Numerical Solutions of Two Point Boundary Value Problems Using Collocation Techniques

Shelly, Inderpreet Kaur

Abstract— A comparative study of weighted residual methods has been made on different types of advection diffusion equations. Both the linear and non-linear models have been discretized by orthogonal collocation method (OCM) and orthogonal collocation on finite elements (OCFE). Model equations have been solved by MATLAB 'ode15s' system solver. Numerical values have been compared with analytic ones and interpreted by relative error and L_2 norm with respect to space variable, in terms of 2D and 3D plots to check the efficiency of numerical techniques. Non linear model equations have been simulated using the experimental data.

Index Terms— Advection diffusion equation, Collocation points, Finite elements, Orthogonal collocation, Peclet number.

1 INTRODUCTION

THE problem of diffusion dispersion in porous solid and semisolid particles has gained momentum in the field of mathematical modeling for the past few years. Variety of numerical and analytic techniques such as Laplace transforms, Variable seperable, Finite difference, tau method, Galerkin method, least square method, spline collocation, orthogonal collocation method, orthogonal collocation on finite elements, spectral methods etc. have been proposed so far to solve model equations. For linear models, analytic techniques such as Laplace transforms [1], [2], [3], [4] are used to solve model equations. However, in case of non linear models, variety of numerical techniques, *e.g.*, Galerkin techniques [5], [6], [7], [8], [9] least square method [10], [11], spline collocation [12], [13], [14], [15], [16], orthogonal collocation [17], [18], [19], [20], [21], [22], orthogonal collocation on finite elements [23], [24], [25], [26], [27], [28], [29] etc. are used to discretize the model equations. Among all these techniques, collocation techniques are the simplest form of weighted residual methods to solve the two point boundary value problems.

Basically in collocation techniques an unknown function $\overline{y}$ is assumed to satisfy the differential equation $£^V(y) = 0$ with boundary conditions $£^B(y) = 0$, where B is the boundary adjoining the volume V and £ be an operator. An unknown trial function y^N is used to discretize the unknown function $\overline{y}$. This unknown trial function y^N is represented by a series of orthogonal polynomials and the residual is defined by $£^V(y^N)$ and $£^B(y^N)$ over its region. This residual is set equal to zero at collocation points which are basically the zeros of the orthogonal polynomials forming the basis. This method is known as orthogonal collocation.

However, for stiff boundary value problems having steep gradients near the boundaries, orthogonal collocation method fails to give results for values of parameters near to singularity. To overcome this problem, Carey & Finlayson [23] has proposed to combine orthogonal collocation technique with finite element method.

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In orthogonal collocation on finite elements (OCFE) the global variable x influences the solutions even at small values. Thus the differential algebraic equations for an element of length Δx are coupled with those of all the other elements. The orthogonal collocation is applied within ℓ^{th} element on local variable u obtained by transforming global variable x using the formula $u = (x - x_\ell)/\Delta x$, where x ε $[x_{\ell-1}, x_\ell]$. In this process it is mandatory that the trial function and its first derivative should be continuous at nodal points.

2 COLLOCATION PROCEDURE

In orthogonal collocation method the trial function $\tilde{y}$ is approximated in terms of Lagrangian interpolation polynomial as:

$$y^n(x) = \sum_{i=1}^{n+1} l_i(x) y(x_i) \tag{1}$$

where, $l_i(x) = \psi(x)/[(x - x_i)\psi'(x_i)]$ (2)

$$\psi(x) = x(1-x)\prod_{j=2}^{n}(x - x_j) \tag{3}$$

where x_j's are the zeros of the orthogonal polynomial $P_n(x)$, x_1=0 and x_{n+1}=1. The discretization matrices for first and second order derivative of approximating function at j^{th} collocation point are obtained by differentiating the interpolating polynomial $\psi(x)$ at j^{th} collocation point. The details of collocation procedure are given in Arora et. al. [25].

2.1 Collocation Point

The base of collocation technique is the choice of collocation points. To study the effect of solution profiles at the boundaries of porous media, zeros of Legendre polynomial which is a special case of Jacobi polynomial are followed and has been calculated from the following recurrence frmula:

$$(j-1)P_{j-1}(x) = (2j-3)xP_{j-2}(x) - (j-2)P_{j-3}(x), \quad j=2,3,\ldots,n+1 \tag{4}$$

where $P_0(x) = 1$ and $P_{-1}(x) = 0$. In case of Legendre polynomial, 0 and 1 are taken to be the boundary points. x_j's are transformed onto the interval [0,1] using the formula given by,

$u_{n+3-j} = \frac{x_j}{2} + \frac{1}{2}$, where u_j is the local variable and x_j is the global variable.

