Analysis of One Dimensional Advection Diffusion Model Using Finite Difference Method

Vijay Kumar Kukreja, Ravneet Kaur

Abstract—In this paper, one dimensional advection diffusion model is analyzed using finite difference method based on Crank-Nicolson scheme. A practical problem of filter cake washing of chemical engineering is analyzed. The model is converted into dimensionless form. For the grid $\Omega \times \omega = [0,1] \times [0,T]$, the Crank-Nicolson spatial derivative scheme is used in space domain and forward difference scheme is used in time domain. The scheme is found to be unconditionally convergent, stable, first order accurate in time and second order accurate in space domain. For a test problem, numerical results are compared with the analytical ones for different values of parameter.

Keywords—Consistency, Crank-Nicolson scheme, Gerschgorin circle, Lax-Richtmyer theorem, Peclet number, stability.

I. Introduction

THE phenomenon of longitudinal mixing can be defined by a parabolic partial differential equation. The displacement of solute from a packed bed of finite thickness is expressed in terms of the following one dimensional advection diffusion equation:

$$\frac{\partial c}{\partial t} = D_L \frac{\partial^2 c}{\partial x^2} - u \frac{\partial c}{\partial x} \tag{1}$$

where c(x,t) is the concentration of the fluid in the packed bed, t is the time of start of displacement of the fluid from the bed, x is the bed thickness, D_L is the axial dispersion coefficient, u is the interstitial velocity.

The initial condition is taken as $c(x,t) = C_0 = \text{constant}$. The boundary conditions are taken to be Robin type as:

$$uc - D_L \frac{\partial c}{\partial x} = uC_f, \text{ at } x = 0$$
 (2)

$$\frac{\partial c}{\partial x} = 0, \quad at \quad x = L$$
 (3)

There are many engineering applications of the above model like extraction of sunflower seed oil [4], flow reactor [6], [16], measuring of neutron flux [7], synthesis of ethylene oxide [8], biogas production by bacteria [9], distillation column [11], sorption characteristics [12], [28], chromatography [13], [24], brown stock washing [14], [15], [21], enzymatic hydrolysis [18], glass beads [20], bio synthesis [23], purification of biological compounds [26] and porous catalyst [29].

The advection diffusion model (1) is solved numerically via finite difference method (FDM) using Crank-Nicolson (CN) scheme. Details about CN scheme and other properties of

V.K. Kukreja is with the Department of Mathematics, Sant Longowal Institute of Engineering and Technology, Longowal, Punjab, 148106 India (e-mail: vkkukreja@gmail.com).

R. Kaur is with the Department of Mathematics, Rayat Bahra University, Mohali, Punjab, 140104 India (e-mail: kaur.ravneet08@gmail.com).

FDM are available in standard books like [10], [19], [25], [27]. In this paper, mathematical analysis in terms of stability, consistency and convergence is presented.

II. DISCRETIZATION OF MODEL

The model is converted into dimensionless form using the different dimensionless parameters:

$$C = \frac{c - C_f}{C_0 - C_f}, \quad X = \frac{x}{L}, \quad T = \frac{ut}{L}, \quad Pe = \frac{uL}{4D_L}.$$
 (4)

The diffusion equation(1) reduces to the following PDE:

$$\frac{\partial C}{\partial T} = \frac{1}{4Pe} \frac{\partial^2 C}{\partial X^2} - \frac{\partial C}{\partial X},\tag{5}$$

along with the initial and the boundary conditions as:

$$C(X,T) = 1, \ \forall X, \ T = 0,$$
 (6)

$$4PeC - \frac{\partial C}{\partial X} = 0, \quad X = 0, \quad T > 0, \tag{7}$$

$$\frac{\partial C}{\partial X} = 0, \quad X = 1, \quad T > 0. \tag{8}$$

In (5), the solution domain is a uniform equidistant grid $\Omega \times \omega = (x_i, t_j)$, where i = 0(1)N, j = 0(1)M. The grid $[0,1] \times [0,T]$ is subdivided into a set of equal rectangles of size $\Delta x = \frac{1}{N}$ and $\Delta t = \frac{T}{M}$ by equi-spaced lines parallel to axis. Further, the steps of discretization are given hereunder.

