

Efficient Numerical Solution of Diffusion Convection Problem of Chemical Engineering

Bharti Gupta V.K. Kukreja *
Department of Mathematics, Sant Longowal Institute of Engineering and Technology
Longowal–148106, Punjab, India
* E-mail of the corresponding author: vkkukreja@gmail.com

Abstract
In this paper, the cubic B-spline collocation scheme is implemented to find numerical solution of diffusion convection problem of chemical engineering. The scheme is based on the Crank–Nicolson formulation for time integration and cubic B-spline functions for space integration. The numerical results are found to be in good agreement with the exact solutions. Results are also shown graphically and are compared with results given in the literature.
Keywords: Diffusion; Cubic B-spline; Collocation; Tridiagonal system; Thomas algorithm.

1. Introduction

Consider a parabolic diffusion convection problem with mixed boundary conditions and initial condition which is encountered in different branches of chemical engineering:

$$\mathbf{L}c = \frac{\partial c}{\partial t}+\frac{\partial c}{\partial x}=\frac{1}{4Pe}\frac{\partial^2 c}{\partial x^2}, \text{ in } \Omega\equiv(0,1), \tag{1}$$

$$\mathbf{B}c = \{\, 4Pe\,c-\frac{\partial c}{\partial x}=0, \text{ at } x=0;\ \frac{\partial c}{\partial x}=0, \text{ at } x=1 \,\}, \tag{2}$$

$$\mathbf{I}c = c(x,0)=1, \text{ for all } x. \tag{3}$$

The problem is used to describe the displacement of an initial homogeneous solute from a medium (called bed in chemistry) of finite length x (in this case $x=1$) at time t $(t\geq 0)$, by the introduction of a solvent. Here $c(x,t)$ represents the concentration profile of the solute and Pe is a constant parameter called the Peclet. Partial differential equations can be solved analytically by using techniques like separation of variables, Laplace transform and also numerically by using a verity of methods. However, some of these techniques have limited applications. In particular, the Laplace transform and numerical techniques, which is a useful tool for solving partial differential equations in chemical engineering, could involve the solution of complicated and transcendental equations which are time consuming [Al-Jabari *et al.* (1994); Brenner (1962); Grahs (1975); Lapidus and Amundson (1952); Potucek (2001)].

In this paper, numerical solution of system (1-3) by using the cubic B-spline collocation method (CSCM) is proposed. The collocation method together with B-spline approximations represents an economical alternative, since it only requires the evaluation of the unknown parameters at the grid points. Numerical results thus obtained are compared with analytic results of Brenner (1962) and 'pdepe' solver results of Singh *et al.* (2008). A good agreement is found with analytic ones whereas significant difference is found with the results obtained using 'pdepe' solver.

2. Numerical Scheme

Consider, a partition of the domain $0\leq x\leq 1$ at knot x_m, $m=0,\ldots,N$, such that $0=x_0<x_1<\ldots<x_N=1$ and $h_i=x_i-x_{i-1}=h$, *i.e.*, uniform partition $i=1,\ldots,N$ has been taken. Each spline can be written as linear combination of basis function of given spline by Prenter (1975) and de Boor (1978). Cubic B-splines B_m, $m=-1,\ldots,N+1$ are defined over the interval [0, 1] by:

$$B_m(x)=\frac{1}{h^3}\begin{cases}(x-x_{m-2})^3 & ,[x_{m-2},x_{m-1}]\\ h^3+3h^2(x-x_{m-1})+3h(x-x_{m-1})^2-3(x-x_{m-1})^3 & ,[x_{m-1},x_m]\\ h^3+3h^2(x_{m+1}-x)+3h(x_{m+1}-x)^2-3(x_{m+1}-x)^3 & ,[x_m,x_{m+1}]\\ (x_{m+2}-x)^3 & ,[x_{m+1},x_{m+2}]\\ 0 & ,otherwise\end{cases}.$$

Each basis function $B_m(x)$ is twice continuously differentiable, and the values of $B_m(x)$, $B'_m(x)$, $B''_m(x)$ may be tabulated as in Table 1.