3 Convergence and Error Analysis

The crest of every numerical technique lies within its convergence and stability analysis. Higher the convergence, more stable will be the method. In this paper, the convergence of OCFE has been checked on the basis of element size. Following formula has been followed to check the convergence of orthogonal collocation on finite elements.

$$L = Kh^2 y \tag{5}$$

where K is any constant depending upon the number of collocation pointsand h is the element size. Convergence of OCFE depends upon the number of elements as well as on the number of collocation points unlike the orthogonal collocation method. For OCFE to be convergent, $\|L\|_2 \leq 1$ i.e.

$$Kh^2 \|y\|_2 \leq 1 \tag{6}$$

The relative error is calculated by using the formulae,

$\frac{y_{ex} - y_{nm}}{y_{ex}}$, where y_{ex} is the exact or analytic value of the problem and y_{nm} is the numerical value calculated by using numerical techniques. The graphs are plotted for different number of elements. It is observed that with the increase in the number of elements the relative error decreases considerably which shows that the discretization error is proportional to h^2.

4 Results and Discussions

To check the convergence and applicability of the OCM and OCFE, both the methods have been applied to different types of advection-diffusion equation as discussed below:

Problem 1

Consider a transient linear advection-diffusion equation involving Peclet number (Pe). It is the ratio of advection to dispersion and is inversely proportional to axial dispersion coefficient. The details of this problem are available in Arora et. al. [25].

$$\frac{\partial C}{\partial t} = \frac{1}{Pe}\frac{\partial^2 C}{\partial x^2} - \frac{\partial C}{\partial x} \qquad (x,t) \in (0,1) \times (0,T] \tag{7}$$

Boundary conditions:

$$C - \frac{1}{Pe}\frac{\partial C}{\partial x} = 0, \qquad \text{at } x = 0, \text{ for all } t \geq 0 \tag{8}$$

$$\frac{\partial C}{\partial x} = 0, \qquad \text{at } x = 1, \text{ for all } t \geq 0 \tag{9}$$

Initial condition: $C = 1$, at $t = 0$, for all x (10)

This problem has been solved by using OCM. The detail of the methodis given in Villadsen& Stewart [17]. In OCM, the number of collocation points hasvaried from 5 to 19. In Fig. 1, the effect of Pe is shown for 5 collocation points. It is observed from this figure that minor oscillations occur at initial stage for Pe=5, whereas sharp oscillations occur at Pe = 10 and 15. For Pe=15, values may go down to negative as time increases from 2, however, this variation is of small order. In Fig. 2 to 5, the behaviour of solution profiles and relative error for different values of Pe is shown in form of 3D graphs.It is observed from these figures that relative error goes upto 2% for Pe= 3.2 and Pe = 4, whereas for Pe=16, it goes upto 4% for 5 collocation points. This effect can be reduced by increasing the number of collocation points. In Table1, the comparison between number of collocation points is shown for Pe=16.One can observe from this Table that for 5 to 9 collocation points, the relative error is very high and is more than 1% for large time period, which reduces considerably with the increase in collocation points from 9 to 11. However, this effect is only for the values of Pe≤ 20. As the value of *Pe* increases, the results obtained even for large number of collocation points do not converge to steady state condition smoothly.

The problem has also been solved using OCFE. The discretized form of equations (7) to (10) for ℓ^{th} element is given as:

$$\frac{dC_j^{\ell}}{dt} = \frac{1}{Pe\,h^2}\sum_{i=1}^{n+1} B_{ji} C_i^{\ell} - \frac{1}{h}\sum_{i=1}^{n+1} A_{ji} C_i^{\ell} , \quad j = 2,3,\ldots,n \ \ \& \ \ \ell = 1,2,\ldots,r \tag{11}$$

$$C_1^1 - \frac{1}{Pe\,h}\sum_{i=1}^{n+1} A_{1i} C_i^1 = 0, \quad \text{at } x = 0 \tag{12}$$

$$\sum_{i=1}^{n+1} A_{n+1i} C_i^r = 0, \quad \text{at } x = 1 \tag{13}$$

$$C_i^{\ell} = 1, \quad \text{at } t = 0, \forall\, i = 1,2,\ldots,n+1 \ \& \ \ell = 1,2,\ldots,r \tag{14}$$

$$C_{n+1}^{\ell} = C_1^{\ell+1} \qquad \ell = 1,2,\ldots,r\text{-}1 \tag{15}$$

$$\sum_{i=1}^{n+1} A_{n+1i} C_i^{\ell} = \sum_{i=1}^{n+1} A_{1i} C_i^{\ell+1} \qquad \ell = 1,2,\ldots,r\text{-}1 \tag{16}$$

This resulting set of differential algebraic equations when clubbed up, reduces into a tri-diagonal matrix structure as shown below, with one side column of differential coefficients of C and other side coefficient matrix of C. Matrix 'M' is the coefficient matrix and matrix D is the matrix of differential coefficients of C. The crosses shows the collocation equations within each element. The single column on the right hand side signifies the time derivatives of the C and the boxes represented by empty circles shows the boundary conditions and continuity conditions.

