International Journal of Applied Mathematics & Statistical Sciences (IJAMSS)
Vol.1, Issue 1 Aug 2012 40-49

International Academy of Science, Engineering and Technology
Connecting Researchers; Nurturing Innovations

NUMERICAL SOLUTION OF ONE-DIMENSIONAL ADVECTION – DISPERSION EQUATION WITH REACTION IN A HOMOGENEOUS POROUS MEDIUM USING DIFFERENTIAL QUADRATURE METHOD (DQM)

SONA RAJ & V.H. PRADHAN

Applied Mathematics & Humanities Department, Sardar Vallabhbhai National Institute of Technology, Surat, Gujarat, India

ABSTRACT

In the present work, one dimensional Advection – Dispersion equation with Reaction in a homogeneous porous medium is solved by using Differential Quadrature Method. Here polynomial based differential quadrature method and fourth order Runge–Kutta scheme for space and time is applied for solving the equation having initial and boundary conditions. Compared to the conventional numerical methods, we obtained accurate solutions for less number of nodes. All computations were carried out using some codes produced in MATLAB. The computed results justify the efficiency of the method.

KEYWORDS: Advection, Differential Quadrature Method, Dispersion, Reaction, Runga- Kutta Method, Shu's General Approach.

INTRODUCTION

Advection-dispersion equation with reaction is applicable various disciplines of engineering such as chemical engineering, petroleum engineering, civil engineering, etc to describe the behaviour of solute concentration. Many authors had contributed their ideas in this field. Warrick et al. (1972) shown the miscible displacement processes with time-varying velocity and dispersion coefficients and solutions are used in the analysis of experimental data. Van Genuchten and Alves (1982) had obtained the solutions for Advection Dispersion equation with reaction analytically. B. Ataie-Ashtiani et.al. (1996) examined an explicit finite difference scheme for the truncation errors on the solution of an advection – dispersion with a first order reaction term. Zoppou and Knight (1997) worked on one-dimensional analytical solutions for equation in which they considered solute dispersion varying with square of position variable while velocity varies with the position variable. H.Saberi Najafi (2008) solved the one – dimensional advection – dispersion with reaction with some finite difference methods. In the present work, we obtain the numerical solution of the equation using Differential Quadrature Method for 11 grid points with good accuracy.

Consider the one-dimensional flow of underground water through fixed soil or rock matrix. In this work, the fixed soil through which water is flowing is represented as saturated homogeneous porous medium. Porosity of the porous medium is 'ω', considering as a constant [1]. Let C(x, t) be the concentration of a chemical or biological tracer dissolved in the water. It is measured as mass of tracer present per unit volume of water. The movement of tracer particles in soil by the bulk motion of water signifies Advection [1,2]. The spreading of tracer in water due to the variability of macroscopic velocities through the pores of the soil is mentioning the Dispersion. Let D be the dispersion coefficient of the dispersion [1]. The tracer created or destroyed with rate k, measured in mass per unit volume of soil per unit time, referred as Reaction term [1]. Using reaction term we can measure the decay rate, the rate of consumption in a chemical reaction and even growth or death rate can obtain if the tracer is biological. The specific discharge of water through the soil is denoted as V, which is the Darcy velocity. Assume V is a constant [1]. The velocity 'v'of the tracer in water is expressed as $v \equiv \frac{V}{\omega}$ known as average velocity. The basic physical law for the flow of fluid through a porous medium is derived from the mass balance of the tracer. By using the Mass Balance Law, we get the equation for one-dimensional advection –dispersion with reaction expressed as [1,3,4],

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - u\frac{\partial C}{\partial x} - kC \tag{1}$$

The initial condition is

$$C(x,0) = 0,\ 0 \le x \le L \tag{2}$$

The boundary conditions are

$$C(0,t) = C_0$$

$$C(L,t) = 0,\ 0 \le t \le T \tag{3}$$

Where

C: is solute concentration, (ML^{-3}), t: is time, (T), x: is the soil depth, (L) , u : is the pore water velocity, (LT^{-1}), D: is the dispersion coefficient, ($L^2\,T^{-1}$), k: is the first order reaction rate coefficient, (T^{-1}).

