IMPLICIT PREDICTOR CORRECTOR METHODS
FOR PDE'S WITH CONVECTION AND DIFFUSION

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SUMMARY.

A modified diagonally implicit Runge-Kutta method for solving PDE's
with convection, diffusion and chemical kinetic interaction terms
is presented. We obtain stability and second order accuracy in both
space and time. An application to the numerical solution of a non-
linear system of equations is also illustrated.

1. INTRODUCTION.

In this paper we do a Fourier stability analysis on a hybrid scheme
based upon Miller's second order diagonally implicit Runge-Kutta me-
thod DIRK2 (see [1], [2]), for solving certain PDE's with convection,
diffusion and chemical kinetic interaction terms.

In this scheme, we treat implicitly only the "stiff" terms in the e-
quations. We obtain stability and second order accuracy in both spa-
ce and time by means of a first order "upwind" predictor followed
by a second order centered corrector.

A typical equation, written for brevity in its one-dimensional form
is

$$(1.1) \qquad \frac{\partial v}{\partial t} = w \frac{\partial v}{\partial x} + \varepsilon \frac{\partial^2 v}{\partial x^2} + f(v)$$

where $v = (v_1, v_2, \ldots, v_n)^T$ describes the n chemical concentrations
convected with velocity w and diffusing according to the "diffusion
coefficient" ε. The nonlinear term $f(v)$ models the chemical reactions.

The spatially semi-discretized approximation to equation (1.1) is
of the form

$$(1.2) \qquad \frac{du}{dt} = Au + B(u)$$

where Au involves the first two terms of (1.1) and has long time

constants since the grid spacing in the x direction is long, and B(u) is stiff due to the presence of the chemical kinetics.

In §2, the modified 2nd order DIRK method is presented and discussed.

In §3, using von Neumann's method (see e.g. [3]), a region of stability is obtained for a certain simplified model of (1.1) with coefficients frozen constant and with the nonlinear operator B(u) replaced by a linear operator with large negative eigenvalues which commutes with A. We also do not bother about boundary conditions, imagining the equation to hold on the entire real line.

In §4 we discuss the error analysis assuming that the nonlinear operator B has an appropriate Lipschitz constant on the order of unity.

Finally, in section 5 we present some numerical results of interest.

2. NUMERICAL METHOD.

The modified 2nd order DIRK method when applied to (1.2) is given by

Predictor

(2.1a) $$u^{n+1/3} = u^n + \frac{\Delta t}{3} A^* u^n + \frac{\Delta t}{3} B\, u^{n+1/3}$$

Extrapolation

(2.1b) $$u^{(n+1)*} = 3u^{n+1/3} - 2u^n$$

Corrector

(2.1c) $$u^{n+1} = u^n + \frac{3}{4} \Delta t (Au^{n+1/3} + Bu^{n+1/3}) +$$
$$+ \frac{\Delta t}{4} Au^{(n+1)*} + \frac{\Delta t}{4} Bu^{n+1}$$

The finite difference operator A indicates the 2nd order *centered* approximations to the convection and diffusion terms in the PDE. However, for the sake of stability we have had to replace A by A* in the explicit $A^* u^n$ term of the predictor formula (2.1a); this indicates that the wv_x convection term has been approximated by the 1st order noncentered *upwind* difference approximation. The predictor-corrector result however, is 2nd order correct in both space and time.

2.1. PRELIMINARIES.

Given the function $f_k = f(kh)$, k integer, defined at the points
x = kh on the whole discrete line, we will use the operators

$$(S_+f)_k = f_{k+1} \qquad \text{(forward shift)}$$

$$(D_+f)_k = \frac{1}{h} (f_{k+1} - f_k) \qquad \text{(forward difference)}$$

$$(D_-f)_k = \frac{1}{h} (f_k - f_{k-1}) \qquad \text{(backward difference)}$$

and

$$(D_0f)_k = \frac{1}{2h} (f_{k+1} - f_{k-1}) \qquad \text{(centered difference)}$$