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<table>
<tr><td>B.C. at x= 0</td><td rowspan="2">0</td></tr>
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<tr><td>B.C. at x=1</td></tr>
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The resulting set of system of differential algebraic equations is solved using MATLAB with ode15s system solver. In Fig. 6, the behaviour of solution profiles is shown for Pe varying from 40 to 100. It is observed from this figure that solutions profiles converge to steady state condition smoothly and no oscillation occur even at initial stage.The behaviour of relative error with respect to time and exit solute concentration is shown in 3D graphs from Fig. 7 to 10, for Pe varying from 40 to 100. It is observed that in no case the relative error increases from 10^{-3} and is therefore, less than 1%.

In Table 2, a comparison between OCM and OCFE is shown for Pe =80. It is quite clear from Table 2 that in case of OCM the relative error is greater than 1% as τ increases from 1.5 even for 19 collocation points, whereas in case of OCFE, the relative error is less than 1% for just 25 elements.

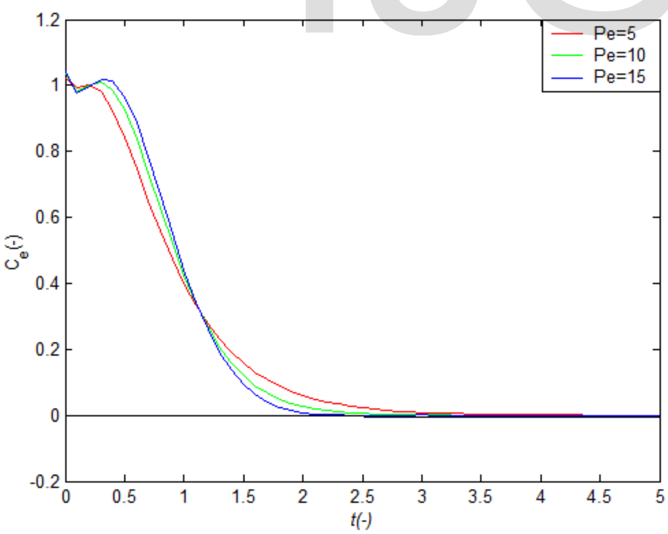


Fig. 1: Behaviour of solution profiles for different values of Pe with 5 collocation points.

