

## DEVELOPMENT OF A NINE-POINT IMPLICIT CONVECTION-DIFFUSION-REACTION SCHEME

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### Abstract

In this paper we develop a two-dimensional scheme for modeling the transport of a passive scalar under the influence of convection, diffusion, and reaction effects. For purposes of computational efficiency, the scheme is constructed within the nine-point implicit finite-difference framework so as to allow use of a computationally efficient direct solver to obtain the solution from the fourth-order scheme. Modified equation analysis is performed to lay the foundation for much of the model development. With a view to validating the proposed scheme, we consider test problems which are amenable to analytic solutions. Good agreement is obtained for all investigated problems, thus demonstrating the integrity of the method.

**Key Words:** Two-dimensional Convection, diffusion and reaction, Nine-point implicit, Modified equation, Analysis, fourth-order

### 1 Introduction

In this paper we present a finite-difference method for solving a practically important convection–diffusion–reaction (CDR) scalar transport equation. Prominent among this subject are simulations of exterior acoustics [1], turbulent kinetic energy and its dissipation [2], extra stresses in non-Newtonian fluid flows [3], and magneto-hydrodynamics [4]. It is this wide application scope that makes numerical prediction of the model equation worthwhile [5]– [11]. Some of the previous studies were focused on developing discontinuity–capturing CDR schemes [12]– [14].

A reliable numerical model must have the ability to simulate transport phenomenon accurately while being able to avoid numerical instabilities in cases of prevailing convection and/or reaction. There is, then, considerable incentive to construct a scheme which can stabilize the finite-difference equation, and this

motivated the present study. In this paper we are also concerned with prediction accuracy and computational performance since we do not regard a scheme as useful if it can not provide accurate solution at a less computing cost.

The rest of this paper is organized as follows. Section 2 presents the working equation. In Section 3 an implicit scheme is presented in two dimensions. Our emphasis is on the use of Taylor series expansion for the investigated differential equation and the modified equation analysis in the development of the proposed discretization scheme. Section 4 presents simulated results that demonstrate the integrity of the method. In Section 5 we give some concluding remarks.

### 2 Working Equations

We consider in this paper the following inhomogeneous scalar convection-diffusion-reaction equation

$$u \phi_x + v \phi_y - k (\phi_{xx} + \phi_{yy}) + K \phi = f . \quad (1)$$

Here,  $u$  and  $v$  represent the velocity components along the  $x$  and  $y$  directions, respectively. In the interest of simplicity, we consider that  $f$ ,  $k$  and  $K$ , which denote the source, diffusion coefficient, and the reaction coefficient, respectively, have constant values throughout. Solution to equation (1) is sought in  $\Omega$  subject to the following boundary condition on  $\partial\Omega$

$$\phi = g . \quad (2)$$

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### 3 Numerical model

Referring to Fig.1, the discrete equation for (1) at an interior point  $(i, j)$  is derived within the nine-point stencil context. Taking eight nodal values adjacent to  $\phi_{i,j}$  into consideration, the discrete equation can be represented by

$$\begin{aligned}
 & c_1\phi_{i-1,j-1} + c_2\phi_{i,j-1} + c_3\phi_{i+1,j-1} + c_4\phi_{i-1,j} \\
 & + c_5\phi_{i,j} + c_6\phi_{i+1,j} + c_7\phi_{i-1,j+1} \\
 & + c_8\phi_{i,j+1} + c_9\phi_{i+1,j+1} = f. \tag{3}
 \end{aligned}$$

The derivation begins with conduct of Taylor series expansion of  $\phi_{i\pm 1,j}$ ,  $\phi_{i,j\pm 1}$ , and  $\phi_{i\pm 1,j\pm 1}$  with respect to  $\phi_{i,j}$ , followed by substitution of them into equation (3). After some algebra, one can obtain the following equivalent representation of equation (3)

$$\begin{aligned}
 & \left( \sum_{n=1}^9 c_n \right) \phi \\
 & + h \left[ (-c_1 + c_3 - c_4 + c_6 - c_7 + c_9) \phi_x \right. \\
 & \quad \left. + (-c_1 - c_2 - c_3 + c_7 + c_8 + c_9) \phi_y \right] \\
 & + \frac{h^2}{2!} \left[ (c_1 + c_3 + c_4 + c_6 + c_7 + c_9) \phi_{xx} \right. \\
 & \quad + 2(c_1 - c_3 - c_7 + c_9) \phi_{xy} \\
 & \quad \left. + (c_1 + c_2 + c_3 + c_7 + c_8 + c_9) \phi_{yy} \right] \\
 & + \frac{h^3}{3!} \left[ (-c_1 + c_3 - c_4 + c_6 - c_7 + c_9) \phi_{xxx} \right. \\
 & \quad \left. + 3(-c_1 - c_3 + c_7 + c_9) \phi_{xxy} \right.
 \end{aligned}$$

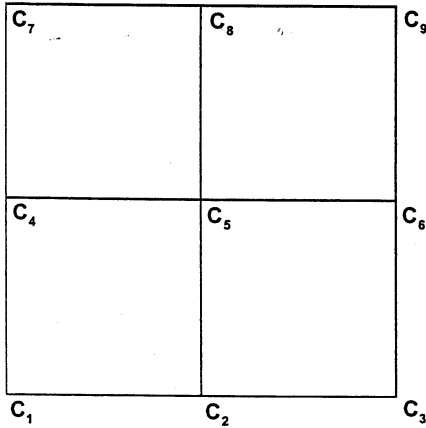


Fig.1: The schematic of the nine-point stencil used in the derivation.

