Solute Transfers Modeling In Layered Porous Media Using Differential Quadrature Method (DQ)

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Abstract: Solute or contaminant transport in porous media can be described by Advection – diffusion equations. In this research, the differential quadrature method (DQM) is employed to solve ADE in solute transport in a double-layered porous medium. This method is applied to two examples with different boundary conditions and the results are compared with analytical solutions. Also, the effect of various parameters on interface conditions are discussed in all examples. Using DQM, provides relatively exact results, while the needed mesh size is much smaller than the traditional approaches which reduces computational time and needed computer storage capacity**.** Another advantage of this numerical method is that applying the boundary and initial conditions can be performed easier than the other numerical methods.

Key-Words: solute transfer, porous media, DQ method, numerical method, analytical solution.

1 Introduction

In a subsurface environment, the characterization of fate and the transfer of solutes is essential for remediation practices specially at last decades . Porous media are seldom homogeneous and the transport properties of these media will vary spatially and sometimes also temporally. Accurate mathematical analyses of transport in heterogeneous media are not easily carried out. However, the formulation and mathematical solution of the transport problem becomes possible if the medium is assumed, somewhat simplistically, to be composed of a series of homogeneous layers. In soil science, composite media have been used for representing stratified soil profiles in which horizons parallel to the soil surface. In order to prevent or make slow the transfer process of a special material, sometimes, this layering in the form of artificial barriers is constructed. Hence, applying the homogeneity assumption for simplifying the problem may lead an inaccurate evaluation of the real case.

Solute transport in soils is usually described deterministically by the Advection - Dispersion Equation (ADE), although alternative stochastic approaches also exist [1]. Exact and approximate analytical solutions for transport in layered soils are now available for a limited number of situations. In most cases. Leij et al investigated the solute transfer in layered soil [2]. They addressed mass balance at the interface between the layers by considering different interface continuity conditions. Leij and van Genuchten presented an analytical solution for the solute transport in a double-layer porous medium with a zero concentration initial condition [3]. Recently, a comprehensive investigation has been conducted by Li et al in which an analytical solution for ADE in a double-layered porous media has been presented [4]. The analytical solutions basically are able to render perception into the governing physical processes, provide useful tools for validating numerical approaches and are rarely applicable to practical problems. Also, finding the simplest and optimal techniques to solve the partial differential equation like ADE has attracted a great importance. A diversity of numerical methods are available now for solving the initial- and/or boundary value problems in physical and engineering science. The frequently used numerical techniques for solving such equations are the standard finite difference method (FDM), finite element method (FEM) and boundary element method (BEM). Usually, above-mentioned methods require a large number of grid points in order to produce a moderately accurate solution and involve complex computer programming algorithms. However, there exist a number of alternative methods such as Differential Quadrature Method which can provide relatively accurate results with inexpensive computation. The method has been applied successfully to solve a wide range of problems, with a diversity of boundary conditions easily and precisely.

After acquiring the correct result as a base in simulations of solute transport which usually is performed by analytical methods, finding the optimal techniques to solve the ADE has attracted a great consideration. One of these effective techniques is the Differential Quadrature Method which in spite of anonymity can provide relatively accurate results depending on the computational efforts. However, there exist a number of alternative methods such as Differential Quadrature Method which can provide relatively accurate results with inexpensive computation. DQM first developed by Bellman and Casti (1971) and has made a noticeable success over the last four decades [5]. The main idea of this method is on the basis of the integral quadrature. Additional developments achieved by Shu et al. (1994) based on Polynomial-based differential quadrature (PDQ) as in [6], [7], [8], Fourier expansion-based differential quadrature (FDQ) as in [9], [10] and Radial basis function based differential quadrature (RBF-DQ) (Shu et al. 2003, 2005) [11], [12].

In this study, the DQM has used to solve one dimensional ADE on solute transport problem in double-layered porous media. Two problems with different boundary conditions was assumed to provide more insight into the solution of the problem. The DQM results are verified to be in an extremely good agreement with the analytical solution by using a small number of grid points.