A. Crank-Nicolson Scheme

In Crank-Nicolson scheme [3] is applied to (5). In which forward difference is applied to approximate the time derivative, Laplacian operator is evaluated at the midpoint $(x_i, t_{j+1/2})$ and forward difference is applied for the spatial derivative. After simplification the problem reduces to:

$$\frac{C_{i,j+1} - C_{i,j}}{\Delta t} = \frac{1}{8Pe} \left[\frac{C_{i-1,j+1} - 2C_{i,j+1} + C_{i+1,j+1}}{\Delta x^2} + \frac{C_{i-1,j} - 2C_{i,j} + C_{i+1,j}}{\Delta x^2} \right] - \frac{1}{2} \left[\frac{C_{i+1,j} - C_{i-1,j}}{2\Delta x} + \frac{C_{i+1,j+1} - C_{i-1,j+1}}{2\Delta x} \right]. \quad (9)$$

By taking $\epsilon=\frac{\Delta t}{8Pe\Delta x^2}$ and $\eta=\frac{\Delta t}{4\Delta x}$, the system can be rewritten as:

$$(-\epsilon - \eta)C_{i-1,j+1} + (1+2\epsilon)C_{i,j+1} + (-\epsilon + \eta)C_{i+1,j+1}$$

= $(\epsilon + \eta)C_{i-1,j} + (1-2\epsilon)C_{i,j} + (\epsilon - \eta)C_{i+1,j}$. (10)

This linear system of equations, after incorporating the boundary condition can be expressed in the matrix form as:

$$PC^{j+1} = QC^j + R \tag{11}$$

$$C^{j+1} = \begin{bmatrix} C_{1,j+1} \\ C_{2,j+1} \\ \vdots \\ C_{N-2,j+1} \\ C_{N-1,j+1} \end{bmatrix}, C^{j} = \begin{bmatrix} C_{1,j} \\ C_{2,j} \\ \vdots \\ C_{N-2,j} \\ C_{N-1,j} \end{bmatrix}, R = \begin{bmatrix} (\epsilon + \eta)C_{0,j} \\ \vdots \\ \vdots \\ (\epsilon - \eta)C_{N,j} \end{bmatrix}$$
 (A) Therefore, for all the dates of Δi , Δi of the finite difference process for (9) is unconditionally stable. IV. ANALYSIS FOR CONSISTENCY Let $F_{i,j}(c) = 0$ represents the difference equation approximating the PDE (5) at the $(i,j)th$ mesh point, with

Here P, Q are non-symmetric and strictly diagonally dominant matrices of order $(N-1) \times (N-1)$. Matrices C^{j} and R are obtained from initial and boundary conditions respectively. The elements of matrix C^{j+1} are unknown. The above tridiagonal matrices can be solved by a variety of numerical methods to generate the output at different grid points. The matrix equation (11) can be written as:

$$C^{j+1} = AC^j + +f_i, (12)$$

where $A = P^{-1}Q$ and $f_j = P^{-1}R$.

The analytic solution [2] of the above problem by using Laplace transform is given as follows:

$$C = e^{Pe(2-T)} \sum_{k=1}^{\infty} \frac{\lambda_k sin(2\lambda_k)}{(\lambda_k^2 + Pe^2 + Pe)} \times \exp\left(\frac{-\lambda_k^2 T}{Pe}\right), (13)$$

where λ_k are positive roots, taken in order of increasing magnitude of the transcendental equation $tan2\lambda = \frac{2\lambda Pe}{\lambda^2 - Pe^2}$. This solution will be used later on for comparison at different Peclet numbers.

III. ANALYSIS FOR STABILITY

For a linear IBVP, stability of the numerical technique is the necessary and sufficient condition for convergence [22], [25]. For a 'nearly diagonal matrix', the diagonal elements are good approximates to the eigenvalues. The Gerschgorin theorem [17] quantifies this as well as provide bounds for the spectrum $\rho(A)$, i.e., eigen values of A.

Theorem1. If $R_i = \sum_{k=1, k \neq i}^{N} |a_{ik}|$ then according to Gerschgorin's circle theorem the spectrum $\rho(A)$ lies in the union of the N disks $|z - a_{ii}| \leq R_i$, in the complex plane. Clearly, if $R_i \ll |a_{ii}|$; $\forall i$ then the matrix may be approximated as diagonal.

Theorem2. Let P_s be the sum of the moduli of the elements along the s^{th} row excluding the diagonal element $a_{s,s}$. Then each eigenvalue of A lies inside or on the boundary of at least one of the circles [25], i.e., $|\lambda - a_{s,s}| \le P_s$.

