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Edited by
C. A. Brebbia, *Southampton University*
W. G. Gray and G. F. Pinder, *Princeton University*

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SOLUTION OF THE CONVECTION - DIFFUSION EQUATION USING A MOVING COORDINATE SYSTEM

O. K. Jensen, B. A. Finlayson

University of Washington, Seattle, WA 98195

INTRODUCTION

The numerical solution of convection-diffusion problems is notoriously difficult when convection dominates because the equation then assumes a hyperbolic character. The convection-diffusion equation is

$$\frac{\partial c}{\partial t} + \lambda \frac{\partial c}{\partial x} = \frac{\partial^2 c}{\partial x^2} \tag{1}$$

The steady state equation is

$$\lambda \frac{\partial c}{\partial x} = \frac{\partial^2 c}{\partial x^2} \tag{2}$$

with the boundary conditions

$$c = 1 \quad \text{at } x = 0$$
$$c = 0 \quad \text{at } x = 1$$

Clearly at high values of λ the transient equation is hyperbolic in character.

Price, et al. (1966) were the first to recognize that the difficulties are mainly due to the spatial discretization. They proved that a finite difference solution with a central difference approximation will not oscillate provided

$$\lambda\Delta x \leqslant 2. \tag{3}$$

Christie, et al. (1976) analyzed the steady state equations (2) in the manner described below. They solved the difference equations and showed that a Galerkin finite element method with linear basis functions will not oscillate if Eq. (3) is satisfied. For quadratic trial functions, they showed that the solution would oscillate unless

$$\lambda\Delta x \leqslant 4 \tag{4}$$

Other methods have been used for examining the oscillations. Stone, et al. (1963) analyzed the transient equation with a Fourier-series. Gray and Pinder (1976/77), Gresho, et al. (1976), and Runchal (1977) made similar comparisons of finite difference formulations with weighted residual methods. The general conclusion is that weighted residual methods are better. Lantz (1971) and Chaudhari (1971) examined the truncation error of the finite difference method applied to the transient equations. They found that backward schemes introduced artificial dispersion and thereby smoothed the front.

Lantz (1971) combined the spatial and temporal truncation errors in Eq. (1) and Van Genuchten (1976) and Laumbach (1975) have both made equivalent combinations (using higher order temporal integrations) to improve the accuracy of the calculations. As yet these manipulations have not been extended to non-linear problems, although Lantz (1971) achieves some success in special non-linear problems.

To summarize, we know how to eliminate oscillations in the solution due to the temporal integration, and for some methods we know the spatial increment needed to eliminate oscillations due to the convective term. Unfortunately, the spatial increment (Δx) needed is frequently much too small and we are forced to degrade the quality of the solution by introducing artificial dispersion in the numerical scheme. We first present the exact solution for the transient problem (1), which gives the eigenvalues for this problem. An extension of the investigation by Christie, et al. (1976) presents the oscillation limits for the steady-state equation and a variety of methods. The eigenvalues of the resulting matrix are calculated to relate the steady-state analysis to the transient analysis. Finally, the new method is explained and illustrated.

Exact solution

The exact solution to Equation (1) can be found by separation of variables after transforming the spatial part to self-adjoint form.

$$c(x,t)= \frac{e^{\lambda}-e^{\lambda x}}{e^{\lambda}-1} - 4e^{\lambda x/2-\lambda^2 t/4}\sum_{n=1}^{\infty} \frac{n\pi}{\lambda^2/4+(n\pi)^2}\, e^{-n^2\pi^2 t} \sin n\pi x \qquad (5)$$

Although not useful for computational purposes, it gives the eigenvalues for this problem.

$$\mu_i = -\lambda^2/4 - n^2\pi^2 \;,\; n = 1,\ 2,\ --- \qquad (6)$$

For computational purposes a solution with Laplace transform is generally used.

Difference Equations and Eigenvalue Analysis

By the numerical solution of the steady-state convection diffusion equation (2) together with an eigenvalue analysis of the equation (1), the importance of mesh spacing can be considered.

The steady state equation (2) when solved by numerical schemes gives a system of equations

$$\underline{\underline{M}} \cdot \underline{c} = \underline{b}$$

As an example, the method of orthogonal collocation on finite elements (Carey and Finlayson, 1975) using Lagrange basis function and one interior collocation point gives

$$\left(\frac{4}{\Delta x} + \lambda\right)c_{i-1} - \frac{8}{\Delta x}c_{1-1/2} + \left(\frac{4}{\Delta x} - \lambda\right)c_i = 0 \text{ (Diff. eqn.)}$$

$$c_{i-1} - 4c_{i-1/2} - 8c_i - 4c_{i+1/2} + c_{i+1} = 0 \text{ (Continuity)}$$

$$\left(\frac{4}{\Delta x} + \lambda\right)c_i - \frac{8}{\Delta x}c_{i+1/2} + \left(\frac{4}{\Delta x} - \lambda\right)c_{i+1} = 0 \text{ (Diff. eqn.)}$$