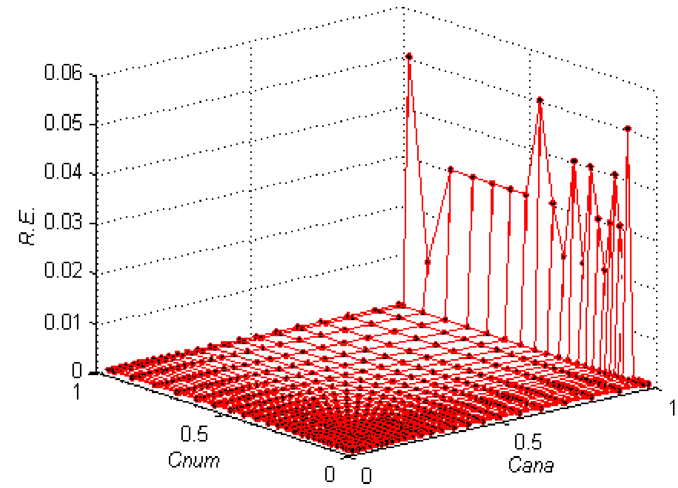


Fig. 2: Behaviour of relative Error for Pe=0.8

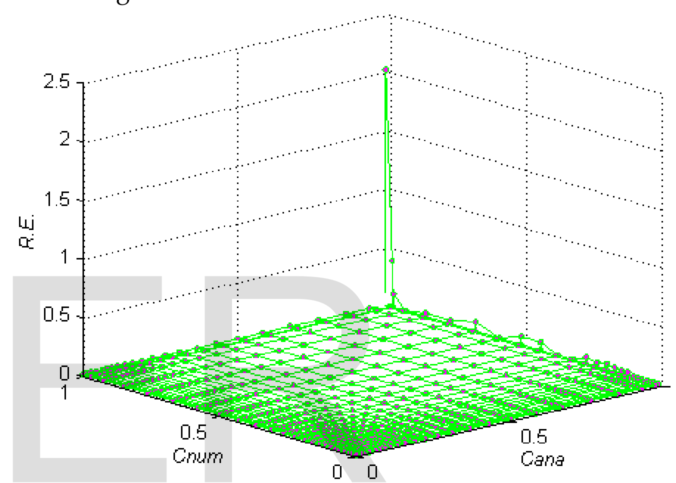


Fig.3: Behaviour of relative Error for Pe=3.2

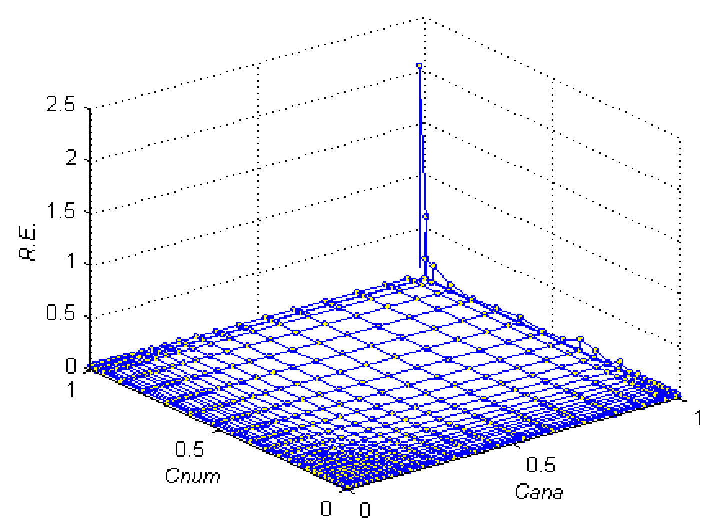


Fig.4: Behaviour of relative Error for Pe=4

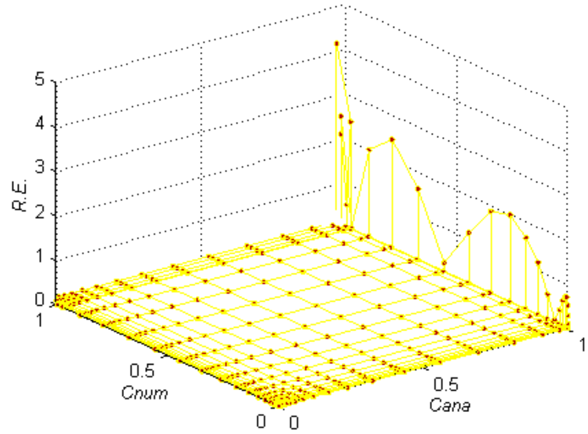


Fig.5: Behaviour of relative Error for Pe=16

Problem 2

Consider a non-linear advection-diffusion equation involving two parameters Peclet number (Pe)and Biot number (Bi). Biot number represents mass transfer resistance inside and on the surface of body. Details of the problem are available in Arora & Potůček [27].

$$\frac{\partial Q}{\partial t}+\frac{1-\beta}{\beta}N'\frac{\partial N}{\partial t}=Bi(C-Q)\ ,$$

$$(x,t)\in(0,1)\times(0,T] \qquad (17)$$

$$\frac{\partial N}{\partial t}=P^{*}\left[Q(1-N)-(N/k^{*})\right]\ ,$$

$$(x,t)\in(0,1)\times(0,T] \qquad (18)$$

$$\frac{\partial C}{\partial t}=\frac{1}{Pe}\frac{\partial^2 C}{\partial x^2}-\frac{\partial C}{\partial x}-2\theta Bi(C-Q)\ ,$$

$$(x,t)\in(0,1)\times(0,T] \qquad (19)$$

The initial and boundary conditions are similar to Problem 1 with Q and N are also equal to unity at t = 0. This problem has been solved by using OCM and OCFE. The model equations have been simulated using the data given in Arora & Potůček [30]. In case of orthogonal collocation, 5 to 11 collocation points have been taken to discretize the system of model equations. In Fig. 11 the behaviour of solution profiles is shown for different values of Pe and Bi in case of OCM. As Pe and Bi increases, wide oscillations are observed at initial stage giving error of more than 4% and for Pe =20.81 and Bi=10, the solution profiles even diverge to negative values as time increases.In Fig. 12, the solution profiles have been plotted using OCFE for 10 elements. This figure not only signify the effect of Pe and Bi but also shows the effect of ε, i.e., bed porosity. As ε lies within 0.67 to 0.69, solution profiles almost overlap each other. However, the values of Pe and Bi are different in all the cases. As ε increases to 0.812, solution profiles converge to steady state condition more rapidly as compare to the case of ε = 0.5561.

From Fig. 13 to 17, the convergence of solution profiles is shown using $||C||_2$ for different values of Pe and Bi. In all the cases it is observed that the $||C||_2$ is less than 1 and smoothly converge to 0 without any oscillation at any stage. It authenticates the fact that at any time period the values of solution profiles are converging to steady state condition without any oscillation.

