to π. Figure 1 is for a constant value of β equal to 0.1 and Figure 2 is for $\beta = 0.3$.

While Figures 1 and 2 provide important data for evaluating the relative velocity factors of the four difference equations in question, it is also helpful to know how their respective decay factors compare with those of the true solution to the partial differential equation for small positive values of D. Such data are presented in Figures 3 and 4. Figure 3 presents data for both $\epsilon = 1/2$ and $\theta = 0$, for β equal to zero. The decay factors for these two equations are insensitive to changes in β, as long as $\beta \leq 1$. Figure 4 consists of decay factor plots for the equation with • $= 2/3$, for a series of values of β, for $0 \leq \beta \leq 1$. No comparable plots were made for the Courant-Isaacson-Rees equation, since the decay factors for this equation were so extremely sensitive to the value of β employed and in general bore little relationship to the correct value.

In Figures 3 and 4, decay factors are plotted as a function of the frequency angle. The decay factor obtained from the analytical solution (Equation 6) is shown on each of these figures. All of these data are for $D = 0.001137$, $V = 1$, and $\Delta x = 0.02$.

The final comparison is shown in Figure 5. This figure shows the velocity factors for the equation with $\epsilon = 1/2$ for two different values of the diffusion coefficient, $D = 0$ and $D = 0.001137$. The data in this plot are for $\beta = 0.25$, $V = 1$, and $\Delta x = 0.02$.

COMPARISON OF SELECTED DIFFERENCE EQUATIONS

When the velocity data presented in Figures 1 and 2 for the four different equations are compared, it should be remembered that the equation with $\epsilon = 2/3$ gives perfect velocities when β equals unity. The Courant-Isaacson-Rees equation gives perfect velocities when β equals unity and also when β equals one-half. In the absence of diffusion, the decay factor, ρ, is identically equal to unity for all equations except that of Courant, Isaacson, and Rees. For this equation, ρ is equal to unity only in the special case in which β is equal to unity; otherwise, ρ is less than unity provided that β is less than unity.

The erratic nature of the velocity factors for the Courant-Isaacson-Rees equation is partially, but not completely, revealed by Figures 1 and 2. These figures show that the factors depart significantly from unity and also vary rapidly with changing β. In addition, they are especially ill-behaved for $1 \geq \beta \geq 0.5$; for $\beta = .7$, the velocity factor at an angle of 2.1 radians suddenly changes from a value greater than one to a negative value. In general, the velocity factors for this equation compare unfavorably to those for the equation with $\epsilon = 1/2$ except for the special case of β near 1/2. Behavior of the decay factors for this equation also is erratic and is a poor approximation of the analytic solution as already mentioned.

Both the velocity factors (Figures 1 and 2) and the decay factors (Figure 3) for the equation with $\theta = 0$ are well behaved, but the velocity factors are unity only for a small range of the frequency angle. It may be seen that these velocity factors are always appreciably lower than those for the equation with $\epsilon = 1/2$, which, in turn, are always lower than the desired value of unity.

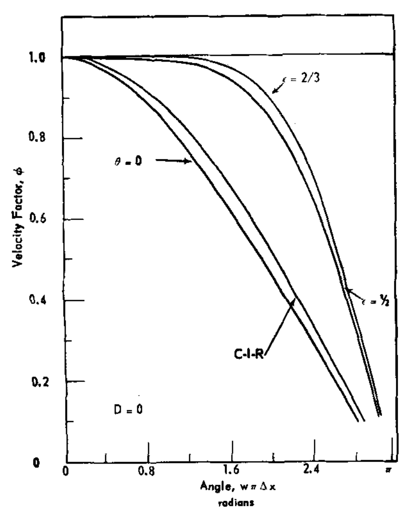

Fig. 1. Velocity factors for $\beta = 0.1$.