2 Mathematical Problem Formulation

Please, A porous medium consisting of two homogeneous layers subject to the steady water flow perpendicular to the layer interface is assumed. The transport and flow properties of both layers are the same in time and space as depicted in Fig. 1. The thickness of the layer is set to *H*, also, $H = h_1 + h_2$. Each layer has its own properties. The z axis is consistent with the constant Darcy velocity. The solute transport in the double layer porous media in one-dimension is well explained by

$$n_{i'} R_{di'} \frac{\partial c_{i'}}{\partial t} = n_{i'} D_{i'}^{*} \frac{\partial^2 c_{i'}}{\partial z^2} - \upsilon \frac{\partial c_{i'}}{\partial z} \quad (i' = 1,2) \qquad (1)$$

Where $n_{i'}$ denotes the porosity, $D_{i'}^{*}$ stand for constant effective diffusion coefficient, $R_{di'}$ is retardation factor, ν denotes the Darcy velocity and $C_{i'}$ provides the solute concentration in layers. It is noteworthy that subscript i' indicates the layer's number. For example $i' = 1$ denotes the inlet layer and $i' = 2$ indicates outlet layer.

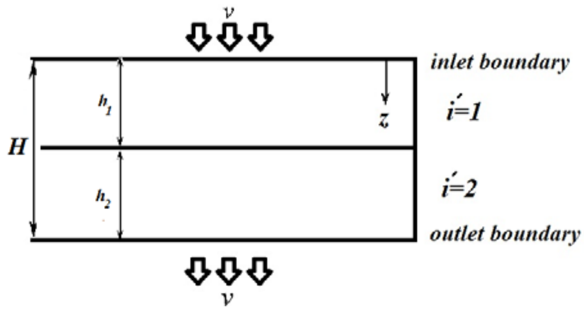

Fig. 1. Schematic of solute transport through a double-layered porous media

Since the apparent velocity in i' th layer is equal to $\nu / n_{i'}$, Eq. (1) can be written as follows:

$$R_{di'} \frac{\partial c_{i'}}{\partial t} = D_{i'}^{*} \frac{\partial^2 c_{i'}}{\partial z^2} - \upsilon_{si'} \frac{\partial c_{i'}}{\partial z} (i' = 1,2) \qquad (2)$$

In this work the initial condition for all problems are the same and is defined by the following function:

$$c_{i'}(z,t) = c_{i'}(z,0), \ i' = 1,2 \qquad (3)$$

The additional continuity conditions are considered at the interface between the layers. The Drichlet and Robin conditions are used to make us sure that both concentration and solute flux continuities are satisfied.

The Drichlet and the Robin continuity conditions at the interface can be conveyed as follows, correspondingly:

$$C_1(h_1, t) = C_2(h_1, t) \qquad (4)$$

$$\begin{aligned} -n_1 D_1^{*} \frac{\partial C_1(z,t)}{\partial z}\bigg|_{z=h_1} + \nu\, C_1(h_1,t) = \\ -n_2 D_2^{*} \frac{\partial C_2(z,t)}{\partial z}\bigg|_{z=h_1} + \nu\, C_2(h_1,t) \end{aligned} \qquad (5)$$

Equation (5) becomes a Neumann continuity condition after substitution of Equation (4) yielding

$$-n_1 D_1^{*} \frac{\partial C_1(z,t)}{\partial z}\bigg|_{z=h_1} = -n_2 D_2^{*} \frac{\partial C_2(z,t)}{\partial z}\bigg|_{z=h_1} \qquad (6)$$

But the boundary conditions for the two problems are quite different and will be investigated separately in three types of problems as follows:

2.1 Problem type 1
Dirichlet or first type inlet and outlet boundary conditions

$$\text{Dirichlet inlet BC: } C_1(0,t) = C_0 \quad (7a)$$

$$\text{Neumann outlet BC: } \left.\frac{\partial C_2(z,t)}{\partial z}\right|_{z=H} = 0 \quad (7b)$$

Which signifies fixed solute concentration situations

2.2 Problem type 2
Dirichlet inlet and Neumann or second type outlet boundary conditions

$$\text{Robin's inlet BC: } -n_1 D^*_1 \left.\frac{\partial C_1(z,t)}{\partial z}\right|_{z=0} + \nu C_1(0,t) = \nu C_0 \quad (8a)$$

$$\text{Neumann outlet BC: } \left.\frac{\partial C_2(z,t)}{\partial z}\right|_{z=H} = 0 \quad (8b)$$

That represents fixed solute concentration and zero gradient condition, respectively.