$$\begin{aligned}
 & + 3(-c_1 + c_3 - c_7 + c_9) \phi_{xyy} \\
 & + (-c_1 - c_2 - c_3 + c_7 + c_8 + c_9) \phi_{yyy} \Big] \\
 & + \frac{h^4}{4!} \left[ (c_1 + c_3 + c_4 + c_6 + c_7 + c_9) \phi_{xxxx} \right. \\
 & \quad + 4(c_1 - c_3 - c_7 + c_9) \phi_{xxx} \\
 & \quad + 6(c_1 + c_3 + c_7 + c_9) \phi_{xxy} \\
 & \quad + 4(c_1 - c_3 - c_7 + c_9) \phi_{xyy} \\
 & \quad \left. + (c_1 + c_2 + c_3 + c_7 + c_8 + c_9) \phi_{yyyy} \right] \\
 & + H.O.T = f. \tag{4}
 \end{aligned}$$

Fulfillment of consistency property, a necessary condition to provide convergent solution, requires that

$$c_1 + c_2 + c_3 + c_4 + c_5 + c_6 + c_7 + c_8 + c_9 = K, \tag{5a}$$

$$-c_1 + c_3 - c_4 + c_6 - c_7 + c_9 = \frac{u}{h} + M, \tag{5b}$$

$$-c_1 - c_2 - c_3 + c_7 + c_8 + c_9 = \frac{v}{h} + N, \tag{5c}$$

$$c_1 + c_3 + c_4 + c_6 + c_7 + c_9 = -\frac{2k}{h^2} + 2G, \tag{5d}$$

$$c_1 + c_2 + c_3 + c_7 + c_8 + c_9 = -\frac{2k}{h^2} + 2A, \tag{5e}$$

$$c_1 - c_3 - c_7 + c_9 = B, \tag{5f}$$

$$c_9 - c_1 = \frac{D}{h}, \tag{5g}$$

$$c_1 + c_9 = \frac{H}{h^2}, \tag{5h}$$

$$c_3 - c_7 = \frac{F}{h}. \tag{5i}$$

In the above,  $M, N, G, A, B, D, H,$  and  $F$  are introduced so as to be able to uniquely determine  $c_1 \sim c_9$ .

With the above simultaneous equations, it follows readily that

$$\begin{aligned}
 & u \phi_x + v \phi_y - k(\phi_{xx} + \phi_{yy}) + K\phi \\
 & + h ( M\phi_x + N\phi_y ) \\
 & + h^2 \left[ (G\phi_{xx} + B\phi_{xy} + A\phi_{yy}) + \frac{1}{6}(u\phi_{xxx} + v\phi_{yyy}) \right. \\
 & \quad - \frac{1}{12}(k\phi_{xxxx} + k\phi_{yyyy} - 6H\phi_{xxy}) \\
 & \quad \left. + \frac{1}{2}(D\phi_{xxy} + D\phi_{xyy} - F\phi_{xxy} + F\phi_{xyy}) \right] \\
 & + \frac{h^3}{6} ( M \phi_{xxx} + N \phi_{yyy} ) \\
 & + h^4 \left[ \frac{G}{12} \phi_{xxxx} + \frac{A}{12} \phi_{yyyy} - \frac{B}{4} \phi_{xxy} \right. \\
 & \quad \left. + \frac{B}{6} (\phi_{xxy} + \phi_{xyy}) \right]
 \end{aligned}$$

$$+ H.O.T. = f. \quad (6)$$

The derivation is followed by differentiating equation (6) with respect to  $xx$  and  $yy$ , yielding

$$u\phi_{xxx} + v\phi_{xxy} - k(\phi_{xxxx} + \phi_{xxyy}) + K\phi_{xx} + h(M\phi_{xxx} + N\phi_{xxy}) + H.O.T. = 0, \quad (7)$$

and

$$u\phi_{xyy} + v\phi_{yyy} - k(\phi_{yyyy} + \phi_{xxyy}) + K\phi_{yy} + h(M\phi_{xyy} + N\phi_{yyy}) + H.O.T. = 0. \quad (8)$$

Summing equations (7) and (8) results in

$$k(\phi_{xxxx} + 2\phi_{xxyy} + \phi_{yyyy}) = K(\phi_{xx} + \phi_{yy}) + Mh(\phi_{xxx} + \phi_{xyy}) + Nh(\phi_{xxy} + \phi_{yyy}) + u(\phi_{xxx} + \phi_{xyy}) + v(\phi_{xxy} + \phi_{yyy}) + H.O.T. \quad (9)$$

Set  $-6H = 2k$  or

$$H = -\frac{k}{3}, \quad (10)$$

we find, with equations (6) and (9), the following equation

$$\begin{aligned} & u\phi_x + v\phi_y - k(\phi_{xx} + \phi_{yy}) + K\phi \\ & + h(M\phi_x + N\phi_y) \\ & + h^2 \left[ \left( G - \frac{K}{12} \right) \phi_{xx} + B\phi_{xy} + \left( A - \frac{K}{12} \right) \phi_{yy} \right. \\ & + \frac{u + Mh}{12} \phi_{xxx} + \frac{v + Nh}{12} \phi_{yyy} \\ & + \frac{1}{2} \left( D - F - \frac{v}{6} - \frac{Nh}{6} \right) \phi_{xxy} \\ & + \left. \frac{1}{2} \left( D + F - \frac{u}{6} - \frac{Mh}{6} \right) \phi_{xyy} \right] \\ & + \frac{h^4}{2} \left[ \frac{1}{6}G \phi_{xxxx} + \frac{1}{6}A \phi_{yyyy} - \frac{1}{2}B \phi_{xxyy} \right. \\ & + \left. \frac{1}{3}B (\phi_{xxxy} + \phi_{xyyy}) \right] \\ & + H.O.T. = f. \quad (11) \end{aligned}$$