DQM METHOD

The Differential Quadrature Method (DQM) is an efficient numerical method for the rapid solution of linear and nonlinear partial differential equations. Compared with the standard methods such as the finite element and finite difference methods, the DQM requires less computer time and storage [5]. In this method a partial derivative of a function is approximated by a weighted linear sum of the function values at given discrete points. The weighting coefficients depend only on the grid spacing. Using these weighting coefficients any partial differential equation can be easily reduced to a set of algebraic equations. Because of their high accuracy, generality in a variety of problems and straightforward implementation Differential quadrature (DQ) methods have been distinguished. The basic procedure in the DQM is the determination of weighting coefficients. Richard Bellman 1972 introduced the DQM.

Bellman used two procedures to obtain the weighting coefficients. In first procedure, he used a simple function as test functions but when the sampling points are relatively large (say 13) the coefficient matrix become ill conditioned [6]. Second procedure has similarity with the first except coordinates of grid points, which should be chosen as the roots of the Nth order Legendre polynomial. C. Shu had given a remarkable contribution to generalize the idea of the DQ.

The present problem is solved by using a Polynomial based Differential Quadrature (PDQ) Method [5, 7]. This method has the basis of the quadrature method in deriving the derivatives of a function and it follows that the partial derivative of a function with respect to a space variable can be approximated by a weighted linear combination of the function values at some intermediate points in that variable. The selection of locations of the sampling points plays an important role in the accuracy of the solution of the differential equations. Shu suggested that the solution of a partial differential equation can be accurately approximated by a polynomial of high degree. Suppose that the degree of the approximated polynomial is N-1. This approximated polynomial constitutes an N-dimensional linear vector space V_N with the operation of vector addition and scalar multiplication , and can be expressed in different forms and N is the total number of grid points[5,8].

For the accuracy, weighting coefficients and choice of sampling points plays a vital role. In the present problem we choosed uniform grid, that means the grid has same step sizes [5].

i.e. $\Delta x = x_k - x_{k-1}$; where k = 1,2,3,..........,11 (4)

For the approximation form for the discretization of first order derivative is given by [5,6,7]

$$C_x^{(1)}(x_i) = \sum_{j=1}^{N} a_{ij}.C(x_j)\,, \quad for \;\; i, j = 1, 2, ...N; \tag{5}$$

By using Bellman's first and second approaches, Shu generalised the weighting coefficients as follows.

The off- diagonal terms of the weighting coefficient matrix of the first order derivative are given by[5]

$$a_{ij} = \frac{M^{(1)}(x_i)}{(x_i - x_j)M^{(1)}(x_j)} \; for\, i \neq j \tag{6}$$

Where $M^{(1)}(x_i) = \prod_{j=1,\, j\neq i}^{N} (x_i - x_k)$ (7)

$$M^{(1)}(x_j) = \prod_{j=1,\, j\neq i}^{N} (x_j - x_k) \tag{8}$$

and diagonal terms are given by

$$a_{ii} = -\sum_{j=1}^{N} a_{ij} \tag{9}$$

Equations (6) & (9) are two formulations to compute the weighting coefficients for first order derivative.

For the discretization of the second order derivative, we can introudce a similar approximation form given by[5,6]

$$C_x^{(2)}(x_i) = \sum_{j=1}^{N} b_{ij}.C(x_j), \text{ for i=1,2,....N} \tag{10}$$

Where $C_x^{(2)}(x_i)$ is the second order derivative of f(x) at x_i , b_{ij} is the weighting coefficient of the second order derivative , is expressed as,

$$b_{ij} = 2a_{ij}\left[a_{ii} - \frac{1}{x_i - x_j}\right], \, for\, i \neq j \tag{11}$$

$$b_{ii} = -\sum_{j=1,\, j\neq 1}^{N} b_{ij} \tag{12}$$

b_{ij} is calculated from Equation (11) when i $\neq$ j and b_{ii} from Equation (12).