If we let $u = \{u_k\}$ and assume that $u_k = e^{ikh\theta}$; $i = \sqrt{-1}$, setting
$\alpha = h\theta$, we can define *the discrete Fourier transform of* u, $\hat{u}$, by

$$\hat{u}(\alpha) = \sum_k u_k \ell^{ik\alpha} \quad ; \quad 0 \leqslant \alpha \leqslant 2\pi \ .$$

It follows that

$$\widehat{S_+u}(\alpha) = \ell^{i\alpha} \hat{u}(\alpha)$$

If we have a difference operator L, linear with constant coeffi-
cients,

$$u^{n+1} = (\sum_{\ell=n_1}^{n_2} a_\ell(S_+)^\ell)u^n = L\ u^n \ ,$$

after applying Fourier transform, we get

$$\widehat{u^{n+1}}(\alpha) = \rho(\alpha)\ \widehat{u^n}(\alpha)$$

If $\rho(\alpha)$, the amplification factor, satisfies the von Neumann condi-
tion

$$|\rho(\alpha)| \leqslant 1 + C\Delta t \ , \quad C \text{ constant} \ ,$$

then

$$\|u^{n+1}\|_2 \leqslant e^{Ct + \Delta t} \|u^0\|_2$$

and we have stability [4].

3. STABILITY ANALYSIS.

We consider first the equation

(3.1) $$v_t = v_x + \varepsilon v_{xx} \quad ; \quad \varepsilon \text{ constant.}$$

Using the modified DIRK method (2.1), we obtain

(3.2) $$u^{n+1} = (I + \Delta t \, A + \frac{\Delta t^2}{2} AA^*) \, u^n \, ,$$

where $A^* = D_+ + \varepsilon \, D_+ D_-$ and $A = D_0 + \varepsilon \, D_+ D_-$. The method is explicit, and we use D_+ as an approximation for v_x in the predictor and D_0 in the corrector. We use the second difference $D_+ D_-$ approximation for v_{xx} in both predictor and corrector.

Setting $k = \Delta t$, $h = \Delta x$, $\lambda = k/u$, $\gamma = k/h^2$ and taking Fourier transform in (3.2), we get

(3.3) $$\rho(\alpha) = 1 - \frac{\lambda^2}{2} \sin^2\alpha + (\cos\alpha - 1)\varepsilon\gamma \, (2 + (\cos\alpha - 1)(\lambda + 2\varepsilon\gamma)) +$$

$$+ \, i \, \lambda \sin\alpha \, ((\cos\alpha - 1)(\frac{\lambda}{2} + 2\varepsilon\gamma) + 1)$$

The area in the $(\varepsilon\gamma, \lambda)$ plane in which $|\rho(\alpha)| \leq 1$, the region of stability (RS), has been determined experimentally and it is shown in Figure 1. In the purely convective case $\varepsilon = 0$, we have stability if $\lambda \leq 2$.

If we plot $\rho(\alpha)$ for a typical value of λ, for example $\lambda = 0.5$ and several values of $\varepsilon\gamma$ we can see how increasing the diffusion affects the amplification factor. We notice that small diffusion helps $\rho(\alpha)$ to remain inside the unit circle (Figures 2 and 3). If we increase the diffusion term, the second loop approaches the boundary again for $\alpha = \pi$ (Figure 4) and finally, if we still increase the diffusion term, the inner loop crosses the boundary and we reach the region of instability (Figure 5).

3.1. THE GENERAL CASE.

We study now the equation

(3.4) $$\frac{\partial v}{\partial t} = \frac{\partial v}{\partial x} + \varepsilon \, \frac{\partial^2 v}{\partial x^2} + f(v)$$

This is of the form $\frac{\partial u}{\partial t} = Au + B(u)$ after space discretization.