This arbitrary set of equations (nodes i-1, i, i+1) can be combined to give

$$\left(1 + \frac{\lambda\Delta x}{2}\right) c_{i-1} - 2c_i + \left(1 - \frac{\lambda\Delta x}{2}\right) c_{i+1} = 0 \tag{7}$$

The theoretical solution is

$$c_i = R + S\,[\phi(\lambda\Delta x)]^i$$
$$\phi(\lambda\Delta x) = (1 + \lambda\Delta x/2)\,/\,(1 - \lambda\Delta x/2) \tag{8}$$

When the function $\phi(\lambda\Delta x)$ changes signs in Eq. (8) [c not monotone] the solution oscillates. Thus the criterion for no oscillations is

$$\phi(\lambda\Delta x) \geqslant 0 \text{ or } \lambda\Delta x \leqslant 2 \tag{9}$$

The same type of analysis has been made for various Galerkin/finite difference schemes by Christie, et al. (1976). The results obtained are summarized in Table 1. New calculations are presented in Table 1 for OCFE Lagrange and Hermite basis functions.

The eigenvalues for the transient equation (1) have been found analytically Eq. (6), but it is of interest to examine eigenvalues of a numerical approximation. Using OCFE to discretize (1) gives a set of coupled ordinary difference equations.

$$\frac{d\underline{c}}{dt} = \underline{\underline{M}} \cdot \underline{c} \tag{10}$$

For large Δx the eigenvalues are complex, but for small enough Δx (depending on the parameters λ) the eigenvalues are real and corresponds to the analytical results. For each method there was a distinct limit between getting real or complex eigenvalues. Price, et al. (1966) found this distinct limit for real or complex eigenvalues theoretically for the finite difference method. We have calculated the limit for other methods as well (see Table 1) and find it corresponds quite

Table 1. Oscillation Limits for Different Methods

Scheme	Criteria Diff. Eqn.	Criteria Eigenvalue	Order of Method (SS)	Reference
Finite Difference				
- Upwind Diff.	None		$O(h)$	Price, et al. (1966)
- Forward	$\lambda\Delta x<1$		$O(h)$	
- Central	$\lambda\Delta x<2$	<2	$O(h^2)$	
Galerkin-FD				
- Var. Upwind linear base functions	$\lambda\Delta x<\frac{2}{1-\alpha}$		$O(h)$ $\alpha=0$ $O(h^2)$	Chien (1977) Christie, et al. (1976) Huyakorn (1976)
Galerkin				
- linear, C^o	$\lambda\Delta x<2$		$O(h^2)$	Christie, et al. (1976)
- Quadratic, C^o	$\lambda\Delta x<4$		$O(h^3)$	
OCFE-Lagrange				
$NCOL^{INT} = 1$	$\lambda\Delta x<2$	$\leq 2.12\pm.04$	$O(h^3)$	This report
$NCOL^{INT} = 2$	$\lambda\Delta x<4.39$	$\leq 4.01\pm.16$	$O(h^4)$	
$NCOL^{INT} = 3$	$\lambda\Delta x<4.64$	$\leq 4.77\pm.23$	$O(h^5)$	
OCFE-Hermite				
1st (cubic)	$\lambda\Delta x<4.39$		$O(h^4)$	This report
2nd (quartic)	$\lambda\Delta x<4.64$		$O(h^5)$	

well to the result expected from the steady-state equations. Consequently, we henceforth use the result from the analysis of steady-state equations as criteria for eliminating oscillations in both steady state and transient calculations.

SOLUTION METHODS

A great variety of solution methods have been applied to the convection-diffusion equation. The finite difference formulation initiated with Peaceman and Rachford (1962) were followed by schemes of increasing complexibility. Stone and Brian (1963) introduced higher order spatial schemes while Laumbach (1975) used high order in both space and time. Unfortunately, the complex schemes cannot always be adopted to more difficult non-linear problems in two dimensions. The Galerkin finite element method was introduced by Price, et al. (1968) and provided better results, especially for large λ, 10^3-10^6.

All conventional schemes can solve the convection-diffusion equation, but they all must use a large number of elements, nodes, and timesteps when convection dominates. Therefore, additional techniques have been tried.