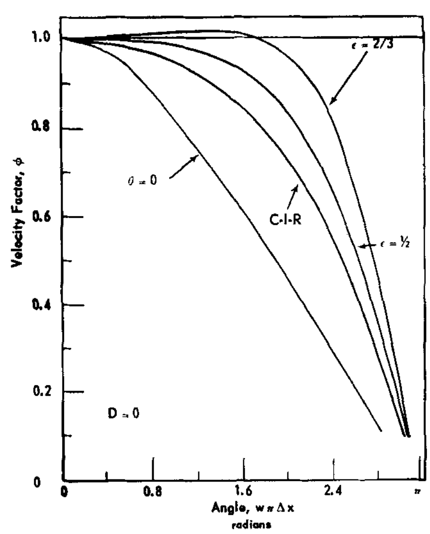

Fig. 2. Velocity factors for $\beta = 0.3$.

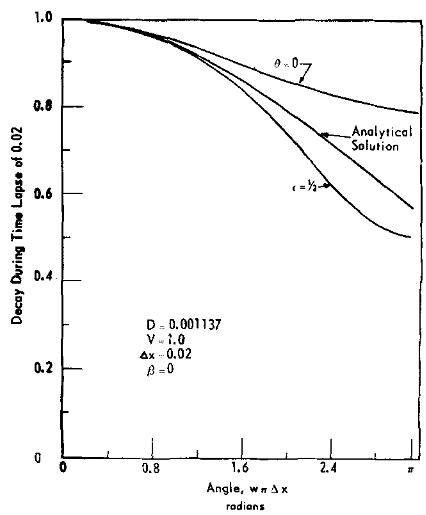

Fig. 3. Harmonic decay for $\epsilon = 1/2$ and $\theta = 0$.

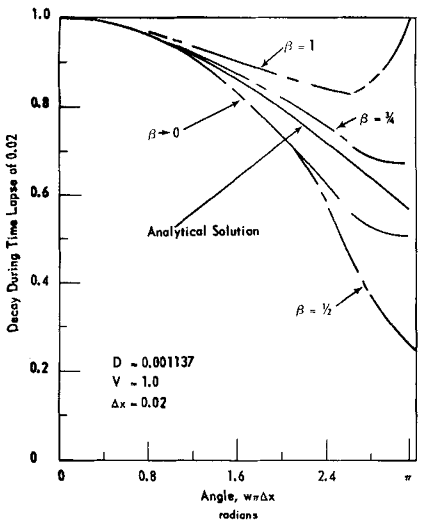

Fig. 4. Harmonic decay for $\epsilon = 2/3$.

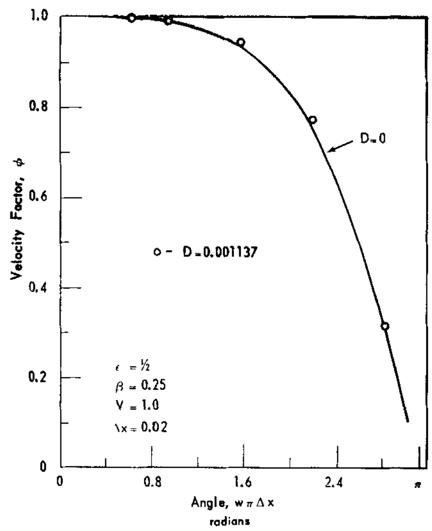

Fig. 5. Effect of diffusion on velocity factors.

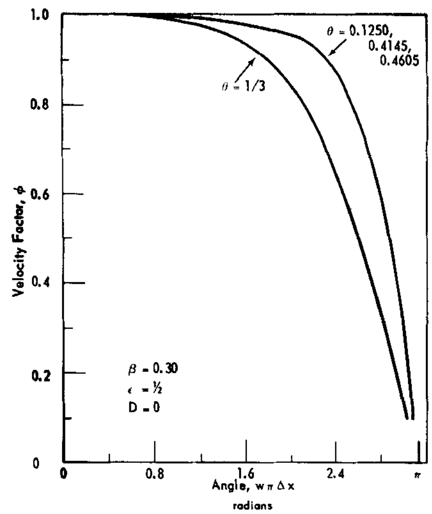

Fig. 6. Velocity factors for cyclical use of three equations.