We then differentiate equation (1) with respect to  $x$  and  $y$  to yield

$$M\phi_x = -\frac{M}{K} (u\phi_{xx} + v\phi_{xy} - k\phi_{xxx} - k\phi_{xxy}), \quad (12a)$$

$$N\phi_y = -\frac{N}{K} (u\phi_{xy} + v\phi_{yy} - k\phi_{xxy} - k\phi_{yyy}). \quad (12b)$$

Upon substituting (12a) and (12b) into (11), it will lead to

$$\begin{aligned} & u\phi_x + v\phi_y - k(\phi_{xx} + \phi_{yy}) + K\phi \\ & + h^2 \left[ \left( G - \frac{K}{12} - \frac{Mu}{hK} \right) \phi_{xx} + \left( A - \frac{K}{12} - \frac{Nv}{hK} \right) \phi_{yy} \right. \\ & + \left( B - \frac{Mv}{hK} - \frac{Nu}{hK} \right) \phi_{xy} \\ & + \left( \frac{u + Mh}{12} + \frac{Mk}{hK} \right) \phi_{xxx} \\ & + \left( \frac{v + Nh}{12} + \frac{Nk}{hK} \right) \phi_{yyy} \\ & + \left( \frac{D}{2} - \frac{F}{2} - \frac{v}{12} - \frac{Nh}{12} + \frac{Nk}{hK} \right) \phi_{xxy} \\ & + \left( \frac{D}{2} + \frac{F}{2} - \frac{u}{12} - \frac{Mh}{12} + \frac{Mk}{hK} \right) \phi_{xyy} \left. \right] \\ & + \frac{h^4}{2} \left[ \frac{1}{6}G \phi_{xxxx} + \frac{1}{6}A \phi_{yyyy} - \frac{1}{2}B \phi_{xxyy} \right. \\ & + \left. \frac{1}{3}B (\phi_{xxxy} + \phi_{xyyy}) \right] \\ & + H.O.T. = f. \quad (13) \end{aligned}$$

We prescribe first the following four equations to eliminate all of the third-order derivative terms :

$$\frac{u - Mh}{12} + \frac{Mk}{hK} = 0, \quad (14a)$$

$$\frac{v - Nh}{12} + \frac{Nk}{hK} = 0, \quad (14b)$$

$$\frac{D}{2} - \frac{F}{2} - \frac{v}{12} - \frac{Nh}{12} + \frac{Nk}{hK} = 0, \quad (14c)$$

$$\frac{D}{2} + \frac{F}{2} - \frac{u}{12} - \frac{Mh}{12} + \frac{Mk}{hK} = 0. \quad (14d)$$

The above four conditions enable us to have the following expressions for determining  $M$ ,  $N$ ,  $D$  and  $F$

$$M = -\frac{huK}{12k + h^2K}, \quad (15)$$

$$N = -\frac{hvK}{12k + h^2K}, \quad (16)$$

$$D = \frac{2k(u+v)}{12k + h^2K}, \quad (17)$$

$$F = \frac{2k(u-v)}{12k + h^2K}. \quad (18)$$

Upon obtaining the above expressions, we are to eliminate the second-order derivative terms shown in equa-

tion (13). By doing so, the remaining three free parameters can be determined as

$$A = \frac{K}{12} - \frac{v^2}{12k + h^2K}, \quad (19)$$

$$B = -\frac{2uv}{12k + h^2K}, \quad (20)$$

$$G = \frac{K}{12} - \frac{u^2}{12k + h^2K}. \quad (21)$$

By substitution of the above derived expressions for  $A, B, D, F, G, H, M, N$  into equation (4), we are led to obtain

$$c_1 = -\frac{12k^2 + h^2kK + 6hku + 6hkv}{6h^2(12k + h^2K)}, \quad (22a)$$

$$c_2 = -\frac{1}{12h^2(12k + h^2K)}(96k^2 - 4h^2kK - h^4K^2 + 48hkv + 12h^2uv + 12h^2v^2), \quad (22b)$$

$$c_3 = -\frac{12k^2 + h^2kK - 6hku + 6hkv - 6h^2uv}{6h^2(12k + h^2K)}, \quad (22c)$$

$$c_4 = -\frac{1}{12h^2(12k + h^2K)}(96k^2 - 4h^2kK - h^4K^2 + 48hku + 12h^2u^2 + 12h^2uv), \quad (22d)$$

$$c_5 = \frac{2}{3h^2(12k + h^2K)}(60k^2 + 17h^2kK + h^4K^2 + 3h^2u^2 + 3h^2uv + 3h^2v^2), \quad (22e)$$

$$c_6 = -\frac{1}{12h^2(12k + h^2K)}(96k^2 - 4h^2kK - h^4K^2 - 48hku + 12h^2u^2 + 12h^2uv), \quad (22f)$$

$$c_7 = -\frac{12k^2 + h^2kK + 6hku - 6hkv - 6h^2uv}{6h^2(12k + h^2K)}, \quad (22g)$$

$$c_8 = -\frac{1}{12h^2(12k + h^2K)}(96k^2 - 4h^2kK - h^4K^2 - 48hkv + 12h^2uv + 12h^2v^2), \quad (22h)$$

$$c_9 = -\frac{12k^2 + h^2kK - 6hku - 6hkv}{6h^2(12k + h^2K)}. \quad (22i)$$

In the limiting case  $K = 0$ , the above weighted coefficients turn out to be exactly the same as those derived by Kolesnikov and Baker [15].