A variable interpolation technique introduced by Price, et al. (1968) improved the efficiency remarkably but it is not easily adopted to more difficult problems. Garder, et al. (1964) solved the convection-diffusion equation by method of characteristics and employing a marker and cell technique to track the concentration front. The accuracy of the calculation is limited to about 2%. Here we employ a moving coordinate system but then we solve the diffusion equation. The basic idea is that if the front has the same shape over a long period of time, the description in a moving coordinate system should be fairly stationary. If this is possible, more points can be located at the front and elsewhere only a few elements are needed. Extension of this method for non-linear problems can be made by introducing a time dependent velocity of the coordinate system. The velocity must then be calculated in order to follow the front. For two dimensional problems the coordinate system can be moved as to locate the front in the region of sharp change of the solution.

Moving Coordinate System

We introduce a moving coordinate system to equation (1) with new coordinates ξ, η

$$\xi = x - \lambda t, \quad \eta = t. \tag{11}$$

Here λ is taken as a constant.

Since $\dfrac{\partial c}{\partial t} = \dfrac{\partial c}{\partial \xi}\dfrac{\partial \xi}{\partial t} + \dfrac{\partial c}{\partial \eta}\dfrac{\partial \eta}{\partial x} = -\lambda\dfrac{\partial c}{\partial \xi} + \dfrac{\partial c}{\partial \eta}$

$$\frac{\partial c}{\partial x} = \frac{\partial c}{\partial \xi}$$

we obtain

$$\frac{\partial c}{\partial \eta} = \frac{\partial^2 c}{\partial \xi^2} \tag{12}$$

The boundary conditions are transformed to

$$\begin{aligned} &c = 0 \quad \xi > 0 \quad \eta = 0 \\ &\left.\begin{aligned} &c = 1 \quad \xi = -\lambda\eta \\ &c = 0 \quad \xi = 1 - \lambda\eta \end{aligned}\right\} \eta > 0 \end{aligned} \tag{13}$$

Now the spatial domain ξ is [$-\infty$, 1] and front will always be near $\xi = 0$ for $\eta < 1/\lambda$.

For almost all purposes computation to $\eta = 1/\lambda$ is sufficient as the solution is then near steady state.

We can apply any numerical method to solve Eq. (12, 13). As we are only interested in $\eta < 1/\lambda$ the discretization only covers [-1, 1]. We choose to apply OCFE, giving a set of ordinary differential equations and algebraic equations and use a Crank-Nicholson time discretization.

All the equations can then be written as

$$\underline{\underline{C}}\ \underline{c}^{n+1} = \underline{\underline{D}}\ \underline{c}^{n} \tag{14}$$

A similar set of equations like (14) could be developed using finite-difference or Galerkin finite-element methods.

The boundary conditions are applied by modifying the matrices $\underline{\underline{C}}$, $\underline{\underline{D}}$ and $\underline{c}^n$ at each timestep. For points to the left of the location of the boundary, $i<I$, $\xi_i < -\lambda\eta$, we replace $\underline{\underline{C}}$ and $\underline{\underline{D}}$ by the identity matrix $\underline{\underline{I}}$ and $\underline{c}^n$ by 1. Since the location of the boundary changes in time, the LU decomposition must be performed every time the boundary locations pass another collocation point.

Results

The advantages of using a MCS for problems with dominating convection is illustrated with comparisons using the same spatial discretization (here collocation) with both a MCS (Moving Coordinate System) and a fixed coordinate system. The convection-diffusion equation is solved with $\lambda = 877.9$ and 87790.

In Fig. 1 is shown a comparison of a conventional scheme versus MCS-scheme. It is apparent that only a relative few number of elements are needed to give a non-oscillatory "fair" solution.

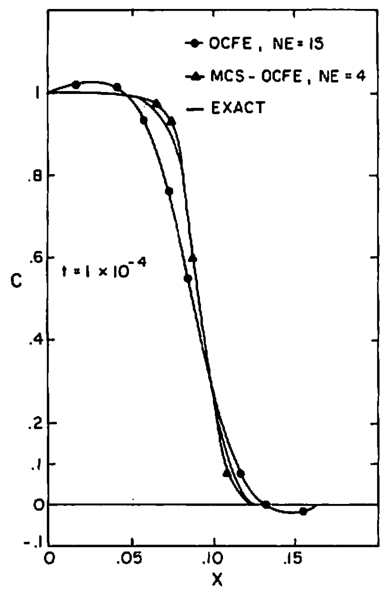

Fig. 1. Comparison of standard OCFE versus moving coordinate system.
λ=877.9, NCOL = 2, Δt=2.5 x 10^{-6}.

In contrast to the method of characteristics by Garder, *et al.*, the error of MCS decreases with increasing number of elements and with smaller timestep. The method of characteristics has a minimum error of 2%. When compared to the method of variable interpolation Price, *et al.* (1968) the MCS is better. Figure 2 shows how the error decreases with time for the same number of elements, and the MCS is very much more accurate at small times (when the front is steepest).