The structure of the nonlinear $B(u)$ is well set up for the Newton's method type of solution of our implicit part of the DIRK method. The Jacobian matrix for the nonlinear term is negative definite and with low profile since the chemical kinetic interaction is sparse.
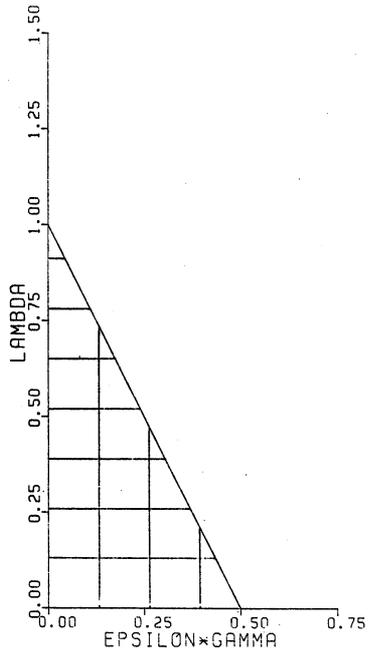
Figure 1

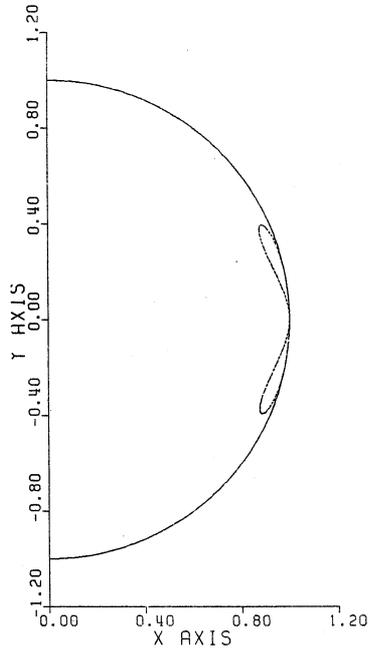Region of Stability in the $(\epsilon\gamma,\lambda)$ plane

Figure 2

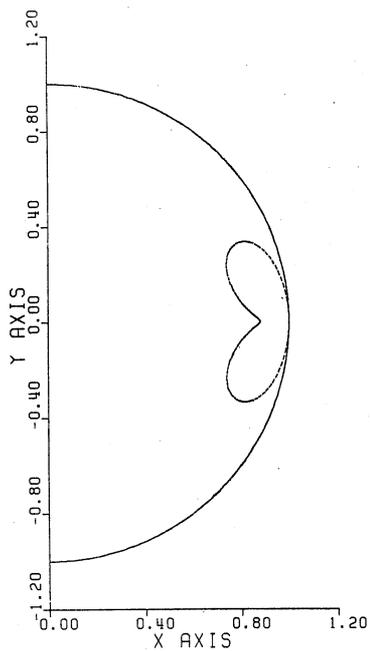Magnification factor for $\lambda = 0.5$ and $\epsilon\gamma = 0.0$

Figure 3

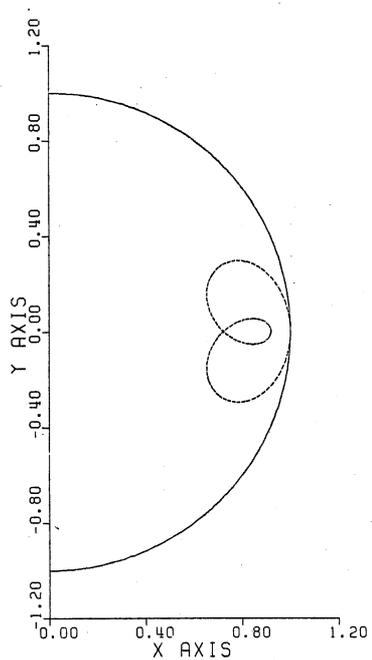Magnification factor for $\lambda = 0.5$ and $\varepsilon\gamma = 0.1$

Figure 4

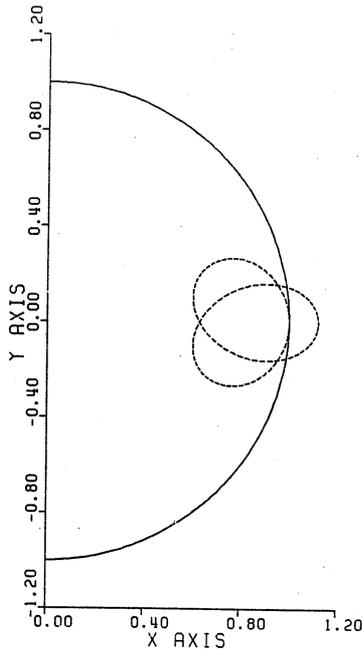Magnification factor for $\lambda = 0.5$ and $\varepsilon\gamma = 0.2$