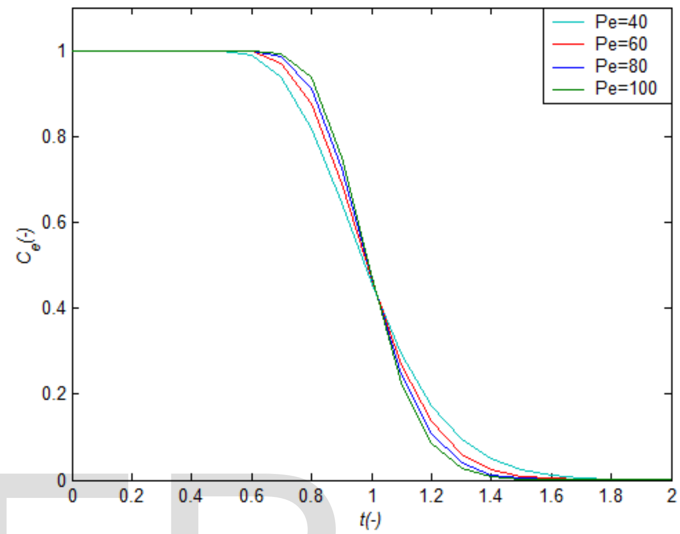
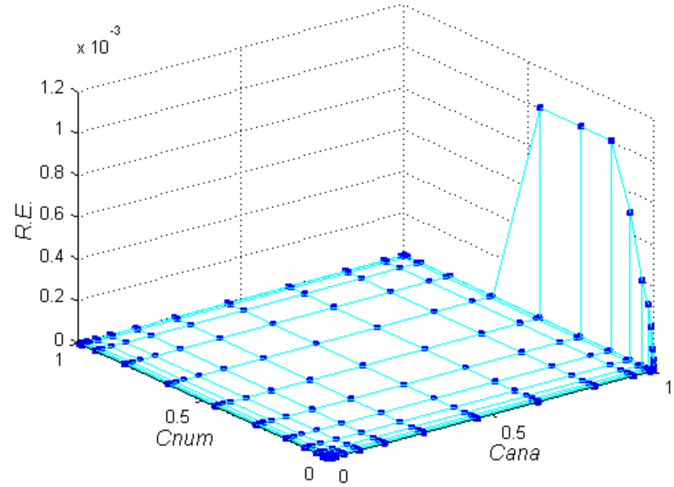


Fig. 6:Behavior of solution profiles for different values of Pe

Fig. 7: Behaviour of relative Error for Pe=40 with 15 elements



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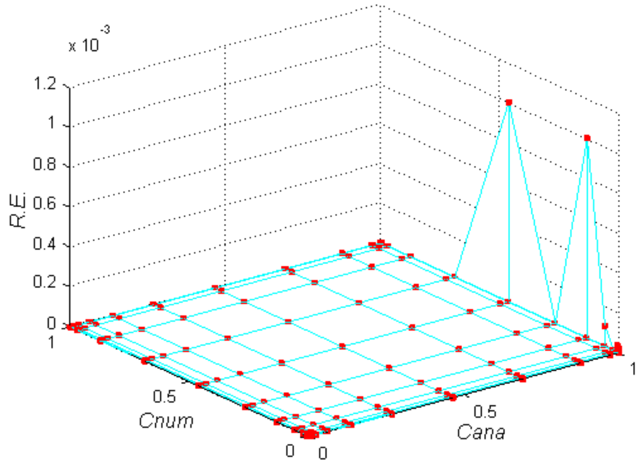