2.3 Problem type 3
Problem 3: Robin's or third type inlet and Neumann outlet boundary conditions

Robin's inlet BC:

$$-n_1 D^*_1 \left.\frac{\partial c_1(z,t)}{\partial z}\right|_{z=0} + \nu c_1(0,t) = \nu c_0 \quad (9a)$$

Neumann outlet BC:

$$\left.\frac{\partial c_2(z,t)}{\partial z}\right|_{z=H} = 0 \quad (9b)$$

Fixed flux and zero gradient condition as shown in (9a) and (9b), respectively.

Where c_0 and c_H stand for constant solute concentrations at the inlet and outlet boundaries, accordingly.

In this paper, the numerical solution for three types of problems subjected to various inlet and outlet boundary conditions are represented (Table 1).

Table 1. Three types of problems with diverse blend of inlet and outlet boundary condition

Problem	Initial condition	Inlet boundary	Outlet boundary
1	$c_1(z,t)=c_1(z,0)=c_0$	$C_1(0,t)=C_0$	$C_2(0,t)=C_H$
2	$c_1(z,t)=c_1(z,0)=c_0$	$C_1(0,t)=C_0$	$\left.\frac{\partial C_2(z,t)}{\partial z}\right\|_{z=H}$
3	$c_1(z,t)=c_1(z,0)=c_0$	$-n_1 D^*_1 \left.\frac{\partial C_1(z,t)}{\partial z}\right\|_{z=0} + \nu C_1(0,t) = \nu C_0$	$\left.\frac{\partial C_2(z,t)}{\partial z}\right\|_{z=H}$

3. Differential Quadrature Method
DQM is a numerical method developed to solve both linear and nonlinear partial differential equations. This method was first proposed by Bellman and Casti and further extended by Shu [13]. Also, many researchers have made important improvements to this method and its applications. For example, to simplify the computational efforts to evaluate weighting coefficients for high order derivatives in DQM, Mingle suggested a linear transformation [14].

Civan and Sliepcevich further extended this method to multi-dimensional problems [15].

In the DQM, a partial derivative of a function with respect to a space variable at a discrete point is approximated as a weighted linear sum of the function values at all discrete points along the corresponding coordinate axes. Its weighting coefficients do not depend to any particular condition and only depend on the grid spacing. Thus, any partial differential equation can be easily reduced to a set of algebraic equations using these coefficients. In this way the n th-order derivative of the function $f(x)$ at point x_i is calculated by Eq. (10).

$$f^n(x_i) = \sum_{j=1}^{N} A^n_{i,j} . f(x_j) \quad for\ i = 1,2,...,N \quad (10)$$

Where

$w^n_{i,j}$ = weighting coefficients, $f(x_j)$ = value of the function at point j, $f^n(x_i)$ = the n th-order derivative value at point x_i.

Calculating the weighting coefficients can be a crucial part of a problem. It influences the accuracy of the results, seriously. The weighting coefficient ($A^n_{i,j}$) can be approximated by a high-order polynomial or by the Fourier series expansion or the harmonic functions as its test functions. In this work Lagrange interpolation basis function is used as the test functions to determine the weighting coefficients [16], [17]:

$$a_{i,j} = \frac{M^{(1)}(x_i)}{(x_i - x_j)\, M^{(1)}(x_j)}, \ for\ j \neq i \quad (11)$$

$$a_{i,i} = -\sum_{j=1, j\neq i}^{N} a_{i,j} \quad (12)$$

$$b_{i,j} = -2a_{i,j}\left(a_{i,i} - \frac{1}{x_i - x_j}\right), \ for\ j \neq i \quad (13)$$

$$b_{i,i} = -\sum_{j=1, j\neq i}^{N} b_{i,j} \quad (14)$$

Where $M^{(1)}(x_i)=-\prod_{k=1,k\neq i}^{N}(x_i-x_k)$, a_{ij} and b_{ij} are the weighted coefficients of first order derivatives and second order derivatives, respectively.