The above comparisons indicate that the equation with $\epsilon = 1/2$ results in velocity factors superior to those for the equation with $\theta = 0$ or the equation of Courant, Isaacson, and Rees. Comparison of the decay factors for small positive values of D for these three equations (Figure 3) reveals that the decay factors for $\epsilon = 1/2$ are as good as those for $\theta = 0$ and superior to those of the Courant-Isaacson-Rees equation. Thus, it may be concluded that in terms of the criteria developed in the second section of this paper, the equation with $\epsilon = 1/2$ is superior to that for $\theta = 0$ or the Courant-Isaacson-Rees equation.

To compare $\epsilon = 1/2$ to $\epsilon = 2/3$, reference is again made to Figures 1 and 2. As $\beta \to 0$ the velocities corresponding to $\epsilon = 1/2$ and $\epsilon = 2/3$ become identical and correspond to those shown for $\epsilon = 1/2$ on Figure 1. For larger values of β, up to $\beta = 1$, $\epsilon = 2/3$ results in velocity factors superior to those for $\epsilon = 1/2$. This advantage of the equation with $\epsilon = 2/3$ is offset by an undesirable characteristic of its decay factors as shown in Figure 4. For large β, the decay factors for the high-frequency harmonics increase rapidly with changing β for $\epsilon = 2/3$. For $\beta = 1$, the highest frequency does not decay at all, and the intermediate frequencies decay slowly. For $\beta > 1$, the equation becomes unstable. In contrast, the decay factors for the equation with $\epsilon = 1/2$ are relatively insensitive to changes in β; and furthermore, they are a better approximation of the true decay factors (Figures 3 and 4).

This insensitivity of the decay factors to changes in β for the equation with $\epsilon = 1/2$ applies also to the velocity factors. However, the velocity factors for $\epsilon = 2/3$ change continually with β. Variation of the decay and velocity factors with changing β (that is, changing Δt or Δx) represents an undesirable property of the equation since in numerical applications a common procedure is to refine Δt and Δx until further refinement causes no appreciable change in the solution.

The above discussion (and limited computing experience) indicates that in practical application, the solutions corresponding to $\epsilon = 1/2$ and $\epsilon = 2/3$ will differ only slightly in accuracy for values of β well below unity. Since $\epsilon = 1/2$ results in an equation which is easier to apply (it is symmetric with respect to the direction of the velocity) and better behaved (its solution is insensitive to changes in $V\dfrac{\Delta t}{\Delta x}$ over a wide range), this value is probably the sounder choice.

One final point for the equations with $\epsilon = 1/2$ should be noted. This is the effect upon the velocity factor curves of a small positive value of the diffusion coefficient. All previous velocity comparisons have been made for $D = 0$. In Figure 5, a comparison of velocities for $D = 0$ and $D = 0.001137$ is made. It may be seen that the positive value of the diffusion coefficient does not appreciably affect the velocities computed for $D = 0$. This can be shown to be true not only for $\epsilon = 1/2$ but also for $\epsilon = 2/3$. Of course, as D becomes relatively large, this will not be the case; but for large D, the problem is dominated by diffusion, decay is rapid, and velocities of the high-frequency components are no longer of critical importance.