Result1. When the eigenvalue λ_i of matrix A are estimated by circle theorem, then $||A||_{\infty}$ or $||A||_{1} \leq 1$ forces the condition $|\lambda_i| \leq 1.$

The matrix method guarantees the stability of (11) as long as the spectral radius $|\rho(A)|<1$. Since $\epsilon=\frac{\Delta t}{8Pe\Delta x^2}$ and $\eta=\frac{\Delta t}{4\Delta x}$, therefore $\epsilon=\beta\eta$, with $\beta=\frac{1}{2Pe\Delta x}>1$. The latter observation is true, since Δx is very small and the denominator is more prominent therefore, it can be concluded that $\epsilon > \eta$. Therefore P and Q can be treated as 'almost diagonal' since $\epsilon, \eta \ll$ 1. Hence $\rho(P^{-1}(P^{-1})') \approx \rho(P^{-2}) = \rho(P^{-1})^2$ and similarly $\rho(QQ^t) \approx \rho(Q^2) = \rho(Q)^2$.

Finally, one gets the necessary bounds for the condition of the stability. Thus, by invoking the spectral norm, it is shown that $\rho(A) < 1$. Result 1 justifies the stability of the equation (11). Hence, for all the values of Δx , $\Delta t > 0$ and P, the finite difference process for (9) is unconditionally stable.

approximating the PDE (5) at the (i,j)th mesh point, with the exact solution. The value of the local truncation error, i.e., $F_{i,j}(C)$ measures the weight by which the analytical solution (C) of the PDE (5), which is represented by the difference equation (9), using finite difference scheme, do not satisfy the difference equation at the mesh point (i, j). A numerical algorithm is successful, if it be possible to make the truncation error as small as possible by using a sufficiently small step size. This further means convergence of the scheme. From (9) the truncation error $T_{i,j}$ of the difference equation at the (i,j)mesh point is taken to be equal to the local truncation error $F_{i,j}(C)$. Therefore:

$$T_{i,j} = F_{i,j}(C) = \frac{C_{i,j+1} - C_{i,j}}{\Delta t}$$

$$-\frac{1}{8Pe} \left[\frac{C_{i-1,j} - 2C_{i,j} + C_{i+1,j}}{\Delta x^2} + \frac{C_{i-1,j+1} - 2C_{i,j+1} + C_{i+1,j+1}}{\Delta x^2} \right]$$

$$+ \left[\frac{C_{i+1,j} - C_{i-1,j}}{2\Delta x} + \frac{C_{i+1,j+1} - C_{i-1,j+1}}{2\Delta x} \right]. \quad (14)$$

Using the Taylor series expansion for different terms of C in (14), the principal component of the local truncation error becomes:

$$T_{i,j} = \left[\frac{\Delta t}{2!} \left(\frac{\partial^2 C}{\partial T^2}\right)_{i,j} - \frac{\Delta x^2}{3!} \left(\frac{\partial^3 C}{\partial X^3}\right)_{i,j}\right].$$

Therefore, the global truncation error is $T_{i,j} = O(\Delta t) +$ $O(\Delta x^2)$. Hence, the numerical scheme is consistent since $T_{i,j} \to 0$, as $\Delta x, \Delta t \to 0$.

V. ANALYSIS FOR CONVERGENCE

Let e be the global error, i.e., e = C - c. At the mesh points $c_{i,j} = C_{i,j} - e_{i,j}$ etc. Substituting these relations in (9) and

further incorporating Taylor's series expansion, one gets:

$$(-\epsilon - \eta)e_{i-1,j+1} + (1 + 2\epsilon)e_{i,j+1} + (-\epsilon + \eta)e_{i+1,j+1}$$

$$= (\epsilon + \eta)e_{i-1,j} + (1 - 2\epsilon)e_{i,j} + (\epsilon - \eta)e_{i+1,j}$$

$$+ \Delta t \left(-\frac{1}{4Pe} \frac{\partial^2 C}{\partial X^2} + \frac{\partial C}{\partial X} + \frac{\partial C}{\partial T} \right)_{(i,j)} + O(\Delta t^2) \quad (15)$$

As proposed by [25], if E_j represents Max $|e_{i,j}|$ at the j^{th} time level, irrespective of i and M_m be the maximum modulus of the PDE in (15), Then

$$E_{i+1} \le E(j) + \Delta t M_m \tag{16}$$

This recursive relation leads to:

$$E_j \le E_0 + j\Delta t M_m = t_j M_m \tag{17}$$

As initial values for c and C are same; $E_0 = 0$. Also M_m tends to zero, as C is the analytical solution of (5), therefore E_j tends to zero as Δt tends to zero. As described above, the relation of the error becomes

$$|C_{i,j} - c_{i,j}| \le E_j$$

and it is proved that E_j tends to zero. Hence, the approximate solution converges to the analytical solution.