Fig. 8: Behaviour of relative Error for Pe=60 with 15 elements

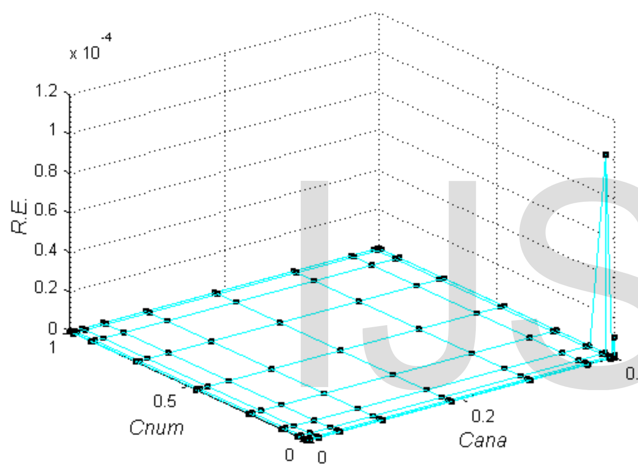

Fig. 9: Behaviour of relative Error for Pe=80 with 50 elements

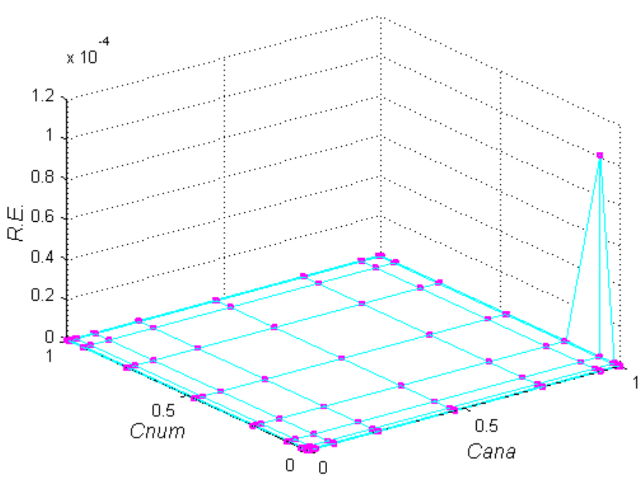

Fig.10: Behaviour of relative Error for Pe=100 with 50 elements

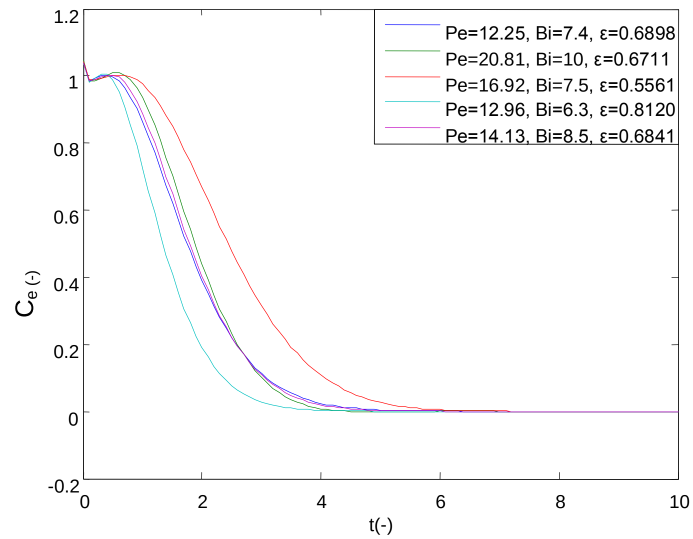

Fig. 11:Behavior of solution profiles for different values of Pe and Bi for OCM

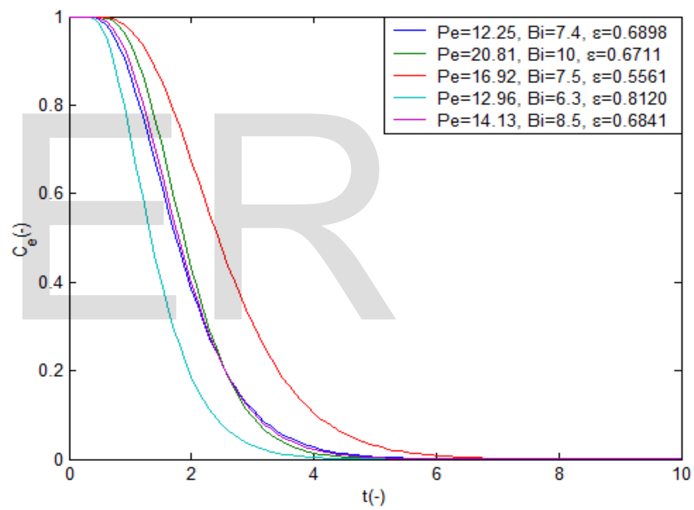

Fig. 12:Behavior of solution profiles for different values of Pe and Bi for OCFE

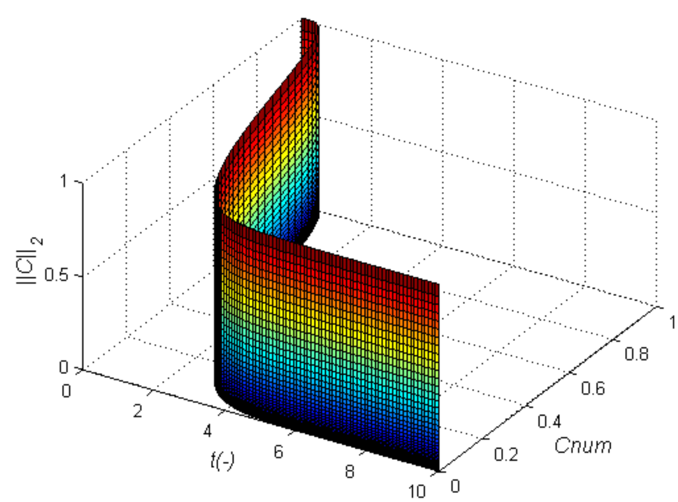

Fig. 13:Behavior of solution profiles for Pe=12.25 andBi=7.4

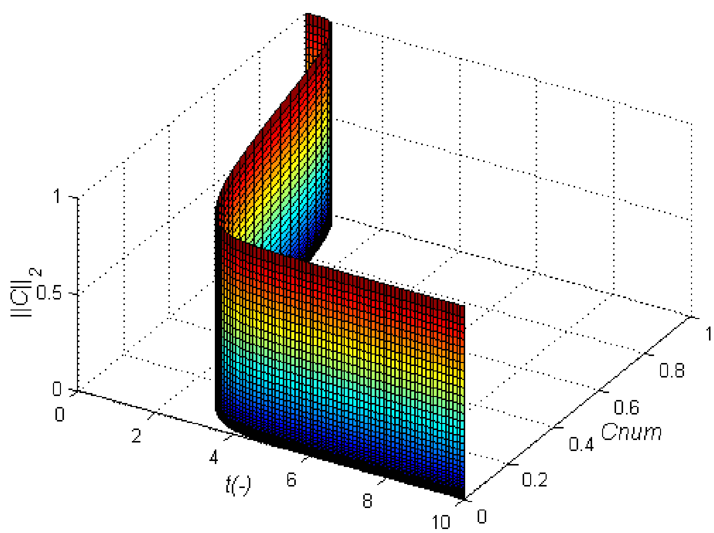

Fig.14:Behavior of solution profiles for Pe=20.81 and Bi=10

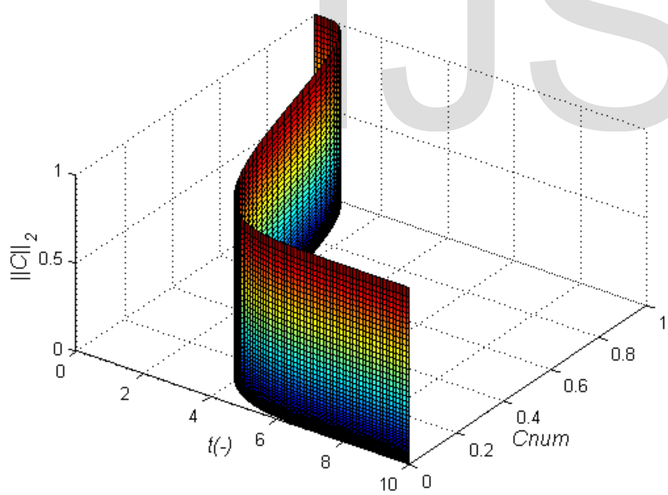

Fig.15:Behavior of solution profiles for Pe=16.92 and Bi=7.5

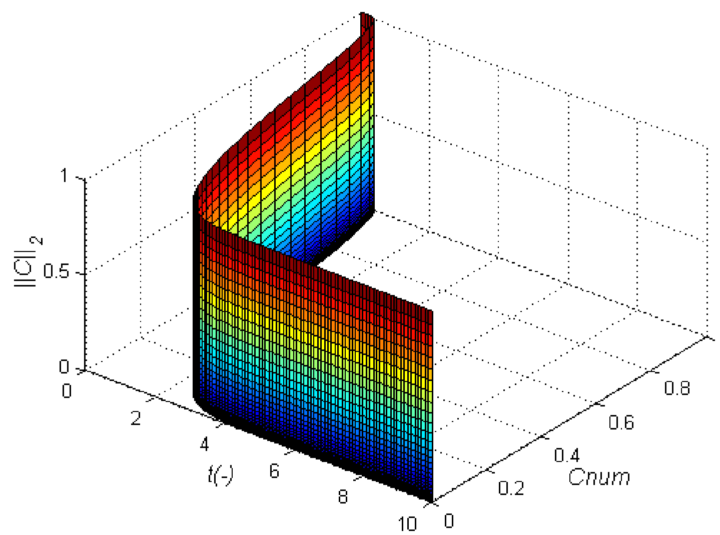

Fig.16:Behavior of solution profiles for Pe=12.96 and Bi=6.3

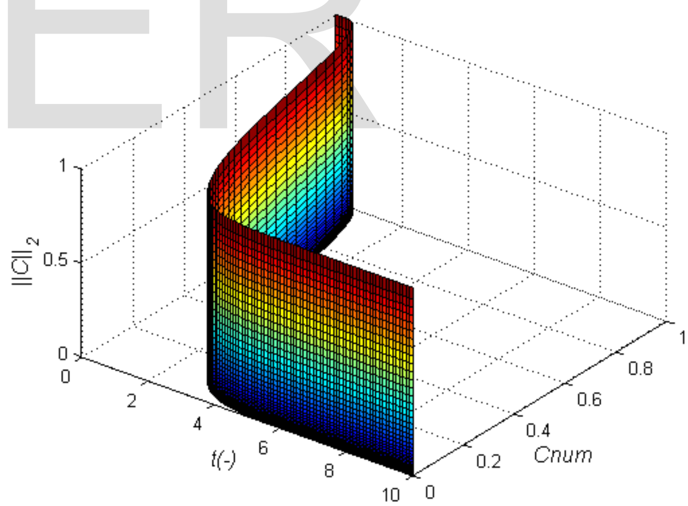

Fig. 17:Behavior of solution profilesfor Pe=14.13 and Bi=8.5

TABLE 1
COMPARISON OF COLLOCATION POINTS FOR PECLET NUMBER=16

t (-)	Analytic solution	5collocation points	9collocation points	11collocation points	% error for 5collocation points	% error for 9collocation points	% error for 11collocation points