4. Problem Solution

In this section, application of DQM in discretization and formulation of the governing equations for three chosen to study problems is presented. In the developed model in this study, all spatial derivatives are discretized by DQM and temporal derivatives by first order forward FD scheme. Since the cited problems are transient they can be solved by each of the explicit, implicit and semi implicit Crank-Nicholson schemes.

In the explicit scheme the value of any parameter of time t^{n+1} or $n+1$-th time step is calculated directly from discretized equations knowing their value in the previous time step n-th or t^n. This method only uses information in time step n for computing parameters in time step $n+1$, so we have to select the small time step Δt ($\Delta t=t^{n+1}-t^n$) to have convergence. **In the implicit scheme** the value of parameters at time step $n+1$ has been used for discretizing spatial derivatives. Therefore, discretized equations represent a set of algebraic equations that must be solved simultaneously to evaluate new values of the parameters in time step $n+1$. The **semi implicit Crank-Nicholson scheme** is similar to an implicit scheme except that in this way, for solving the problem, the value of parameters in both time step n and $n+1$ is used for discretizing spatial derivatives.

The general form of discretized Eq. (2) can produce Eq. (15) and Eq. (16):

$$R_{di'}\left[\frac{C_{i'}^{\,n+1}-C_{i'}^{\,n}}{\Delta T}\right]_i=\theta\left[D_{i'}^{*}\frac{\partial^2 C_{i'}}{\partial Z}-v_{si'}\left(\frac{\partial C_{i'}}{\partial Z}\right)\right]_i^{n+1}$$

$$+(1-\theta)\left[D_{i'}^{*}\frac{\partial^2 C_{i'}}{\partial Z}-v_{si'}\left(\frac{\partial C_{i'}}{\partial Z}\right)\right]_i^{n} \qquad (15)$$

$for\ i=1,2,...,N$ and $i'=1$.

$$R_{di'}\left[\frac{c_{i'}^{\,n+1}-c_{i'}^{\,n}}{\Delta t}\right]_j=\theta\left[D_{i'}^{*}\frac{\partial^2 c_{i'}}{\partial z^2}-v_{si'}\left(\frac{\partial c_{i'}}{\partial z}\right)\right]_j^{n+1}$$

$$+(1-\theta)\left[D_{i'}^{*}\frac{\partial^2 c_{i'}}{\partial z^2}-v_{si'}\left(\frac{\partial c_{i'}}{\partial z}\right)\right]_j^{n} \qquad (16)$$

$for\ j=1,2,...,M$ and $i'=2$.

Which Eq.(15), Eq.(16) are applied to the inlet and outlet layer, correspondingly and $\theta=0$, $\theta=1$ and $\theta=0.5$ result in explicit, implicit and semi implicit Crank-Nicholson scheme respectively. In order to establish an equation for water solute concentration calculation, DQ will be used to discretize spatial derivatives in time step n and $n+1$ in Eq. (17) and Eq.(18) for any scheme. The form of spatial discretization is depicted in Fig. 2. The first subscript of C indicates the layer number and the second subscript denotes the grid point number which N, M show that how many grid points are recognized in inlet and outlet layer, respectively.

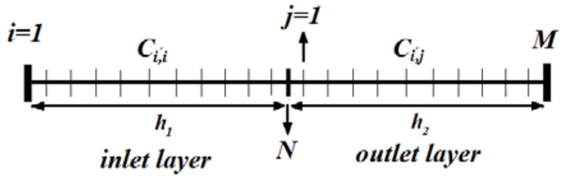

Fig 2. The form of spatial discretization

The general equation then would be:

$$R_{di'}\frac{C_{i',j}^{n+1}-C_{i',j}^{n}}{\Delta T}=D_{i',j}^{*}\sum_{k=1}^{M}b_{i',j,k}\left[\theta C_{i',k}^{n+1}+(1-\theta)C_{i',k}^{n}\right]$$

$$-v_{si'}\sum_{k=1}^{M}a_{i',j,k}\left[\theta C_{i',k}^{n+1}+(1-\theta)C_{i',k}^{n}\right] \qquad (17)$$

$for\ j=1,3,...,M-1$ and $i'=2$.