It is instructive to introduce three dimensionless parameters

$$R_1 = \frac{Kh^2}{2k}, \quad (23)$$

$$(R_{2u}, R_{2v}) = \left(\frac{uh}{2k}, \frac{vh}{2k}\right), \quad (24)$$

to represent the relative importance of convection, reaction, and diffusion terms. This gives us the ratio of reaction and convection terms as  $R_{3u} = R_1 / R_{2u}$  and  $R_{3v} = R_1 / R_{2v}$ . For purposes of generality, nine coefficients shown in the following discrete equation

$$\begin{aligned} &\bar{c}_1\phi_{i-1,j-1} + \bar{c}_2\phi_{i,j-1} + \bar{c}_3\phi_{i+1,j-1} + \bar{c}_4\phi_{i-1,j} \\ &+ \bar{c}_5\phi_{i,j} + \bar{c}_6\phi_{i+1,j} + \bar{c}_7\phi_{i-1,j+1} \\ &+ \bar{c}_8\phi_{i,j+1} + \bar{c}_9\phi_{i+1,j+1} = \frac{f}{K}. \end{aligned} \quad (25)$$

are rewritten in terms of  $R_1, R_{2u}$  and  $R_{2v}$  as follows :

$$\bar{c}_1 = -\frac{(6 + R_1 + 6R_{2u} + 6R_{2v})}{12R_1(6 + R_1)}, \quad (26a)$$

$$\bar{c}_2 = -\frac{(24 - 2R_1 - R_1^2 + 24R_{2v} + 12R_{2u}R_{2v} + 12R_{2v}^2)}{12R_1(6 + R_1)}, \quad (26b)$$

$$\bar{c}_3 = -\frac{(6 + R_1 - 6R_{2u} + 6R_{2v} - 12R_{2u}R_{2v})}{12R_1(6 + R_1)}, \quad (26c)$$

$$\bar{c}_4 = -\frac{(24 - 2R_1 - R_1^2 + 24R_{2u} + 12R_{2u}R_{2v} + 12R_{2u}^2)}{12R_1(6 + R_1)}, \quad (26d)$$

$$\bar{c}_5 = \frac{(30 + 17R_1 + 2R_1^2 + 6R_{2u}^2 + 6R_{2u}R_{2v} + 6R_{2v}^2)}{3R_1(6 + R_1)}, \quad (26e)$$

$$\bar{c}_6 = -\frac{(24 - 2R_1 - R_1^2 - 24R_{2u} + 12R_{2u}R_{2v} + 12R_{2u}^2)}{12R_1(6 + R_1)}, \quad (26f)$$

$$\bar{c}_7 = -\frac{(6 + R_1 + 6R_{2u} - 6R_{2v} - 12R_{2u}R_{2v})}{12R_1(6 + R_1)}, \quad (26g)$$

$$\bar{c}_8 = -\frac{(24 - 2R_1 - R_1^2 - 24R_{2v} + 12R_{2u}R_{2v} + 12R_{2v}^2)}{12R_1(6 + R_1)}, \quad (26h)$$

$$\bar{c}_9 = -\frac{(6 + R_1 - 6R_{2u} - 6R_{2v})}{12R_1(6 + R_1)}. \quad (26i)$$

With  $\bar{c}_1 \sim \bar{c}_9$  chosen above, the modified equation for the proposed finite-difference scheme turns out to be

$$\begin{aligned}
 & u \phi_x + v \phi_y - k (\phi_{xx} + \phi_{yy}) + K \phi - f \\
 &= \frac{h^4}{12} \left[ \left( \frac{u^2}{12k + h^2 K} - \frac{K}{12} \right) \phi_{xxxx} \right. \\
 &\quad + \left( \frac{v^2}{12k + h^2 K} - \frac{K}{12} \right) \phi_{yyyy} \\
 &\quad - \left( \frac{2uv}{12k + h^2 K} \right) \phi_{xxyy} \\
 &\quad \left. + \frac{4uv}{12k + h^2 K} (\phi_{xxyy} + \phi_{xyyy}) \right] \\
 &\quad + H.O.T. \tag{27}
 \end{aligned}$$

Note that the right-hand side represents the discretization error that may produce. It is seen that these terms approach zero as  $h \rightarrow 0$ , thus demonstrating the consistency of the proposed unconditionally stable implicit scheme. Thanks to the Lax equivalent theorem [16], convergent solution having an accuracy order of  $O(h^4)$  can be obtained from equations (25-26). To avoid adding too much damping in the convection dominated case, grid sizes should be chosen to render  $\frac{h^4}{k} \ll k$  or  $h^2 \ll k$ .

4 Numerical results

The proposed numerical method must be validated through comparison to known solutions. For this purpose, we will employ test problems which are amenable to analytic solutions. In this paper, the diffusion-reaction equation is solved in the square  $0 \leq x, y \leq 1$  so as to justify the use of the proposed scheme [17]:

$$\phi_{xx} + \phi_{yy} - H^2 \phi = -1. \tag{28}$$

Provided that the boundary values for  $\phi$  are specified as  $\phi(0, y) = \phi(1, y) = \phi(x, 0) = 1/H^2$ , and  $\phi(x, 1) = \frac{1}{H^2} + \sin \pi x$ , the exact solution to the above equation can be derived as

$$\phi(x, y) = \frac{\sin \pi x \sinh(\alpha y)}{\sinh \alpha} + \frac{1}{H^2}, \tag{29}$$

where  $\alpha^2 = (\pi^2 + H^2)$ .