In general, for the discretization of mth order derivative [5,7]

$$C_x^{(m)}(x_i) = \sum_{j=1}^{N} w_{ij}^{(m)}.C(x_j),\; for \;\; i, j = 1, 2, ...N;\; m = 2, 3, ..., N-1 \tag{13}$$

the weighting coefficient matrix of higher order derivative may obtained through the recurrence relationship expressed as [6,7],

$$w_{ij}^{(m)} = m\left(a_{ij} w_{ii}^{(m-1)} - \frac{w_{ij}^{(m-1)}}{x_i - x_j}\right) \;;\; for \;\; i, j = 1, 2, ...N;\; m = 2, 3, ..., N-1 \tag{14}$$

and the diagonal terms of the weighting coefficients are,

$$w_{ii}^{(m)} = -\sum_{j=1, i\neq j}^{N} w_{ij}^{(m)} \;;\; for \;\; i, j = 1, 2, ...N;\; m = 2, 3, ..., N-1 \tag{15}$$

After applying Differential Quadrature Method equation (1) becomes system of ordinary differential equations of the form

$$\frac{dC_i}{dt} = D\sum_{j=1}^{N} b_{ij} C_j - u\sum_{j=1}^{N} a_{ij} C_j - kC_i \qquad , \text{for i} = 1, 2, ...\text{N} \tag{16}$$

Where a_{ij} and b_{ij} are the first and second order weighting coefficients and C_i is the concentration of solute at the node x_i; i=1,2,...............,N

NUMERICAL ILLUSTRATIONS

The system of ordinary differential equations[9] obtained by PDQ method is solved by using fourth order Runga- Kutta Method[10] for the initial condition(2) and boundary conditions(3) using MATLAB. The following set of values is considered for obtaining the required numerical results.

N=11, D = 1 cm^2, u= 0.5cmh^{-1}, k= 0.1 h^{-1} , Δx = 2 cm , Δt =1 h , L=20 cm, C_0 =1000 mg / l , T=25 h.

For checking the accuracy of method the numerical results are compared with the analytic solution which is expressed as [1,5,6]

$$C(x,t)=\frac{C_0}{2}\left[\exp\left(\frac{(u-v)x}{2D}\right)erfc\left(\frac{x-vt}{2(Dt)^{\frac{1}{2}}}\right)+\exp\left(\frac{(u+v)x}{2D}\right)erfc\left(\frac{x+vt}{2(Dt)^{\frac{1}{2}}}\right)\right] \tag{17}$$

Where $v=\left(u^2+4kD\right)^{\frac{1}{2}}$

The numerical results are shown in Table I to VI. The absolute error is shown in Fig.1. The behaviour of solute concentration with respect to depth and time is shown in Fig.2, Fig.3and Fig.4 respectively.

Table 1 The Absolute Errors for Different Values of X at Time T=5 H

Values of x	Exact values at t=5	DQM values at t=5	Absolute error at t=5
	1.0e+003 *	1.0e+003 *	
x = 6	0.1445439	0.1440285	5.15E-04
x = 8	0.0439684	0.0433135	6.55E-04
x = 10	0.00952	0.0094629	5.70E-05
x = 12	0.0014398	0.001486	4.62E-05
x = 14	0.0001503	0.000179	2.87E-05

Table 2 The Absolute Errors for Different Values of X at Time T=10 H

Values of x	Exact values at t=10	DQM values at t=10	Absolute error at t=10
	1.0e+003 *	1.0e+003 *	
x = 6	0.3123135	0.3118717	4.42E-04
x = 8	0.1790724	0.1791775	1.05E-04
x = 10	0.0903314	0.0904814	1.50E-04
x = 12	0.0393365	0.0393543	1.78E-05
x = 14	0.0145848	0.014555	2.98E-05

Table 3 The Absolute Errors for Different Values of X at Time T=15 H

Values of x	Exact values at t=15	DQM values at t=15	Absolute error at t=15
	1.0e+003 *	1.0e+003 *	
x = 6	0.3700538	0.3700612	7.44E-06
x = 8	0.2496601	0.2496152	4.49E-05
x = 10	0.1591935	0.159146	4.74 e-005
x = 12	0.0944992	0.0944806	1.86 e-005
x = 14	0.0515434	0.0515393	4.06E-06