Using equations in the form of Equations (17, 18) for each grid, a set of nonlinear equations will be assembled that must be solved simultaneously for each layer.

$$R_{di'}\frac{C_{i',j}^{n+1}-C_{i',j}^{n}}{\Delta T}=D_{i',j}^{*}\sum_{k=1}^{M}b_{i',j,k}\left[\theta C_{i',k}^{n+1}+(1-\theta)C_{i',k}^{n}\right]$$

$$-v_{si'}\sum_{k=1}^{M}a_{i',j,k}\left[\theta C_{i',k}^{n+1}+(1-\theta)C_{i',k}^{n}\right] \qquad (18)$$

$for\ j=1,3,...,M-1$ and $i'=2$.

By some simplifications, a set of equations will be acquired in the following:

$$C_{i',i}^{n+1}+\frac{\Delta T}{R_{di}}(1-\theta)\sum_{k=1}^{N}\left[v_{si'}a_{i',i,k}-D_{i',i}^{*}b_{i',i,k}\right]C_{i',i}^{n+1}=$$

$$C_{i',i}^{n}+\frac{\Delta T}{R_{di'}}\theta\sum_{k=1}^{N}\left[D_{i',i}^{*}b_{i',i,k}-v_{si'}a_{i',i,k}\right]C_{i',i}^{n} \qquad (19)$$

$for\ i=2,3,...,N-1$ and $i'=1$

$$C_{i',j}^{n+1}+\frac{\Delta T}{R_{di'}}(1-\theta)\sum_{k=1}^{M}\left[v_{si'}a_{i',j,k}-D_{i',j}^{*}b_{i',j,k}\right]C_{i',j}^{n+1}=$$

$$C_{i',j}^{n}+\frac{\Delta T}{R_{di'}}\theta\sum_{k=1}^{M}\left[D_{i',j}^{*}b_{i',j,k}-v_{si'}a_{i',j,k}\right]C_{i',j}^{n} \qquad (20)$$

$for\ j=1,3,...,M-1$ and $i'=2$

Using DQM to discretize different type of boundary condition equations, a set of linear equation is created to determine the boundary values of solute concentration in time step $n+1$.

Problem type 1 boundary values:

$$C_{1,1}^{n+1} = C_0 \quad (21a)$$

$$\sum_{k=1}^{M} A_{M,k} C_{2,k}^{n+1} = 0 \quad (21b)$$

Problem type 2 boundary values:

$$c_{1,1}^{n+1} = c_0 \quad (22a)$$

$$\sum_{k=1}^{M} A_{M,k} c_{2,k}^{n+1} = 0 \quad (22b)$$

Problem type 3 boundary values:

$$(v - n_1 D_1^* A_{1,1}) C_{1,1}^{n+1} - n_1 D_1^* \sum_{k=2}^{N} A_{1,k} C_{1,k}^{n+1} = v\, C_0 \quad (23a)$$

$$\sum_{k=1}^{M} A_{M,k} C_{2,k}^{n+1} = 0 \quad (23b)$$

Which are corresponding to Eqs.(7 and 8).

5. Simulation Results

Two types of problem are considered to verify the correctness of the proposed numerical method and also to investigate the influence of various parameters on the transport process in a double-layer porous medium. The numerical results will be compared with the analytical results presented by Li and Cleall and Leij and van Genuchten [18], [19].

In all cases the effect of various parameters on transport process regarding the dimensionless relative parameters $\delta, \rho, \theta, \varphi$ is investigated. These parameters are assumed to provide more insight into the solution of the problem and are obtained as

$$\theta = \frac{h_2}{h_1},\ \varphi = \frac{n_2}{n_1},\ \rho = \frac{R_{d2}}{R_{d1}},\ \delta = \frac{D_2^*}{D_1^*} \quad (24)$$

5.1 Problem 1

For the first problem, the two layers are defined to initially have a zero solute concentration. The solute concentration at the inlet boundary is equal to zero and at outlet boundary solute concentration gradient is fixed to zero, which is often considered as appropriate. The effect of various parameters on the interface and the transport process are shown in Figs. 3a, 3b, 3c and 3d by dimensionless relative parameters $\delta, \rho, \theta, \varphi$ to provide more insight into the solution of the problem. These dimensionless parameters are:

$$\theta = \frac{h_2}{h_1},\ \varphi = \frac{n_2}{n_1},\ \rho = \frac{R_{d2}}{R_{d1}},\ \delta = \frac{D_2^*}{D_1^*} \quad (25)$$

In this investigation each parameter varies, while others are assigned constant values. the effect of the effective dispersion coefficient (D^*) on transport process in the double-layered porous medium with constant values of $\rho = \theta = \varphi = 1$, $v = 4\times10^{-9} m/s$ and $H = 1m$ at the 2 years is depicted in Fig. 3a. It is clear from Fig. 3a that the change of the relative effective dispersion coefficient (δ), will vary the concentration gradient between the two layers. This show that interface condition depends on the effective dispersion coefficient.