We computed solutions on the two-dimensional uniform grids with the size of  $\Delta x = \Delta y = \frac{1}{60}$  and plotted  $\phi$  for the cases with  $H = 1, 10, 10^2$  and  $10^3$  in their contour-valued format. As Figs. 2-5 show, good agreement between the simulated and analytic solutions is

obtained. The computed  $L_2$ -error norms were also shown in each figure. We also carried out computations on continuously refined grids, namely  $h = \frac{1}{10}, \frac{1}{20}, \frac{1}{40}, \frac{1}{80}$  and  $\frac{1}{100}$ . This was followed by plotting  $\log(\frac{err_1}{err_2})$  against  $\log(\frac{h_1}{h_2})$ . Here, the  $L_2$ -error norms  $err_1$  and  $err_2$  were computed at two continuously refined grids  $h_1$  and  $h_2$ . Figures 6-9 show that the schemes rates of convergence for all test cases were predicted as expected.

Our attention is now drawn to validate the two-dimensional convection-diffusion equation. For this reason, we solve for the following equation which is

$L_2$ - error norm =  $0.1063 \times 10^{-8}$   
 mesh =  $80 \times 80$

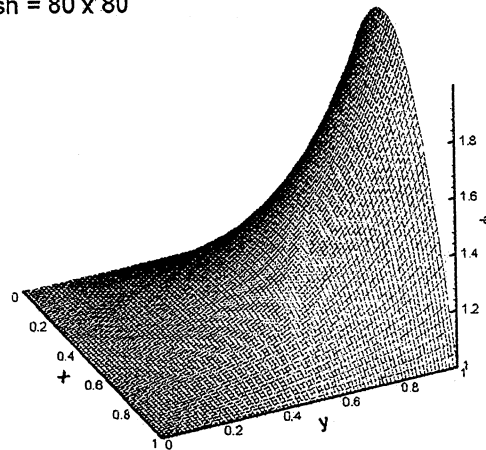


Fig.2: The computed results for the test problem given in (28), where  $H = 1$ .

$L_2$ -error norm =  $0.7439 \times 10^{-7}$   
 mesh =  $80 \times 80$

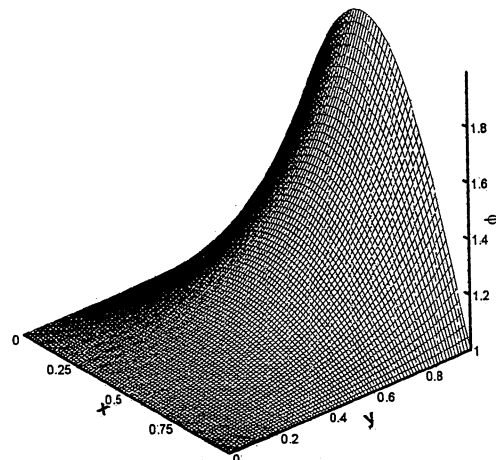


Fig.3: The computed results for the test problem given in (28), where  $H = 10$ .

also amenable to the analytical solution in  $0 \leq x, y \leq 1$ :

$$a \phi_x + b \phi_y = k (\phi_{xx} + \phi_{yy}). \quad (30)$$

For simplicity,  $a$  and  $b$  are assumed to be constant with  $a = 1$  and  $b = 1$ . Subject to the analytic boundary values of  $\phi$ , the exact solution to this linear viscous Burgers equation is given by [18] :

$$L_2\text{-error norm} = 0.1608 \times 10^{-3}$$

$$\text{mesh} = 80 \times 80$$

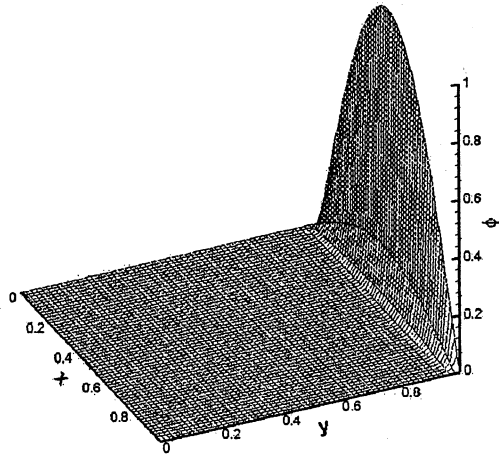


Fig.4: The computed results for the test problem given in (28), where  $H = 100$ .

$$L_2\text{-error norm} = 0.7191 \times 10^{-2}$$

$$\text{mesh} = 80 \times 80$$

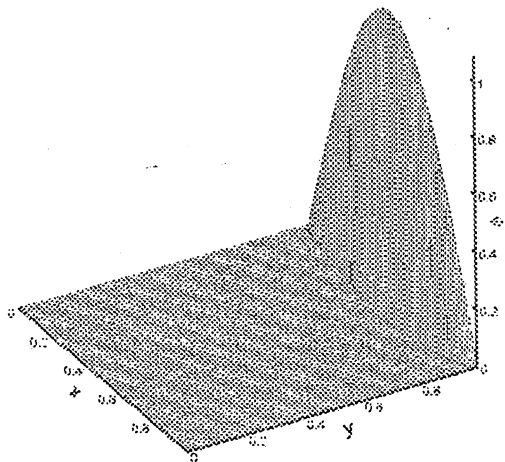


Fig.5: The computed results for the test problem given in (28), where  $H = 1000$ .