VI. RESULTS AND DISCUSSION

A comparison of numerical (present) and analytic [2] is given in Tables and for a wide range of parameter namely, Peclet number (Pe). The values are matching appreciably for the entire range of Peclet numbers, practically from 0 to ∞ . Based on this analysis, different figures are drawn. In Figure 1 to 3, at a fixed Peclet number, relative error between the analytic results and the numeric ones is plotted for different mesh lengths in space and time domains. For different Peclet numbers (Pe=0,40,160), it is found that the value of relative error decreases as the values of Δx and Δt are becoming smaller and smaller.

In Figs. 4-6, 3D mesh diagrams indicating the behaviour of the solute removal process over the entire range of dimensionless distance and time $(0 \le X \le 1, \ 0 \le T \le 2)$ for Peclet numbers Pe=1,10,80 are plotted. It is observed as time is increasing, the solute concentration is approaching to zero. It is happening at a slow rate for small Peclet number (Pe=0), where as for higher Peclet number (Pe=80), it is fast approaching to zero.

VII. CONCLUSION

In this paper, a numerical method is discussed for the advection diffusion problem over a finite slab, where the partial time derivative is interpreted in the sense of forward difference. The stability, consistency and convergence of the method are estimated. The method is unconditionally stable for any time and space steps. The results obtained by the Crank-Nicolson scheme for a test problem are compared with the analytic solution. The scheme is found to be simple, elegant and easy to use. The scheme is second order stable in space domain and first order in time domain. Further the scheme can be extended for linear and non linear PDEs. For the test example, the numeric results are matching with the analytic ones.

TABLE I COMPARISON OF ANALYTIC AND NUMERIC VALUES FOR SMALL Pe

	Pe = 1		Pe = 6		Pe = 40	
t	Analytic	Present	Analytic	Present	Analytic	Present
	[2]	N=1000	[2]	N=1000	[2]	N=1500
		M=6000		M=6000		M=5000
0.0	1.000E+0	1.000E+0	1.000E+0	1.000E+0	1.000E+0	1.000E+0
0.2	9.951E-1	9.951E-1	1.000E+0	1.000E+0	1.000E+0	1.000E+0
0.4	8.985E-1	8.986E-1	1.000E+0	9.994E-1	1.000E+0	1.000E+0
0.6	7.177E-1	7.177E-1	9.559E-1	9.960E-1	1.000E+0	1.000E+0
0.8	5.378E-1	5.377E-1	7.455E-1	7.455E-1	9.747E-1	9.748E-1
1.0	3.909E-1	3.909E-1	4.448E-1	4.448E-1	4.778E-1	4.781E-1
1.2	2.801E-1	2.800E-1	2.144E-1	2.144E-1	4.493E-2	4.504E-2
1.4	1.992E-1	1.992E-1	8.905E-2	8.908E-2	9.904E-4	9.952E-4
1.6	1.412E-1	1.412E-1	3.341E-2	3.342E-2	7.900E-6	7.935E-6
1.8	9.987E-2	9.985E-2	1.168E-2	1.168E-2	3.111E-8	3.120E-8
2.0	7.058E-2	7.057E-2	3.882E-3	3.884E-3	7.41E-11	7.41E-11