CYCLIC USE OF A SET OF DIFFERENCE EQUATIONS

Consider the use of two distinct difference equations on alternate time steps; let ρ_I and ϕ_I be the decay and velocity factors corresponding to the first finite-difference equation, and ρ_{II} and ϕ_{II} be the factors for the second equation. It is readily shown that Equation (20) applies at the end of two time steps:

$$u_{j,2} = \sum_{w=1}^{J-1} A_w \, \rho_I \, \rho_{II} \sin w\pi \, (j\Delta x - V\,[\phi_I + \phi_{II}]\,\Delta t) \tag{20}$$

It may be seen that Equation (20) is a generalization of Equation (12). In general, if a different finite-difference equation is used for each of the first N time steps, and then the pattern is repeated in cycles of N time steps, the u values at the end of any cycle will be given by Equation (12) with ρ and ϕ replaced by $\overline{\rho}$ and $\overline{\phi}$, respectively, where

$$\overline{\rho} = (\rho_I \, \rho_{II} \, \rho_{III} \cdots \rho_N)^{\frac{1}{N}} \tag{21}$$

$$\overline{\phi} = \frac{(\phi_I + \phi_{II} + \phi_{III} + \cdots \phi_N)}{N} \tag{22}$$

Thus, $\overline{\rho}$ is the geometric mean of the decay factors for the N different finite-difference equations, and $\overline{\phi}$ is the arithmetic mean of the velocity factors.

When $N = 3$ and the three different finite-difference equations all have $\epsilon = 1/2$*, but each has a different value of θ, $\rho = 1$ for all three equations when $D = 0$.

* An alternate approach which utilizes the relationships of Equations (21) and (22) is discussed in the data which has been deposited with the American Documentation Institute. See footnote on page 683.

The three values of θ will be chosen so that the arithmetic mean of the three ϕ values will be close to unity for the low-frequency harmonics. For the limiting case in which $\beta \to 0$, an equation is obtained which is similar to Equation (18), but which expresses the mean of three ϕ values and thus contains three θ values. When this equation is expressed as the ratio of two power series in $(w\pi\Delta x)$, three simultaneous equations may be written to determine the three θ values such that the coefficients of the first three powers of $(w\pi\Delta x)$ are equal in the numerator and the denominator. The resulting values of θ are 0.1250, 0.4145, and 0.4605. The average velocity factor for the cycle of three time steps for $D = 0$, $\beta = 0.30$, and $\epsilon = 1/2$ is shown as a function of the frequency angle in Figure 6. Also shown on this figure is the comparable curve for a constant value of θ equal to one-third.. It is apparent that the use of a cycle of values of θ instead of one constant value enhances the convection properties of finite-difference analogues of Equation (1). Since the θ's all lie between zero and one-half and have an average value of one-third, there is little change in the average decay factors for each cycle as compared to using a constant value of θ equal to one-third.

Even better average velocity factors result from the use of more than three equations in each cycle. In fact, it may be shown that if a number of equations of the order of $\frac{1}{\Delta x}$ are employed in each cycle, and small time steps are used, nearly perfect velocities for all of the harmonic frequencies will result.

COMPARISON OF NUMERICAL SOLUTIONS OBTAINED BY DIFFERENT METHODS

The mode of derivation of the new difference equations presented in this paper is designed to yield equations with optimum harmonic decay and propagation rates when applied to linear problems. In the previous sections it is demonstrated that the new equations are indeed superior in this regard to two commonly used equations, and this demonstration is easily extended to include other difference equations. However, since the degree of improvement in the quality of the numerical solution resulting from the observed differences in the harmonic decay and propagation properties is not readily apparent, a sample problem has been solved numerically. The problem solved was as follows:

$$\begin{aligned} &u_x + u_t = 0 \\ &u = 0 \text{ for } 0 \leq x \leq 1 \text{ at } t = 0 \\ &u = 1 \text{ for } 0 \leq t \leq .2 \text{ at } x = 0 \\ &u = 0 \text{ for } 0.2 < t \text{ at } x = 0 \end{aligned} \qquad (23)$$

Equations (23) correspond to a system of unit length through which a fluid flows with unit velocity. The dependent variable u represents a concentration which is initially zero, but u equals unity on the inflow boundary ($x = 0$) from zero time to time $t = 0.2$. Thereafter, u equals zero on this boundary. To arrive at Equations (23), it has been assumed that concentrations are not affected by diffusion(that is, the diffusion coefficient is zero).