$$\phi(x, y) = \left\{ \frac{1 - \exp\left[-(x-1)\frac{a}{k}\right]}{1 - \exp\left(-\frac{a}{k}\right)} \right\} \left\{ \frac{1 - \exp\left[-(y-1)\frac{b}{k}\right]}{1 - \exp\left(-\frac{b}{k}\right)} \right\}. \quad (31)$$

Calculations at  $k = 10^{-3}, 10^{-2}, 10^{-1}$  and 1 have been carried out at mesh sizes  $h = \frac{1}{8}, \frac{1}{16}, \frac{1}{32}, \frac{1}{64}$  and  $\frac{1}{128}$ . Upon obtaining the corresponding solutions, we can compute the  $L_2$ -error norms  $err_1$  and  $err_2$  at each two consecutively refined meshes  $h = h_1$  and  $h = h_2$  and then plot  $\log\left(\frac{err_1}{err_2}\right)$  against  $\log\left(\frac{h_1}{h_2}\right)$ . With these error norms, the rates of convergence of the convection-diffusion scheme were obtained and plot-

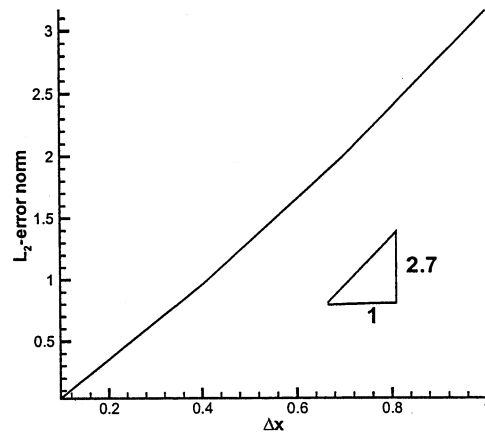


Fig.6: The computed rate of convergence for the test problem given in (28), where  $H = 1$ .

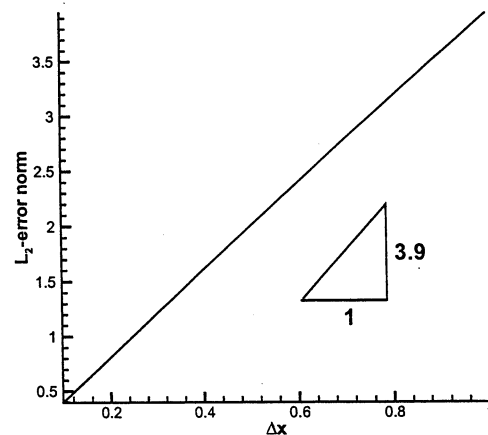


Fig.7: The computed rate of convergence for the test problem given in (28), where  $H = 10$ .

ted in Figs. 10-13. Good agreement with the results and fast convergence to the analytic solutions were both demonstrated.

Having verified the applicability of the proposed scheme to smooth problems, a more stringent test case was considered. We shall in what follows assume that  $f = 1$  and  $k = 10^{-4}$ . For simplicity, velocity vector was assumed to have the constant values of  $u = |\bar{u}| \cos(\frac{\pi}{3})$  and  $v = |\bar{u}| \sin(\frac{\pi}{3})$ . Three cases considered by Codina [14] were investigated here :

(a)  $|\bar{u}| = 1, K = 10^{-4};$  (32a)

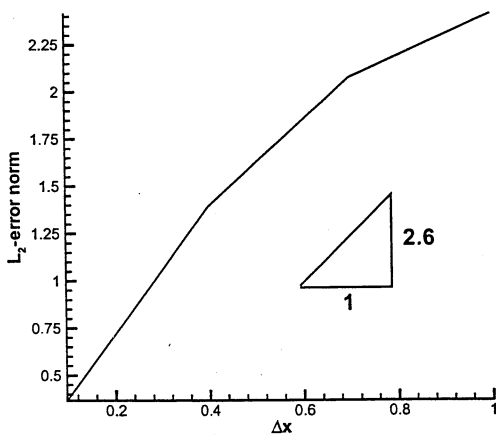


Fig.8: The computed rate of convergence for the test problem given in (28), where  $H = 100$ ,

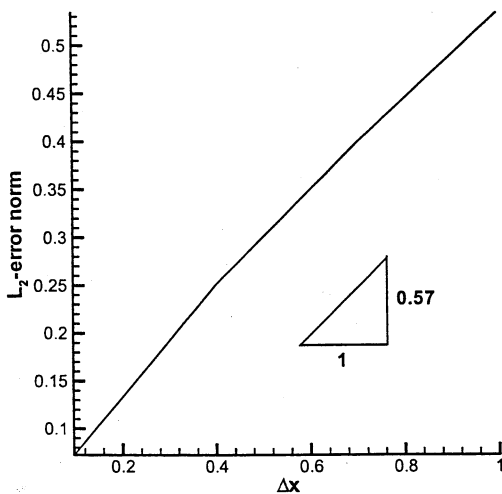


Fig.9: The computed rate of convergence for the test problem given in (28), where  $H = 1000$ .