Figure 5

Magnification factor for $\lambda = 0.5$ and $\varepsilon\gamma = 0.3$

In what follows we will instead assume (for the purposes of stability analysis only) that B is linear, commutes with A and A* and has full real negative eigenvalues b, some of which might be expected to be quite large since the chemical kinetic terms may be quite stiff. We want to show that we have stability for all negative b.

Using the modified DIRK method (2.1), we obtain

$$(3.5) \qquad u^{n+1} = (I - \frac{k}{4} B)^{-1} [(I - \frac{k}{2} A) + (\frac{3}{2} kA + \frac{3}{4} kB) .$$

$$. \; (I - \frac{k}{3} B)^{-1} (I + \frac{k}{3} A*)] u^n$$

Using the fact that B has negative eigenvalues b and that it commutes with A and A* and assuming that $(\varepsilon\gamma,\lambda)$ belongs to the region of stability (RS), after taking Fourier transform in (3.5) we get

$$(3.6) \qquad |\rho(\alpha)| \leqslant \frac{1 + \frac{kb}{12} \; |5 + (\cos \alpha - 1)(3\lambda + 10\varepsilon\gamma) + i \; 5\lambda \sin \alpha |}{1 + \frac{7}{12} kb + \frac{1}{12} k^2 b^2}$$

For $(\varepsilon\gamma,\lambda)$ in the region of stability

$$0 \leqslant 3\lambda + 10\varepsilon\gamma \leqslant 5$$

and if

(3.7) $\qquad \lambda \leqslant (24/25)^{1/2}$,

it follows that

(3.8) $\qquad |15 + (\cos \alpha - 1)(3\lambda + 10\varepsilon\gamma) + i\, 5\lambda \sin\alpha| \leqslant 7$

Using (3.6) and (3.8) we obtain stability for all $b \leqslant 0$ if λ satisfies (3.7) and $(\varepsilon\gamma, \lambda)$ belongs to the region of stability.

4. ERROR ANALYSIS.

In this section we perform the error analysis for the equation

(4.1) $\qquad \dfrac{\partial v}{\partial t} = \dfrac{\partial v}{\partial x} + \varepsilon\, \dfrac{\partial^2 v}{\partial x^2} + f(v)$

where we assume that the solution v is sufficiently smooth in both space and time and also that the nonlinear term f has an appropriate Lipschitz constant on the order of unity.

The modified DIRK method is given by

Predictor

(4.2a) $\qquad u^{n+1/3} = u^n + \dfrac{k}{3}(D_+ + \varepsilon\, D_+D_-)u^n + \dfrac{k}{3} Bu^{n+1/3}$

Extrapolation

(4.2b) $\qquad u^{(n+1)*} = 3u^{n+1/3} - 2u^n$

Corrector

(4.2c) $\qquad u^{n+1} = u^n + \dfrac{3}{4} k(D_0 + \varepsilon\, D_+D_-)u^{n+1/3} + \dfrac{3}{4} kBu^{n+1/3} +$

$\qquad\qquad + \dfrac{k}{4}(D_0 + \varepsilon\, D_+D_-)u^{(n+1)*} + \dfrac{k}{4} Bu^{n+1}$

The restriction of the smooth true solution $v(x,t)$ to the grid domain will be noted by $v_j^n = v(nk, jh)$. We now try to write v itself as a solution of the difference equations plus a uniformly small local truncation error.