The global approximation c_N to the exact solution c can be given by:

$$c_N(x,t) = \sum_{m=-1}^{N+1} \delta_m(t) B_m(x) ,$$

where δ_m are time dependent parameters to be determined using cubic B-spline collocation method. The collocation points are selected in order to coincide with knots x_m. Using the approximate solution and cubic B-splines $B_m(x)$, nodal values c, c' (first derivative) and c'' (second derivative) at knots x_m are obtained in terms of the element parameters by:

$$c_m = \delta_{m-1} + 4\delta_m + \delta_{m+1} ,$$

$$c'_m = \frac{3}{h}(\delta_{m+1} - \delta_{m-1}) ,$$

$$c''_m = \frac{6}{h^2}(\delta_{m-1} - 2\delta_m + \delta_{m+1}) .$$

3. Discretization of Model

The solution of given model Eqs. (1-3) can be obtained by assuming that the parameters δ_m and its time derivatives are linearly interpolated between two time levels n and n +1,

$$\frac{\partial c^n}{\partial t} = \theta F^n(c,x,t) + (1-\theta) F^{n+1}(c,x,t) \text{, where } F(c,x,t) = \frac{1}{4Pe}\frac{\partial^2 c}{\partial x^2} - \frac{\partial c}{\partial x} .$$

The time derivative is discretized in the usual finite difference way and applying Crank–Nicolson scheme to Eq. (1), it becomes:

$$\frac{c_m^{n+1} - c_m^n}{\Delta t} = \frac{1}{4Pe}\left(\frac{(c_{xx})_m^{n+1} + (c_{xx})_m^n}{2}\right) - \left(\frac{(c_x)_m^{n+1} + (c_x)_m^n}{2}\right).$$

Separating the terms of advanced and initial level:

$$\delta_{m-1}^{n+1}(1-\alpha_1) + \delta_m^{n+1}(4+\alpha_2) + \delta_{m+1}^{n+1}(1-\alpha_3) = \delta_{m-1}^n(1+\alpha_1) + \delta_m^n(4-\alpha_2) + \delta_{m+1}^n(1+\alpha_3) , \quad (4)$$

where $\alpha_1 = \left(\frac{6}{8Peh^2} + \frac{3}{2h}\right)\Delta t;\ \alpha_2 = \left(\frac{12}{8Peh^2}\right)\Delta t;\ \alpha_3 = \left(\frac{6}{8Peh^2} - \frac{3}{2h}\right)\Delta t$.

Boundary conditions are:

$$4Pe(\delta_{-1} + 4\delta_0 + \delta_1) - \frac{3}{h}(\delta_1 - \delta_{-1}) = 0 \text{, at x = 0,} \quad (5)$$

$$\frac{3}{h}(\delta_{N+1} - \delta_{N-1}) = 0 \text{, at x =1.} \quad (6)$$

Initial condition is:

$$\delta_{m-1} + 4\delta_m + \delta_{m+1} = 1 \text{, at t = 0, } m = 0,1,...,N . \quad (7)$$

Now using initial condition (7) and eliminating δ_{-1} and δ_{N+1} from boundary conditions (5) and (6), we can find initial approximation δ_m^0 from the tri-diagonal matrix:

$$\begin{bmatrix} 4-\alpha_5 & 1+\alpha_4 & 0 & . & . & . & . \\ 1 & 4 & 1 & . & . & . & . \\ 0 & 1 & 4 & 1 & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & 0 & 1 & 4 & 1 \\ . & . & . & . & 0 & 2 & 4 \end{bmatrix} \begin{bmatrix} \delta_0 \\ \delta_1 \\ . \\ . \\ . \\ \delta_{N-1} \\ \delta_N \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ . \\ . \\ . \\ 1 \\ 1 \end{bmatrix},$$

where $\alpha_4 = \left(\frac{3-4Peh}{3+4Peh}\right);\ \alpha_5 = \left(\frac{16Peh}{4Peh+3}\right)$.