The analytical solution of this problem, after $t = 0.2$, is simply a concentration band of unit height, with a length of 0.2, which is propagated through the column with unit velocity. Elsewhere the concentrations are zero. This solution for $t = 0.4$ is shown as the heavy curve on both Figures 7 and 8. Also shown on Figure 7 are two numerical solutions obtained for 25 grid intervals and $\frac{\Delta t}{\Delta x}$ equal to 0.1042. The light solid line is the result of using the Courant-Isaacson-Rees equation, while the light dashed line is the result of using the equation with $\theta = 0$. These numerical solutions may be compared to the corresponding numerical solution obtained by use of the equations presented in this paper and shown as the light line on Figure 8. This solution was obtained through cyclic use of three equations with $\epsilon = 1/2$, corresponding to θ equal to 0.1250, 0.4145, and 0.4605.

The solution obtained by use of the Courant-Isaacson-Rees equation clearly shows the effect of the implicit diffusion term discussed in an earlier section. Although the peak concentration is at the right location, it has declined from the correct value of 1 to about 0.745. Nonzero concentrations exist from $x = 0$ to $x = 0.65$ instead of from 0.2 to 0.4. This spreading of the concentration band is progressive with time. At later times the maximum concentration is even lower, and the band width even greater.

The solution obtained with the $\theta = 0$ equation is better in some respects than the Courant-Isaacson-Rees equation but worse in others. It shows less diffusion-like spreading of the band; but the maximum concentration is greater than one, and the minimum is significantly less than zero. Also, the low harmonic velocities for this equation, indicated by the analysis of this paper, are revealed by the

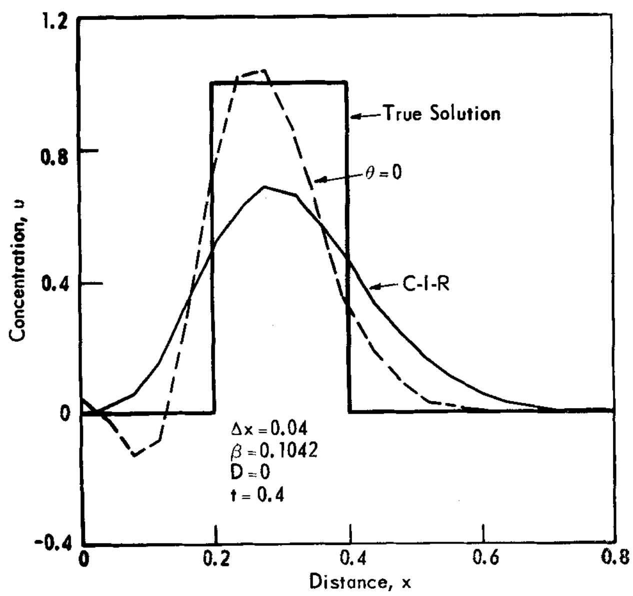

Fig. 7. Numerical solutions of $u_x + u_t = 0$ for $\theta = 0$ and C-I-R equations.