TABLE II COMPARISON OF ANALYTIC AND NUMERIC VALUES FOR LARGE Pe

	Pe = 80		Pe = 160		Pe = 320	
t	Analytic	Present	Analytic	Present	Analytic	Present
	[2]	N=2000	[2]	N=2000	[2]	N=2000
		M=10000		M=10000		M=10000
0.0	1.000E+0	1.0000+0	1.000E+0	1.000E+0	1.000E+0	1.000E+0
0.2	1.000E+0	1.000E+0	1.000E+0	1.000E+0	1.000E+0	1.000E+0
0.4	1.000E+0	1.000E+0	1.000E+0	1.000E+0	1.000E+0	1.000E+0
0.6	1.000E+0	1.000E+0	1.000E+0	1.000E+0	1.000E+0	1.000E+0
0.8	9.974E-1	9.974E-1	9.999E-1	9.999E-1	1.000E+0	1.000E+0
1.0	4.843E-1	4.846E-1	4.889E-1	4.893E-1	5.000E-1	4.929E-1
1.2	9.282E-3	9.288E-3	4.874E-4	4.852E-4	0.000E+0	1.638E-6
1.4	7.615E-6	7.594E-6	5.92E-10	5.70E-10	0.000E+0	3.45E-18
1.6	7.12E-10	7.05E-10	7.79E-18	7.04E-18	0.000E+0	5.36E-34
1.8	1.50E-14	1.47E-14	4.76E-27	3.93E-27	0.000E+0	1.31E-52
2.0	1.10E-19	1.06E-19	3.33E-19	2.47E-37	0.000E+0	3.39E-73

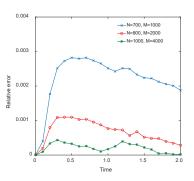


Fig. 1 Relative Error for different Δx and Δt at Pe=0

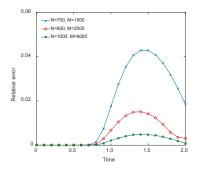


Fig. 2 Relative Error for different Δx and Δt at Pe=40

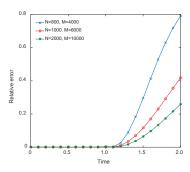


Fig. 3 Relative Error for different Δx and Δt at Pe=160

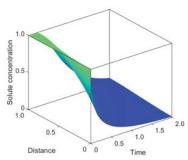


Fig. 4 Mesh Diagram at Pe=0 for $\Delta x=\frac{1}{1000}$ and $\Delta t=\frac{1}{3000}$

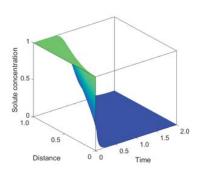


Fig. 5 Mesh Diagram at Pe=10 for $\Delta x=\frac{1}{1000}$ and $\Delta t=\frac{1}{3000}$

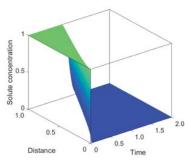


Fig. 6 Mesh Diagram at Pe=80 for $\Delta x=\frac{1}{2000}$ and $\Delta t=\frac{1}{5000}$