Predictor

(4.3) $\qquad v^{n+1/3} = v^n + \dfrac{k}{3}(v_x^n + \varepsilon\, v_{xx}^n) + \dfrac{k}{3} Bv^{n+1/3} + O(k^2)$

Since

$$v_x^n = D_+ v^n + O(u)$$

and $\qquad\qquad \varepsilon\, v_{xx}^n = \varepsilon\, D_+D_- v^n + O(u^2)$

After replacing these terms in (4.3) we get

(4.4) $\qquad v^{n+1/2} = v^n + \frac{k}{3} (D_+ + \varepsilon D_+D_-)v^n + \frac{k}{3} Bv^{n+1/3} +$

$\qquad\qquad\qquad + O(k^2 + kh + kh^2)$

From (4.4) and (4.2a) we have

(4.5) $\qquad\qquad v^{n+1/3} = u^{n+1/3} + O(k^2 + kh + kh^2)$

Extrapolation:

(4.6) $\qquad\qquad v^{(n+1)*} = 3v^{n+1/3} - 2v^n =$

$\qquad\qquad\qquad = 3u^{n+1/3} - 2u^n + O(k^2 + kh + kh^2).$

From (4.2b) and (4.6), we have

(4.7) $\qquad\qquad v^{(n+1)*} = u^{(n+1)*} + O(k^2 + kh + kh^2).$

Corrector:

(4.8) $\qquad v^{n+1} = v^n + \frac{3}{4} k(v_x^{n+1/3} + \varepsilon v_{xx}^{n+1/3} + Bv^{n+1/3}) +$

$\qquad\qquad\qquad + \frac{k}{4} (v_x^{(n+1)*} + \varepsilon v_{xx}^{(n+1)*}) + \frac{k}{4} Bv^{n+1}$

Using the smoothness of the solution, (4.5) and the fact that B has a Lipschitz constant on the order of unity, the second term in (4.8) can be replaced by

(4.9) $\qquad \frac{3}{4} k(D_0 + \varepsilon D_+D_-)u^{n+1/3} + \frac{3}{4} kBu^{n+1/3} +$

$\qquad\qquad\qquad + O(k^3 + k^2h + k^2h^2 + kh^2)$

Analogously, using (4.7), the third term in (4.8) can be replaced by

(4.10) $\qquad \frac{k}{4} (D_0 + \varepsilon D_+D_-)u^{(n+1)*} + O(k^3 + k^2h + k^2h^2 + kh^2)$

From (4.2c), (4.9) and (4.10), assuming k/h bounded, we have

(4.11) $\qquad\qquad v^{n+1} = u^{n+1} + k \, O(k^2 + h^2)$

In this equation, u^{n+1} denotes the approximate value that we would compute in one step of our method. We see that the method has local truncation error which is uniformly bounded by k times $O(k^2 + h^2)$. The method is 2nd order correct both in space and time.

5. A NUMERICAL EXAMPLE.

A diffusion-convection reaction process involving three substances of concentrations v_1, v_2 and v_3 respectively, leading to the system

$$\frac{\partial v_1}{\partial t} = - \frac{\partial v_1}{\partial x} + \varepsilon \frac{\partial^2 v_1}{\partial x^2} + v_3 - 10^4 v_1 v_2$$

$$\frac{\partial v_2}{\partial t} = - \frac{\partial v_2}{\partial x} + \varepsilon \frac{\partial^2 v_2}{\partial x^2} + v_3 - 10^4 v_1 v_2$$

$$\frac{\partial v_3}{\partial t} = - \frac{\partial v_3}{\partial x} + \varepsilon \frac{\partial^2 v_3}{\partial x^2} - v_3 + 10^4 v_1 v_2$$

is integrated using the following boundary and initial conditions

$$v_i(0,t) = 0 \;, \; t > 0 \;, \; i = 1,2,3 \quad, \quad \frac{\partial v_i}{\partial x}(1,t) = 0 \;, \; t > 0 \;, \; i = 1,2,3$$

$$v_1(x,0) = \begin{cases} 20x & , \quad 0 < x \leqslant 0.1 \\ -20x + 4 & , \quad 0.1 < x \leqslant 0.2 \\ 0 & , \quad 0.2 < x < 1 \end{cases}$$

$$v_2(x,0) = \begin{cases} 10x & , \quad 0 < x \leqslant 0.1 \\ -10x + 2 & , \quad 0.1 < x \leqslant 0.2 \\ 0 & , \quad 0.2 < x < 1 \end{cases}$$

$$v_3(x,0) = 0 \;, \quad 0 < x < 1 \;,$$

and with the physical parameter $\varepsilon = 10^{-2}$. We notice that the first order spatial derivatives are large in relation to the second order ones and, consequently, we expect the solution to behave like the solution of the limiting purely convective case.