Table-4.The Absolute Errors for Different Values of X at Time T=20 H

Values of x	Exact values at t=20	DQM values at t=20	Absolute error at t=20
	1.0e+003 *	1.0e+003 *	|C num.-C anal.|
x = 6	0.3890326	0.3890291	3.47E-06
x = 8	0.2772744	0.2772636	1.07E-05
x = 10	0.1927266	0.1927084	1.81 e-005
x = 12	0.1293428	0.1293131	2.97 e-005
x = 14	0.0829654	0.0828758	8.95E-05

Table-5.The Absolute Errors for Different Values of X at Time T=25 H

Values of x	Exact values at t = 25	DQM values at t= 25	Absolute error at t = 25
	1.0e+003 *	1.0e+003 *	|C num.-C anal.|
x = 6	0.3954871	0.395488	8.95E-07
x = 8	0.2875953	0.2875849	1.03E-05
x = 10	0.206862	0.2068416	2.03E-05
x = 12	0.14633	0.1462737	5.63E-05
x = 14	0.1011159	0.1008698	2.46E-04

Table-6.The Absolute Errors for Different Values of X at Different Time

Values of x	Absolute error at t=1h	Absolute error at t=5h	Absolute error at t=10 h	Absolute error at t=15 h	Absolute error at t=20 h	Absolute error at t=25 h
x = 6cm	8.26E-05	5.15E-04	4.13E-04	7.44E-06	3.47E-06	8.95E-07
x = 8cm	3.83E-05	6.54E-04	1.27E-04	4.49E-05	1.07E-05	1.03E-05
x = 10cm	2.23E-05	5.70E-05	1.68E-04	4.74 e-005	1.81 e-005	2.03E-05
x = 12cm	9.08E-06	4.62E-05	6.35E-05	1.86 e-005	2.97 e-005	5.63E-05
x = 14cm	5.09E-06	2.87E-05	1.52E-05	4.06E-06	8.95E-05	2.46E-04