Also Eq. (4) is reduced to a $(N+1)\times(N+1)$ matrix system as:

$$\begin{bmatrix} 4+\alpha_2-\alpha_5+\alpha_5\alpha_1 & 1-\alpha_3+\alpha_4-\alpha_4\alpha_1 & 0 & . & . & . & . \\ 1-\alpha_1 & 4+\alpha_2 & 1-\alpha_3 & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & 0 & 1-\alpha_1 & 4+\alpha_2 & 1-\alpha_3 \\ . & . & . & . & 0 & 2-\alpha_1-\alpha_3 & 4+\alpha_2 \end{bmatrix} \begin{bmatrix} \delta_0^{n+1} \\ \delta_1^{n+1} \\ . \\ . \\ . \\ \delta_{N-1}^{n+1} \\ \delta_N^{n+1} \end{bmatrix}$$

$$= \begin{bmatrix} -\alpha_5-\alpha_5\alpha_1+4-\alpha_2 & \alpha_4+\alpha_4\alpha_1+1+\alpha_3 & 0 & . & . & . & . \\ 1+\alpha_1 & 4-\alpha_2 & 1+\alpha_3 & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & 0 & 1+\alpha_1 & 4-\alpha_2 & 1+\alpha_3 \\ . & . & . & . & 0 & 2+\alpha_1+\alpha_3 & 4-\alpha_2 \end{bmatrix} \begin{bmatrix} \delta_0^{n} \\ \delta_1^{n} \\ . \\ . \\ . \\ \delta_{N-1}^{n} \\ \delta_N^{n} \end{bmatrix}.$$

By using δ_m^0, the above matrix is solved for δ_m^n's by using Thomas algorithm (see Appendix A.). By putting δ_m^n's in the approximate solution, exit concentration c_N can be determined.

4. Results and Discussion

Chemical engineers are particularly interested in the exit solute concentration. Stiff system of Eqs. (1-3) have been solved analytically up to acceptable accuracy by Brenner (1962). A comparison of analytic results of Brenner (1962), results of Singh *et al.* (2008) and results obtained using CSCM for wide range of Pe are given in Table 2. The Exit concentration profiles are drawn for different values of Peclet number, as shown in Figure. 1, 2 and 3. For $Pe \le 10$, the transport by axial dispersion becomes stronger than convective transport, which causes more back mixing, resulting in more dispersion of solute, leading to longer period for solute to leach out from fibers. For large $Pe(=40)$, solution profile is converging to steady-state condition sharply, because dispersion becomes smaller thereby increasing the solute removal rate. However, no significant effect is observed on solution profiles for $Pe > 40$. Al-Jabari *et al.* (1994) have established that efficient washing operations can be achieved for $\text{Pe} \le 40$.

5. Conclusions

CSCM is used due to its conceptual simplicity, wide applicability and ease of implementation. Breakthrough curves indicates, that an increase in the Pe causes the area under the curve to increase, resulting in less dispersion and lesser back mixing which leads to more removal of solute adsorbed on the particle surface. CSCM gave good results for large values of Pe also where as Brenner (1962) has given asymptotic expression for such large values of Pe. Results are compared with Singh *et al.* (2008) also and from error analysis it is observed that CSCM is giving much more accurate results than MATLAB 'pdepe' solver.

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Appendix A.

For the tri-diagonal matrix equation,

$$\begin{bmatrix} b_1 & c_1 & 0 & \cdots & \cdots & 0 \\ a_2 & b_2 & c_2 & 0 & \cdots & 0 \\ 0 & a_3 & b_3 & c_3 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & a_{n-1} & b_{n-1} & c_{n-1} \\ 0 & \cdots & \cdots & 0 & a_n & b_n \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_{n-1} \\ y_n \end{bmatrix} = \begin{bmatrix} r_1 \\ r_2 \\ r_3 \\ \vdots \\ r_{n-1} \\ r_n \end{bmatrix},$$

the steps of Thomas algorithm to obtain the solutions are as follows:

Step 1: $\beta_1 = b_1$

Step 2: $\gamma_1 = r_1/\beta_1$

Step 3: For i = 2, …, n

$\beta_i = b_i - (a_i\, c_{i-1}/\beta_{i-1})$

$\gamma_i = (r_i - a_i\, \gamma_{i-1})/\beta_i$

End

Step 4: $y_n = \gamma_n$

Step 5: For j = 1, …, n−1

$y_{n-j} = \gamma_{n-j} - c_{n-j}\, y_{n-j+1}/\beta_{n-j}$

End

Table 1. Values of $B_m(x)$, $B'_m(x)$, $B''_m(x)$.

	x_{i-2}	x_{i-1}	x_i	x_{i+1}	x_{i+2}
$B_m(x)$	0	1	4	1	0
$B'_m(x)$	0	-3/h	0	3/h	0
$B''_m(x)$	0	$6/h^2$	$-12/h^2$	$6/h^2$	0