We use the modified DIRK method with fixed $\Delta x = 1/20$ and variable step size Δt. Because of the chemical kinetics and in order to save computer time, the initial step size is chosen fairly small (10^{-6}).

We impose a rather conservative upper bound (2×10^{-2}) for the maximum size to which the step would be increased, satisfying the stability conditions of section 3. To automatically adjust the step size, the difference between the solution after one step of size Δt and two steps of size $\Delta t/2$ is taken as an estimate of the local truncation error. If this difference is within the prescribed tolerance δ, the step size is doubled. Otherwise the step size is halved. We use Newton's method for the solution of our implicit part of the modified DIRK method, and a solution is accepted when two successive iterations

satisfy $\|v^{k+1}-v^k\|_2 \leqslant \delta \times 10^{-1}$. Several runs, with different tolerances, show only the predictable changes in accuracy. However, for $\delta = 10^{-4}$, the average step size is about 4×10^{-3} while for $\delta = 10^{-2}$, the average step size coincides with the maximum step size 2×10^{-2}.
The initial data and the solution at different times are shown in Figures 6 to 10. We notice the sharp transition from the initial concentrations (Figure 6) to the state at time $\cong 0.20$ (Figure 8), due to the chemical reactions. In all the plots, the solution for v_1 is represented by a solid curve, for v_2 by a dashed curve and for v_3 by a solid curve with a symbol. Figures 9 and 10 show the outgoing waves travelling with speed less than 1, as expected, due to the presence of diffusion.
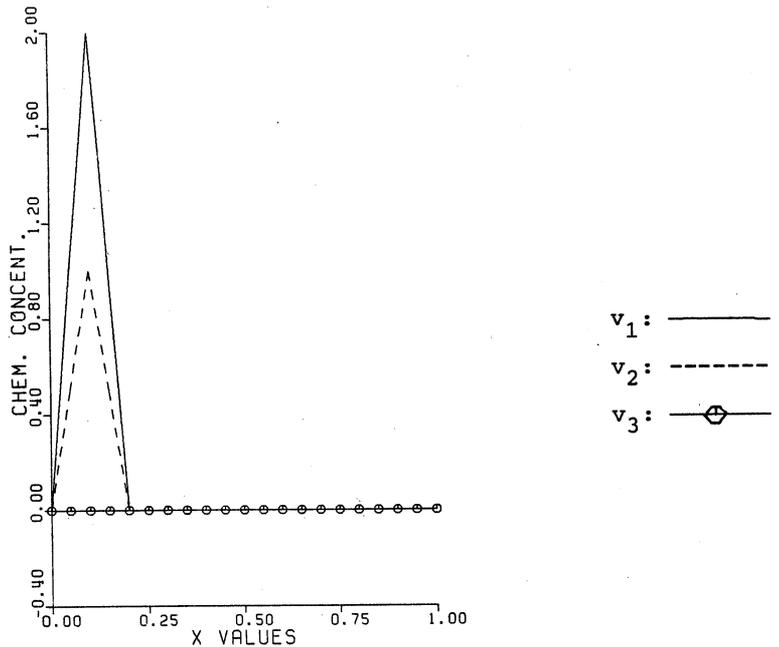
Figure 6