(b)  $|\bar{u}| = 10^{-4}, K = 1;$  (32b)

(c)  $|\bar{u}| = 0.5, K = 1.$  (32c)

All three test cases were investigated subject to the homogeneous Dirichlet-type boundary condition  $\phi(\bar{x} \in \partial\Omega)$ . Simulations were performed on uniform grids  $\Delta x = \Delta y = \frac{1}{20}, \frac{1}{52}, \frac{1}{80}$  and  $\frac{1}{100}$ . The steady-state solutions obtained for these test conditions were plotted in Figs.14-16, respectively. The resolved sharp profiles demonstrated the ability of the present scheme in providing strong stability. While solutions for three test cases are shown to be non-oscillatory, this does not mean that the proposed two-

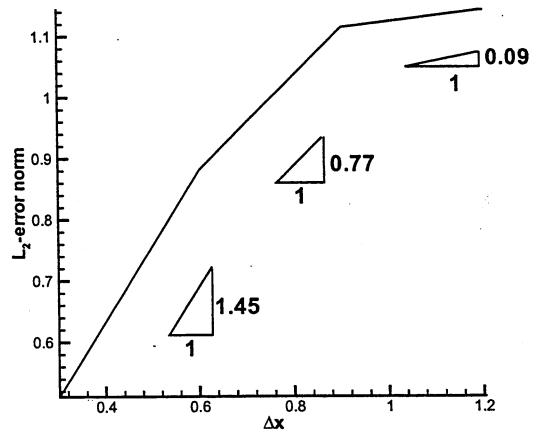


Fig.10: The computed rate of convergence for the test problem given in (30), where  $k = 0.001$ .

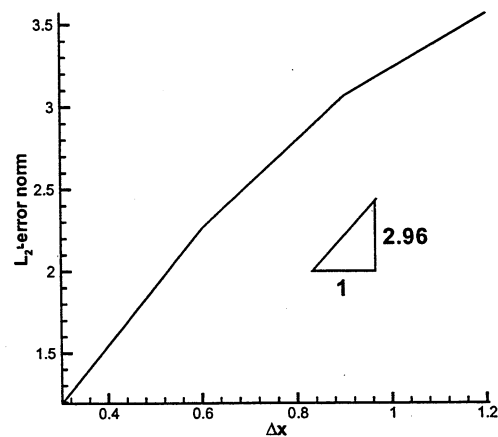


Fig.11: The computed rate of convergence for the test problem given in (30), where  $k = 0.01$ .

dimensional finite-difference scheme is classified to be monotonic. The reason is that the matrix equation of the proposed implicit scheme is conditionally classified as an  $M$ -matrix.

### 5 Concluding Remarks

We have presented in this paper a finite-difference scheme for solving the two-dimensional convection-diffusion-reaction equation. To gain computational efficiency in solving this discrete equation, we have constructed the nine-point stencil scheme on the basis of modified equation analysis. The fourth order accurate discretization scheme has been validated against analytic test cases for the investigated equation.

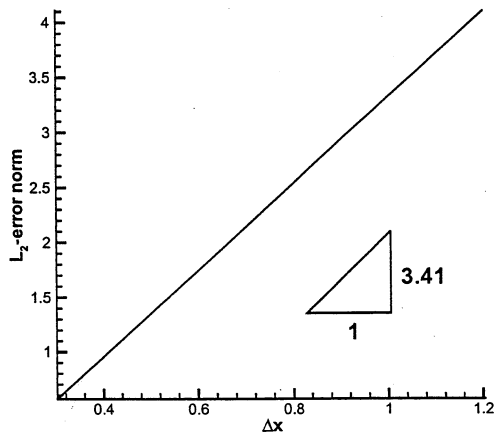


Fig.12: The computed rate of convergence for the test problem given in (30), where  $k = 0.1$ .

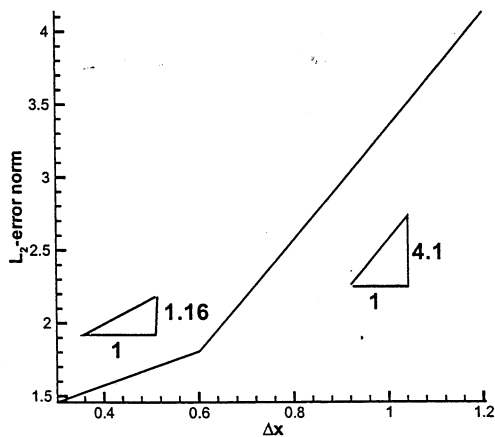


Fig.13: The computed rate of convergence for the test problem given in (30), where  $k = 1$ .

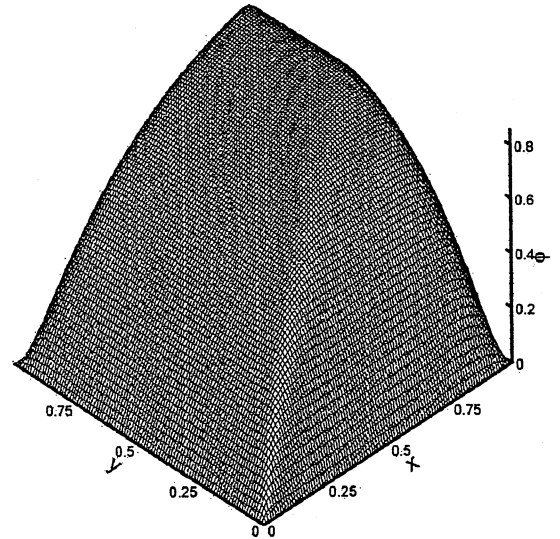


Fig.14: The result for the Codina problem, where  $u = 1$ ,  $K = 10^{-4}$ .