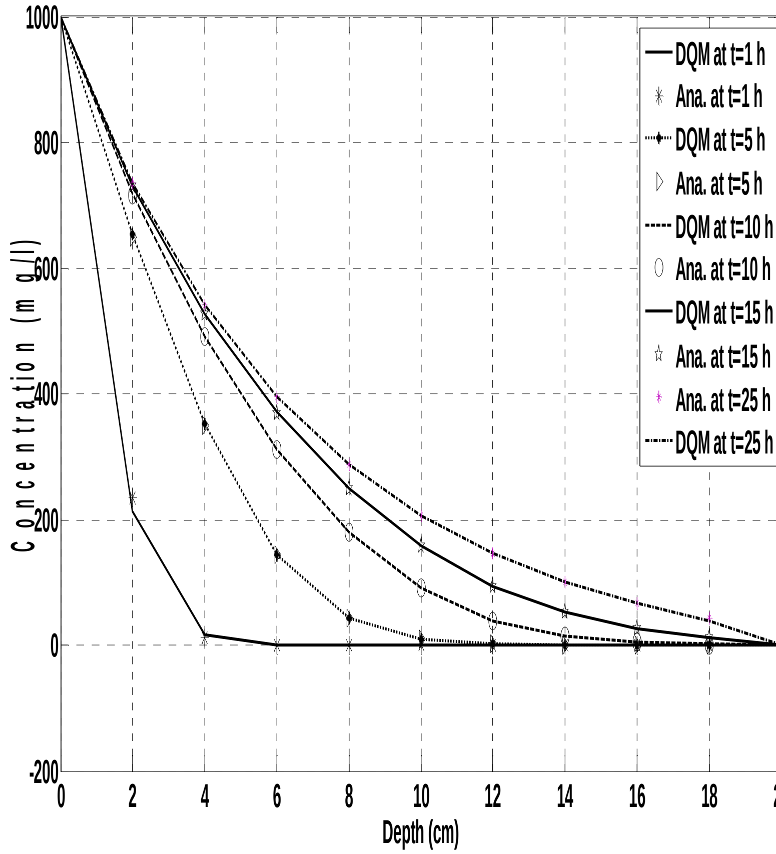

Figure 1: Comparative Results of DQM and Analytical Solution for Different Time

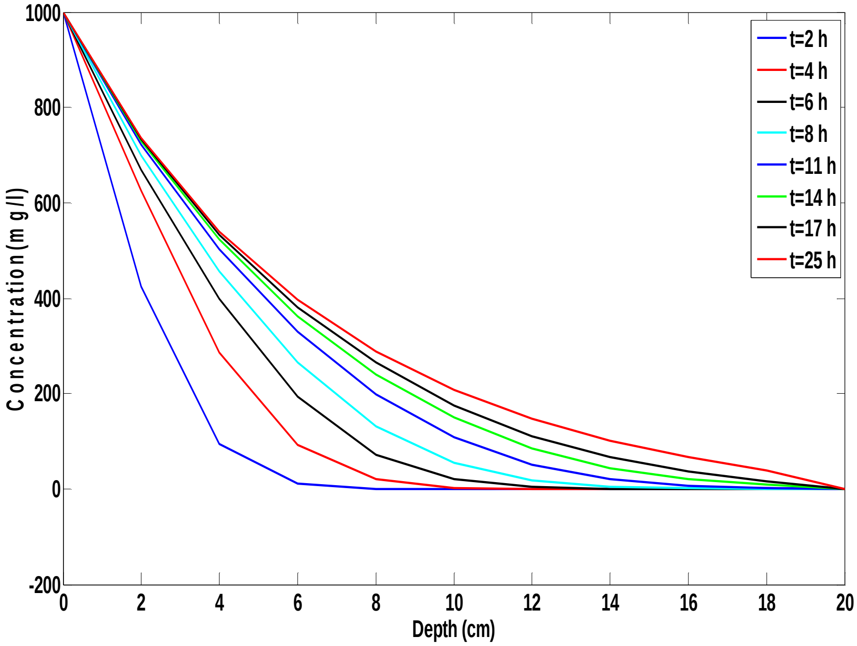

Figure 2: Change in Concentration C(X ,T) with Respect to Depth of Soil at Different Time

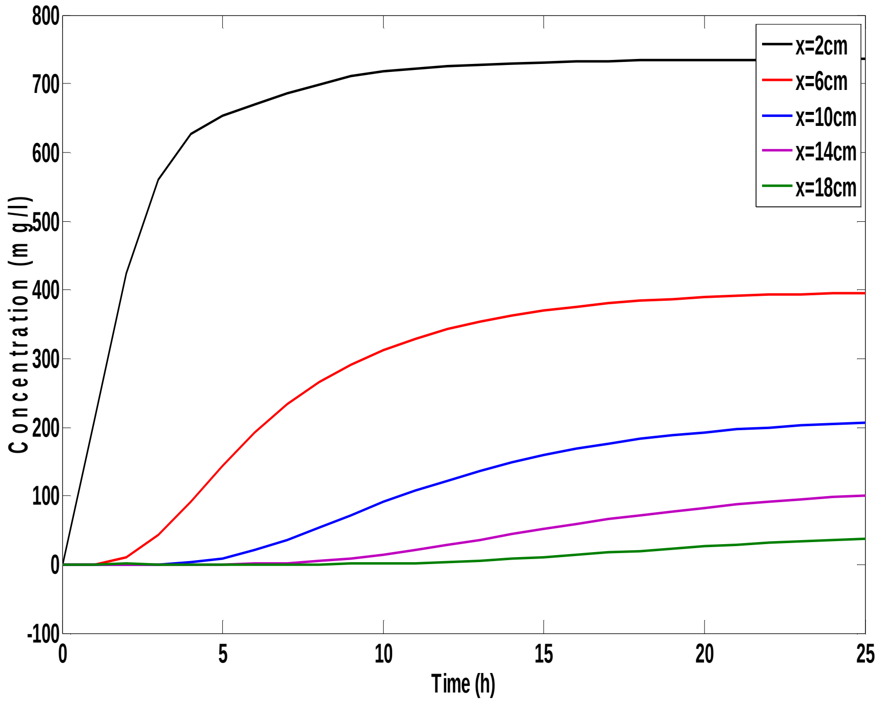

Figure 3: Change of Concentration C(X ,T) with Respect to Time at Different Points of Depth of Soil