0	1.000	1.0426	1.0038	1.0017	4.2600	3.8000×10^{-1}	1.7000×10^{-1}
0.2	9.999×10^{-1}	9.9523×10^{-1}	1.0001	1.0002	4.6705×10^{-1}	2.0002×10^{-2}	3.0003×10^{-2}
0.5	9.716×10^{-1}	9.7213×10^{-1}	9.7281×10^{-1}	9.7302×10^{-1}	5.4549×10^{-2}	1.2454×10^{-1}	1.4615×10^{-1}
1.0	4.338×10^{-1}	4.4455×10^{-1}	4.3393×10^{-1}	4.3406×10^{-1}	2.4781	2.9968×10^{-2}	5.9935×10^{-2}
1.2	2.396×10^{-1}	2.5886×10^{-1}	2.3968×10^{-1}	2.3975×10^{-1}	8.0384	3.3389×10^{-2}	6.2604×10^{-2}
1.4	1.214×10^{-1}	1.3265×10^{-1}	1.2143×10^{-1}	1.2147×10^{-1}	9.2669	2.4712×10^{-2}	5.7661×10^{-2}
1.6	5.807×10^{-2}	5.8590×10^{-2}	5.8075×10^{-2}	5.8096×10^{-2}	8.9547×10^{-1}	8.6103×10^{-3}	4.4774×10^{-2}
2.0	1.195×10^{-2}	5.2137×10^{-3}	1.1945×10^{-2}	1.1953×10^{-2}	5.6371×10^{1}	4.1841×10^{-2}	2.5105×10^{-2}
2.2	5.242×10^{-3}	1.5708×10^{-4}	5.2382×10^{-3}	5.2453×10^{-3}	9.7003×10^{1}	7.2491×10^{-2}	6.2953×10^{-2}
2.8	4.128×10^{-4}	5.2275×10^{-4}	4.1000×10^{-4}	4.1316×10^{-4}	2.6635×10^{1}	6.7829×10^{-1}	8.7209×10^{-2}
3.0	1.744×10^{-4}	7.0061×10^{-4}	1.7261×10^{-4}	1.7461×10^{-4}	3.0173×10^{2}	1.0264×10^{0}	1.2041×10^{-1}

TABLE 2
COMPARISON BETWEEN OCM AND OCFE FOR PECLET NUMBER= 80

t (-)	Analytic solution	OCM	OCFE	% Error for OCM	% Error for OCFE
0	1.0000	1.0008	1.0000	8.0000×10^{-2}	0.0000
0.2	1.0000	9.9978×10^{-1}	1.0000	2.2000×10^{-2}	0.0000