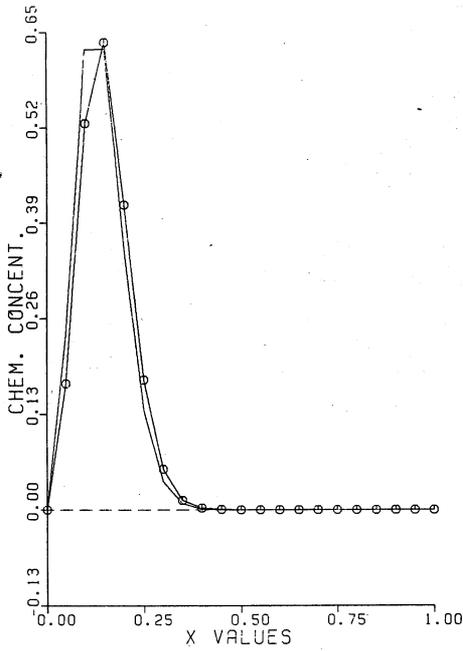Chemical concentrations at time 0.000

Figure 7

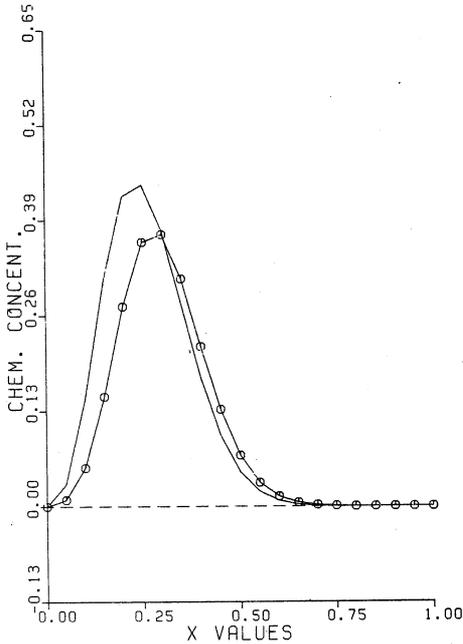Chemical concentrations at time 0.053

v_1: ——————

v_2: - - - - - - -

v_3: ——⬡——

Figure 8

Chemical concentrations at time 0.203
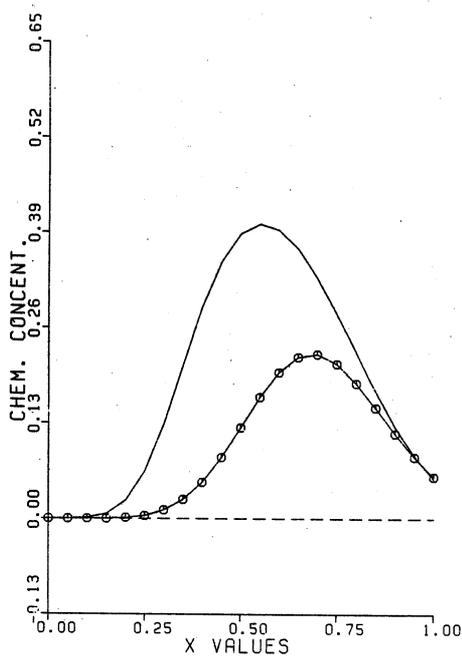
Figure 9

Chemical concentrations at time 0.608

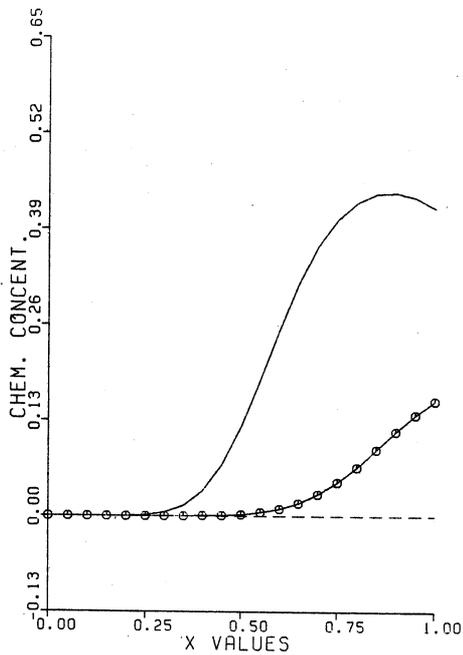v_1: ————————

v_2: — — — — — —

v_3: ———⬡———

Figure 10

Chemical concentrations at time 1.026

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