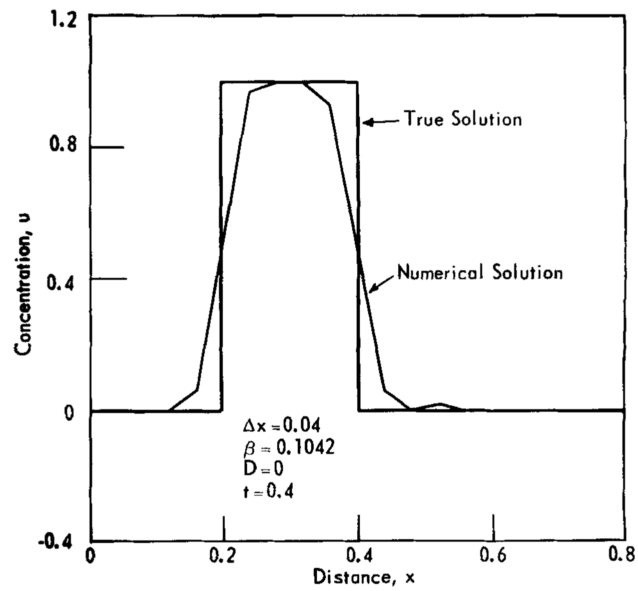

Fig. 8. Numerical solutions of $u_x + u_t = 0$ for $\epsilon = 1/2$, three equations per cycle.

fact that the maximum concentration is behind the center of the true solution band. The oscillation of the numerical solution about the true solution, which is quite pronounced behind the band, would have been greater within the band (around $u = 1$) if the band width of the example problem had been greater. This oscillation is the result of the different velocities of the individual harmonics; thus, after a short time they become out of phase with their correct location.

The solution obtained by the authors' method (Figure 8) does not have the diffused appearance of the Courant-Isaacson-Rees solution, and it minimizes the concentration oscillations and slow propagation velocity observed for the $\theta = 0$ solution. Mild oscillations occur in the solution, but only one of them is large enough to be evident in Figure 8. The solutions for the single equation methods which correspond to $\theta = 1/3$ and $\epsilon = 1/2$ or $2/3$ were obtained but are not shown on Figures 7 and 8. These two solutions were essentially identical, and their quality was between those of the solution shown on Figure 8 and solution for $\theta = 0$. The general shape of these solutions was near that of the solution on Figure 8, but oscillations in the solution were more severe. In fact, each of these solutions showed one positive and one negative deviation of magnitude approaching 0.1.

CONCLUSIONS

A rigorous method has been developed for analyzing the accuracy of finite-difference approximations to the linear differential equations which characterize many convective flow problems. This method has been used to determine for this class of problems approximating equations superior to those heretofore described in the literature. In particular, it has been used to show that the cyclic use of a set of difference equations is superior to the repeated use of a single difference equation for each time step. Since the analysis used to derive the present equations applies only to linear equations, computational studies in which the new equations are applied to nonlinear convective transport problems must be made before their utility for this class of problems can be fully assessed. Suitable computations are currently being made by the authors and will be reported at a later date. However, it may be noted that results to date indicate that the desirable features of solutions obtained by the new equations for linear problems are to a large degree found in solutions of nonlinear problems.

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NOTATION

a, c, d, g, m = arbitrary weighting coefficients in difference equations
f = $f(u)$, a function of u
j = distance index, also used as a subscript $x_j = j\Delta x$
k = a real constant, appearing in definition of ξ
n = time index, appearing in $t_n = n\Delta t$
q = a real constant, appearing in definition of ξ
r = a real constant, appearing in definition of ξ
s = a real constant, appearing in definition of ξ
t = independent variable, time
u = dependent variable, concentration
w = harmonic number
x = independent variable, distance
A_w = a constant dependent upon w
D = dispersion coefficient
J = number of segments into which distance scale is divided
$L_x(u)$ = difference approximation to $\frac{\partial u}{\partial x}$
$L_{x^2}(u)$ = difference approximation to $\frac{\partial^2 u}{\partial x^2}$
$L_t(u)$ = difference approximation to $\frac{\partial u}{\partial t}$
V = velocity

Greek Letters

$\alpha = \frac{2D\Delta t}{\Delta x^2}$
$\beta = \frac{V\Delta t}{\Delta x}$
$\frac{\epsilon}{2}, \frac{\theta}{2}$ = arbitrary weighting coefficients in difference equations
ξ = a complex number, appearing in solution of difference equation
Δt = time step
Δx = distance interval
ρ = decay factor
ϕ = velocity factor
$\phi^* = \lim_{\beta \to 0} \phi$

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