0.4	1.0000	9.9963×10^{-1}	1.0000	3.7000×10^{-2}	0.0000
0.8	9.1140×10^{-1}	9.1106×10^{-1}	9.1140×10^{-1}	3.7305×10^{-2}	0.0000
1.0	4.6890×10^{-1}	4.6872×10^{-1}	4.6886×10^{-1}	3.8388×10^{-2}	8.5306×10^{-3}
1.4	1.2680×10^{-2}	1.2667×10^{-2}	1.2680×10^{-2}	1.0252×10^{-1}	0.0000
1.5	3.6410×10^{-3}	3.6314×10^{-3}	3.6411×10^{-3}	2.6366×10^{-1}	2.7465×10^{-3}
1.6	9.5070×10^{-4}	9.4390×10^{-4}	9.5069×10^{-4}	7.1526×10^{-1}	1.0519×10^{-3}
1.7	2.2910×10^{-4}	2.2515×10^{-4}	2.2919×10^{-4}	1.7241×10^{0}	3.9284×10^{-2}
1.8	5.1630×10^{-5}	4.9606×10^{-5}	5.1654×10^{-5}	3.9202×10^{0}	4.6485×10^{-2}
1.9	1.0990×10^{-5}	9.9680×10^{-6}	1.0997×10^{-5}	9.2994×10^{0}	6.3694×10^{-2}
2.0	2.2260×10^{-6}	1.5372×10^{-6}	2.2321×10^{-6}	3.0943×10^{1}	2.7403×10^{-1}

5 Conclusion

Different types of advection diffusion equations have been solved using OCM and OCFE. Numerical results have been compared with analytic ones for different values of Pe ranging from small to large. It has been observed that OCFE gives less error as compared to OCM even for large values of Pe. Both the concentration-time graphs as well as the numerical values presented in Tables authenticate this fact. In case of non linear problems also the $||C||_2$ smoothly approaches to zeros even for large values of parameters.

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