Table 2. Comparison of CSCM with results of Brenner (1962) and Singh *et al.* (2008).

t (Time)	Pe = 0			Pe = 40			Pe = 100		
	Brenner (1962)	Singh *et al.* (2008)	CSCM	Brenner (1962)	Singh *et al.* (2008)	CSCM	Brenner (1962)	Singh *et al.* (2008)	CSCM
0.0	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
0.1	0.9048	0.9815	0.9054	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
0.2	0.8187	0.9398	0.8192	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
0.3	0.7408	0.8977	0.7412	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
0.4	0.6703	0.8572	0.6706	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
0.5	0.6065	0.8186	0.6067	1.0000	0.9998	1.0000	1.0000	1.0000	1.0000
0.6	0.5488	0.7817	0.5490	1.0000	0.9978	1.0000	1.0000	0.9991	1.0000
0.7	0.4966	0.7465	0.4967	0.9992	0.9837	0.9993	1.0000	0.9920	1.0000
0.8	0.4493	0.7128	0.4494	0.9746	0.9264	0.9750	0.9991	0.9552	0.9992
0.9	0.4066	0.6807	0.4066	0.8137	0.7785	0.8151	0.9276	0.8355	0.9303
1.0	0.3679	0.6500	0.3679	0.4778	0.5254	0.4800	0.4859	0.5815	0.4946

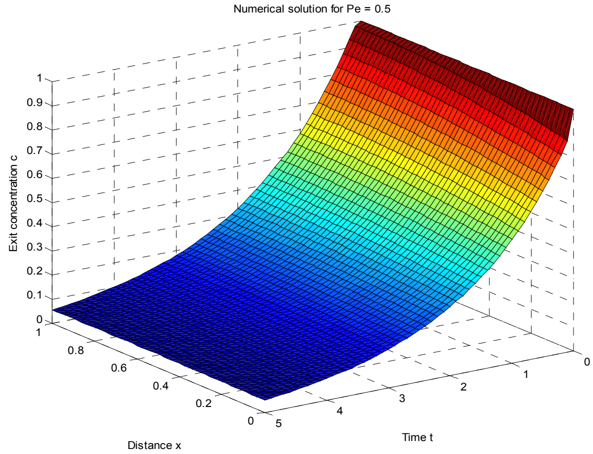

Figure. 1. Solution profile for Peclet number 0.5.

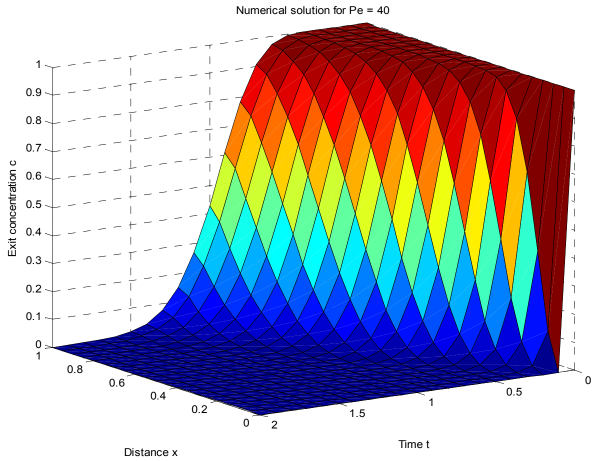

Figure. 2. Solution profile for Peclet number 40.

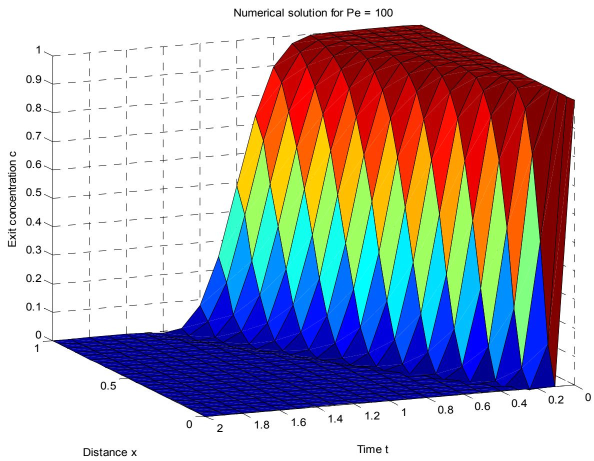

Figure. 3. Solution profile for Peclet number 100.