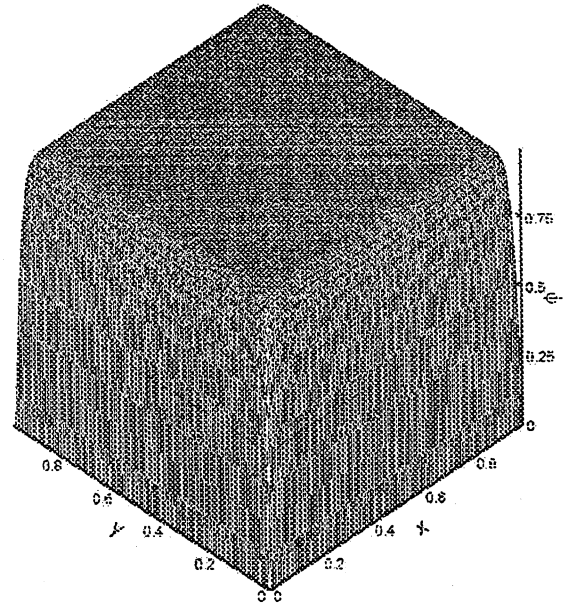


Fig.15: The result for the Codina problem, where  $u = 10^{-4}$ ,  $K = 1$ .

### Acknowledgments

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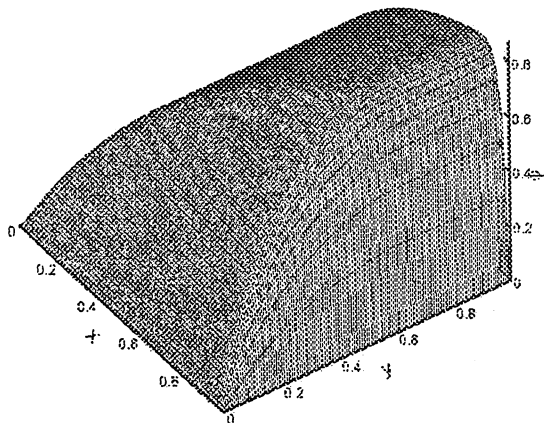


Fig.16: The result for the Codina problem, where  $u = 0.5$ ,  $K = 1$ .

## REFERENCES

- [1] I. Harari and T. J. R. Hughes, Finite element methods for the Helmholtz equation in an exterior domain : model problems, *Comput. Methods Appl. Mech. Engrg.* 87 (1991) 59-96.
- [2] F. Ilinca and D. Pelletier, Positivity preservation and adaptive solution for the  $k - \epsilon$  model of turbulence, *AIAA J.* 36(1) (1998) 44-50.
- [3] M. J. Crochet, A. R. Davies and K. Walters, *Numerical Simulation of Non-Newtonian Flow*, Elsevier Publisher, New York, 1984.
- [4] L. Leboucher, Monotone scheme and boundary conditions for finite volume simulation of magnetohydrodynamic internal flows at high Hartmann number, *J. Comput. Phys.* 150 (1999) 181-198.
- [5] B. Ataie-Ashtini, D. A. Lockington and R. E. Volker, Numerical correction of finite difference solution of the advection-dispersion equation with reaction, *J. Cont. Hydrology.* 23 (1996) 149-156.
- [6] Hossain, M. A. (1999), "Modeling advective-dispersive transport with reaction : An accurate explicit finite difference model", *Applied Mathematics and Computation.*, 102, pp. 101-108.
- [7] Hossain, M. A., Yonge, D. R. (1999), "On Galerkin models for transport in groundwater", *Applied Mathematics and Computation.*, 100, pp. 249-263.
- [8] Harari, I., Hughes. T. J. R. (1994), "Stabilized finite element methods for steady advection-diffusion with production", *Comput. Methods Appl. Mech. Engrg.*, 115, pp. 165-191.
- [9] Idelsohn, S., Nigro, N., Storti, M., Buscaglia, G. (1996), "A Petrov-Galerkin formulation for advection-reaction-diffusion problems", *Comput. Methods Appl. Mech. Engrg.*, 136, pp. 27-46.
- [10] Uri M. Ascher, Robert M. M. Mattheij, and Robert D. Russell (1988), "Numerical Solution of Boundary Value Problems for Ordinary Differential Equations", *Prentice-Hall Inc.*, New Jersey, pp. 454-456.
- [11] Doolan, E. P., Miller, J. J. H., and Schilders, W. H. A. (1980), "Uniform Numerical Methods for Problems with Initial and Boundary Layers", *Dublin: Boole Press.*
- [12] Tezdugar, T. and Park, Y. (1986), "Discontinuity capturing finite element formulations for nonlinear convection-diffusion-reaction equations", *Comput. Methods Appl. Mech. Engrg.*, 59, pp. 307-325.
- [13] Codina, R. (1993), "A shock-capturing anisotropic diffusion for the finite element solution of the diffusion-convection-reaction equation", *Finite Elements in Fluids, New Trends and Applications.*, K. Morgan (Eds.), Pineridge, Part 1, pp. 67-75.
- [14] Codina, R. (1998), "Comparison of some finite element methods for solving the diffusion-convection-reaction equation", *Comput. Methods Appl. Mech. Engrg.* 156, pp. 185-210.
- [15] Kolesnikov, A. and Baker, A.J. (2000), "Efficient implementation of high order methods for the advection-diffusion equation", *Comput. Methods Appl. Mech. Engrg.* 189, pp. 701-722.
- [16] Richtmyer, R. D. and Morton, K. W. (1967), "Difference Methods for Initial-Value Problems", 2nd ed., Interscience Publishers, Wiley, New York.
- [17] Arad, M., Yakhot, A. and Ben-Dor, G. (1996), "High-Order-Accurate Discretization Stencil for An Elliptic Equation", *International Journal for Numerical Methods in Fluids.* 23, pp. 367-377.
- [18] Tannehill, J.C., Anderson, D.A. and Pletcher, R.H. (1997), "Computational Fluid Mechanics and Heat Transfer", 2nd ed., Taylor & Francis, U.K.