The elements are not all the same size in MCS-OCFE. If small elements are used near the front the solution will be good at small times (when all changes occur near the front). At later times, however, the changes also occur near the front. Thus the best discretization may depend on time, and this is shown in Figure 3.

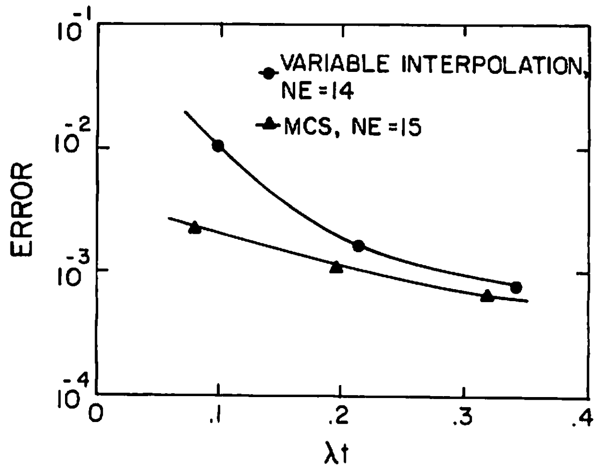

Fig. 2. Comparison of moving coordinate system versus variable interpolation (Price, et al. (1968).) λ=877.9

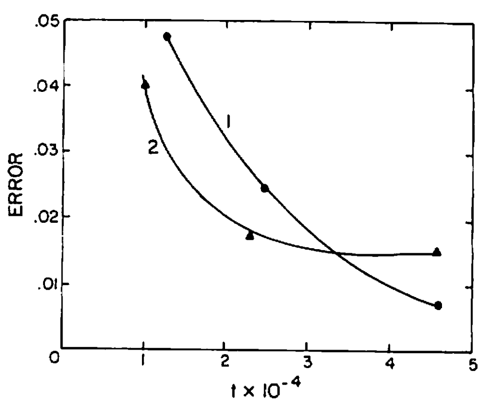

Fig. 3. Error as function of time. Effect of mesh location. λ=877.9, NE=5, Δt=2.5 x 10^{-6}.
Curve 1 element nodes at ξ=-1., -.2, -.05, .05, .2, 1
2 element nodes at ξ=-1., -.12, -.04, .04, .12,

In Table 2 are shown results, errors, computation time, numbers of elements and Δt. It is clear that MCS is superior to the conventional schemes. By having the same number of elements (entries 5 and 8 for 15 elements) the error is decreased by a factor 20-40, but the computation time is only two times longer. For the same computation time (entries 1 and 6 for ~3 secs.) the conventional scheme is unreliable (10%) while MCS gives fairly accurate results (3%). Comparing at 16 secs. (entries 5 and 8) the error is decreased by a factor of 4-12 and MCS gives no oscillations while the conventional scheme does.

For λ = 87790 the MCS is even better. Table 2 shows results for both MCS and conventional OCFE. Comparing entries 5 and 2 the standard OCFE gives excessive oscillation, but MCS gives only 1% error and used 20 times less computer time.

CONCLUSIONS

The steady state convection-diffusion equation is used to provide criteria for the elimination of oscillations. Small element sizes (Δx) are necessary and criteria are given for finite difference, Galerkin and collocation methods.

Solving the convection diffusion equation on a moving coordinate system rather than a fixed coordinate system can give better solutions at less cost. Often factors of 10 or higher in improved accuracy or reduced cost are possible.

TABLE 2

Comparison of MCS with Conventional Scheme (Both using OCFE)

Entry	Scheme	NCOL	NE	for $\lambda=877.9$ $\Delta t x 10^6$	CPU*	Error at $t=1x10^{-4}$	Error at $t=5x10^{-4}$	Maximum Oscillations at $t=5x10^{-4}$
1	MCS	2	4	2.5	3.3	.03	.04	-
2		2	6	2.5	5.1	.01	.005	-
3		2	6	10	1.0	.04	.01	-
4		2	8	2.5	6.7	.008	.006	-
5		2	15	1.25	15.1	.004	.001	-
6	OCFE	2	5	2	3.2	~.1	~.1	~.1
7		2	15	2.5	8.1	.07	.04	.04
8		3	20	2.5	17.0	.03	.004	.0022
				for $\lambda=87790$ $\Delta t x 10^8$			Error at $t=5x10^{-8}$	
1	MCS	2	12	5	4.5	.5	.02	.005
2	-	2	14	2.5	8.1	.5	.01	.004
3	-	2	16	1.25	17.0	.5	.004	-
4	OCFE	3	50	1	70.5	0.0	.003	.004
5	-	3	50	.5	152.0	.5	~.1	~.1
6	-	5	50	1	140.0	0.0	.003	-

*CPU on CDC 6400

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