REFERENCES

- [1] H. Kopka and P. W. Daly, A Guide to ETEX, 3rd ed. Harlow, England: Addison-Wesley, 1999.
- H. Brenner, The diffusion model of longitudinal mixing in beds of finite length. Numerical values, Chem. Eng. Sci. 17(4) (1962) 229-243.
- J. Crank, P. Nicolson, A practical method for numerical evaluation of solutions of partial differential equations of the heat conduction type, Proc. Cambridge Philosophy Soc. 43(1) (1947) 50-67.
- [4] M.J. Cocero, J. Garcia, Mathematical model of supercritical extraction applied to oil seed extraction by CO2+ saturated alcohol I.Desorption model, J. Supercritical Fluids 20(3) (2001) 229-243.
- P.V. Danckwerts, Continuous flow systems distribution of residence times, Chem. Eng. Sci. 2(1) (1953) 1-44.
- S. Farooq, I.A. Karimi, Dispersed plug flow model for steady-state laminar flow in a tube with a first order sink at the wall, Chem. Eng. Sci. 58(1) (2003) 7180.
- [7] M. Feiz, A 1-D multigroup diffusion equation nodal model using the orthogonal collocation method, Annals of Nuclear Energy 24(3) (1997)
- [8] L. Gardini, A. Servida, M. Morbidelli, S. Carra, Use of orthogonal collocation on finite elements with moving boundaries for fixed bed catalytic reactor simulation, Comp. Chem. Eng. 9(1) (1985) 1-17.
- [9] B. Giojelli, C. Verdier, J.Y. Hihn, J.F. Beteau, A. Rozzi, Identification of axial dispersion coefficients by model method in gas/liquid/solid fluidised beds, Chem. Eng. P. 40(2) (2001) 159-166.
- C. Grossman, H.G. Roos, M. Stynes, Numerical Treatment of Partial Differential Equations, Springer-Verlag, Heidelberg 2007.
 [11] S. Karacan, Y. Cabbar, M. Alpbaz, H. Hapoglu, The steady-state
- and dynamic analysis of packed distillation column based on partial differential approach, Chem Eng. P. 37(5) (1998) 379-388.
- [12] I.A. Khan, K.F. Loughlin, Kinetics of sorption in deactivated zeolite
- crystal adsorbents, Comp. Chem. Eng. 27(5) (2003) 689-696. J.H. Koh, P.C. Wankat, N.H.L. Wang, Pore and surface diffusion and bulk-phase mass transfer in packed and fluidized beds, Ind. Eng. Chem. Res. 37(1) (1998) 228-239.
- [14] V.K. Kukreja, A.K. Ray, V.P. Singh, N.J. Rao, A mathematical model for pulp washing on different zones of a rotary vacuum filter, Indian Chem. Eng., Sec- A 37(3) (1995) 113-124.
- [15] V.K. Kukreja, A.K. Ray, Mathematical modeling of a rotary vacuum washer used for pulp washing: A case study of a lab scale washer, Cell. Chem. Tech. 43(1-3) (2009) 25-36.
- [16] L. Lefevre, D. Dochain, S.F. Azevedo, A. Magnus, Optimal selection of orthogonal polynomials applied to the integration of chemical reactor equations by collocation methods, Comp. Chem. Eng. 24(12) (2000) 2571-2588.
- [17] J.R. LeVeque, R. Bali, Finite Difference Methods for Ordinary and Partial Differential Equations Steady-State and Time-Dependent Problems, SIAM, Philadelphia, 2007.
- W.S. Long, S. Bhatia, A. Kamaruddin, Modeling and simulation of enzymatic membrane reactor forkinetic resolution of ibuprofen ester, J. Membrane Sci. 219(1-2) (2003) 69-88.
- C.G. Mingham, D.M. Causon, Introductory Finite Difference Methods for PDEs, Ventus Publishing, 2010.
- F. Potucek, Washing of pulp fibre beds, Collect. Czech. Chem. Commun. 62(4) (1997) 626-644.
- A.K. Ray, V.K. Kukreja, Solving pulp washing problems through mathematical models, AIChE Symposium Series, 96(324) (2000) 42-47.
- R.D. Richtmyer, K.W. Morton, Difference Methods for Initial Value Problems, Interscience Publishers, John Wiley & Sons, New York, 1967.
- L. Sajc, G.V. Novakovic, Extractive bioconversion in a four-phase external-loop airlift bioreactor, AIChE J. 46(7) (2000) 1368-1375.
- [24] N.V. Saritha, G. Madras, Modeling the chromatographic response of inverse size-exclusion chromatography, Chem. Eng. Sci. 56(23) (2001) 6511-6524.
- [25] G.D. Smith, Numerical Solutions of Partial Differential Equations: Finite Difference Methods, Clarendon press-Oxford, New York, 1985.
- [26] P. Sridhar, Implementation of the one point orthogonal collocation method to an affinity packed bed model, Ind. Chem. Eng., Sec. A 41(1) (1999) 39-46.
- J.C. Strikwerda, Finite Difference Schemes and Partial Differential Equations, SIAM, Philadelphia 2004.
- L.M. Sun, F. Meunier, An improved finite difference method for fixed bed multicomponent sorption, AIChE J. 37(2) (1991) 244-254.
- [29] M.K. Szukiewicz, New approximate model for diffusion and reaction in a porous catalyst, AIChE J. 46(3) (2000) 661-665.

International Journal of Engineering, Mathematical and Physical Sciences

ISSN: 2517-9934 Vol:13, No:10, 2019



Vijay K. Kukreja did his Ph.D. from University of Roorkee, India in 1997. Presently he is Professor at Department of Mathematics, SLIET Longowal, India. His areas of interest are mathematical modelling and numerical analysis. He has handled two research projects. Based on this he has published 50 research papers in journals of international repute. He has guided 4 Ph.D. students. He has presented papers in conferences like ICM-06, ICIAM-07, CMAM-10, ICIAM-11 and ICNAAM-13.



Ravneet Kaur is an Associate Professor at Department of Mathematics, Rayat Bahra University, Mohali, India. Her area of interest is numerical analysis. Presently she is pursuing her Ph.D. on the topic 'Solution of some partial differential equations using finite difference method' from SLIET Longowal under the supervision of Prof. V.K. Kukreja. She has extensively participated in conferences and presented research papers.