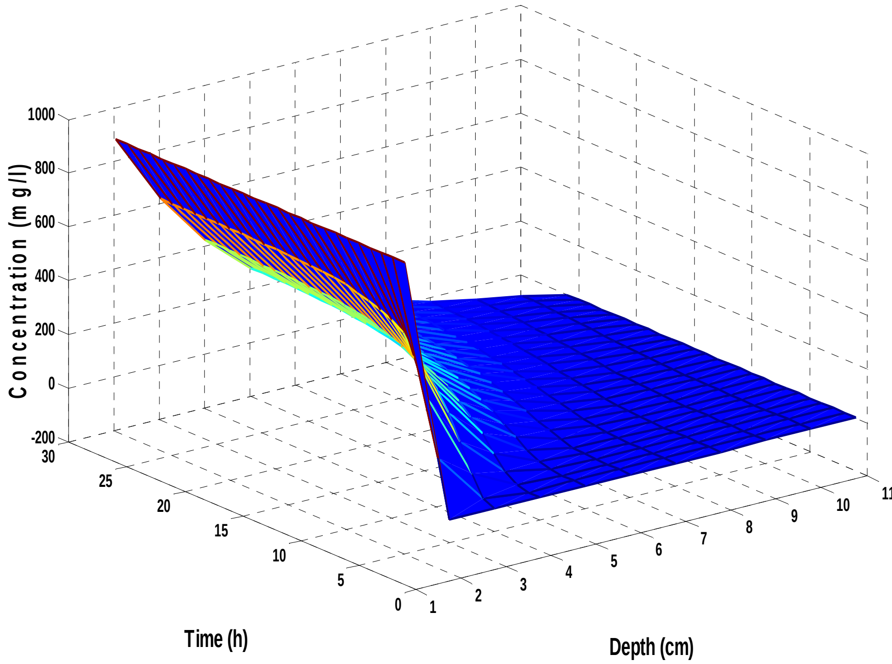

Figure 4: Change in Concentration with Respect to Time and Depth in Three – Dimensional Form

CONCLUSIONS

The solutions to the one – dimensional advection dispersion equation with reaction in a homogeneous porous medium for a very less number of nodes obtained through this method shows that, PDQ method is successfully working. The value of absolute error shows that the method is giving much accurate solutions. The advantages of the method is justifying through the computed results.

ACKNOWLEDGEMENTS

One of the authors (Sona Raj) acknowledges the financial assistance provided by Ministry of Human Resource and Development (MHRD), Government of India, India.

REFERENCES

1. Logan JD. Transport modeling in Hydrogeochemical Systems, Springer, 2001; 15 (223): 50.
2. Cussier EL, Diffusion- Mass Transfer in fluid systems, Cambridge University, 2007; 3: 1-57.
3. Saberi Najafi H. Solving One-Dimensional Advection – Dispersion with Reaction using some Finite – Difference Methods. Applied Mathematical Sciences, Hikari Ltd, 2008; 2(53): 2611-2618.
4. Ataie-Ashtiani B, Lokhington DA, Volker RE. Numerical correction for finite difference solution of the advection-dispersion equation with reaction, J. Contaminant Hydrology, Elsevier: 1996; 23: 149-156.

5. Chang Shu. Differential Quadrature and its Applications in Engineering. Springer: Great Britain, 2000; 1-174.
6. Bellman RE, Kashef BG, Casti J. Differential Quadrature: A technique for the rapid solution of nonlinear partial differential equations. J Computational physics, Elsevier: 1972; 10: 40-52.
7. Charles Bert W. and Moinuddin Malik. Differential Quadrature Method in computational mechanics: A review, J Applied Mechanics Reviews, ASME, 1996; 49 (1):1.
8. Bellomo N. Nonlinear Models and Problems in Applied Sciences from Differential Quadrature to Generalized Collocation Methods. Mathl. Comput. Modelling, Elsevier 1997; 26 (4): 13-34.
9. Larry Andrews C., Ronald Phillips L. Mathematical Techniques for Engineers and Scientists, Prentice – Hall of India: Delhi, 2006; 114-132.
10. Terrence Akai J. Applied Numerical Methods for Engineers. Wiley: Singapore, 1994; 229-242.