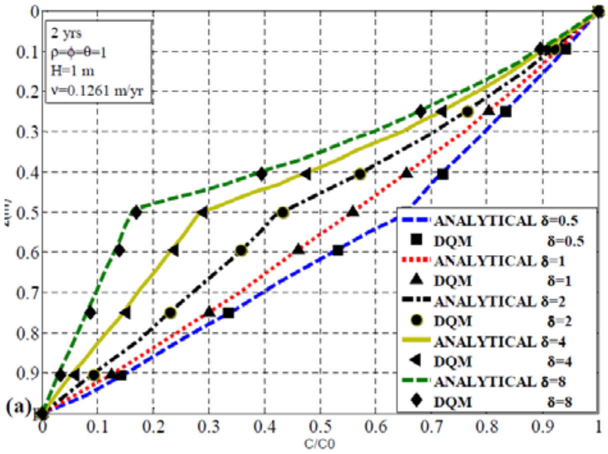

Fig. 3a. Solute concentration profiles in problem 1 with various δ

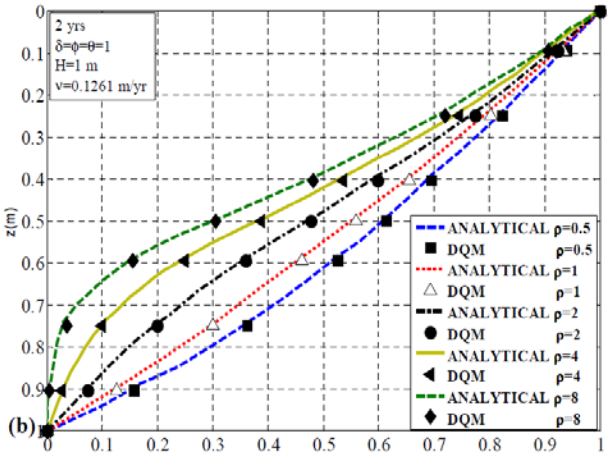

Fig. 3b. Solute concentration profiles in problem 1 with various ρ

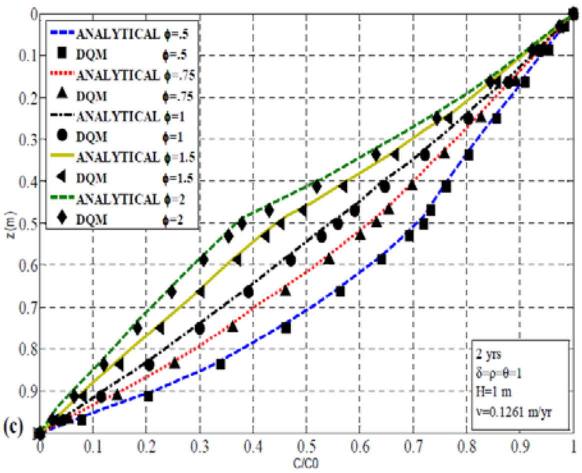

Fig. 3c. Solute concentration profiles in problem 1 with various φ

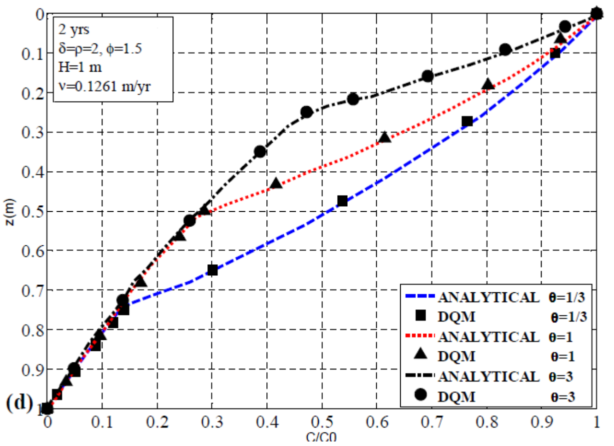

Fig. 3d. Solute concentration profiles in problem 1 with various θ

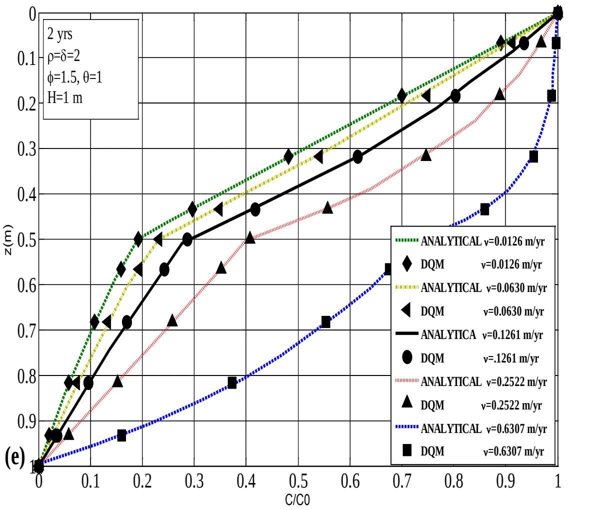

Fig. 3e. Solute concentration profiles in problem 1 with various v

The further results represent the effect of retardation factor on solute transport and is provided in Fig. 3b using following simulation parameters $\rho=\theta=\varphi=1$, Darcy velocity $=4\times10^{-9}\,m/s$, thickness of the layer is 1m and time is 2 years. Next, φ is assumed to be variable and the rest of the relative variable are assumed fixed ($\rho=\theta=\delta=1$).

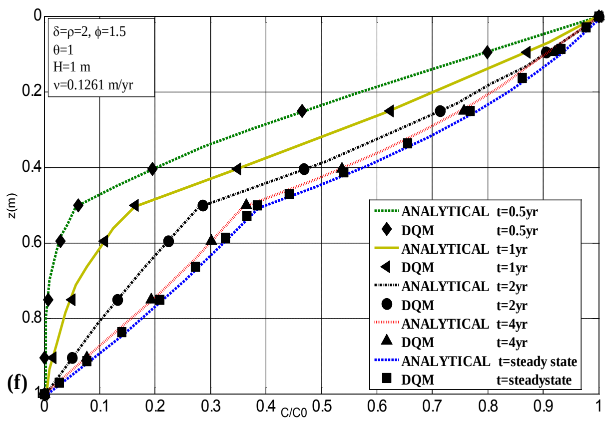

Fig. 3f. Solute concentration profiles in problem 1 at various times

These parameters are kept the same to know the impact of the porosity of layers on solute transport process (Fig. 3c). The impact of the variation of the porosities between the two layers can be clearly seen with a distinct change in the concentration gradient at the interface in Fig. 3c. to show the impact of the layer thickness of concentration profile the following values for parameters are used $\rho=\delta=2$, $H=1m$ $v=4\times10^{-9}\,m/s$ and the processing time is considered 2 years. The results are shown in Fig. 3d. In Fig. 3e the velocity effect on the layer thickness are demonstrated. The solute transport at various times are also investigated using $\theta=1$, $\varphi=1.5$ $\rho=\delta=2$, $H=1m$ at 0.5, 1, 2, 4 years period while steady state is assumed. Simulation results are provided in Fig. 3f.

In the numerical solution, different number of grid points were used. Selecting the different number of grid points reveals that mesh size can affect the accuracy of the results. To confirm the validity of the results, they are compared with the analytical solution results. Root Mean Square Error (RMS) values for DQ method are calculated for different grid numbers and are given in Table 2 in the Fig. 3a with $\delta=8$ as a case.

From different grid numbers, RMS Error is calculated using Eq. 26 as follows:

$$\Delta h=h_{analytical}-h_{\text{numerical}}\;;\;RMS=\sqrt{\frac{1}{R}\sum_{i=1}^{R}\left|\Delta h_i\right|^2} \qquad (26)$$

Where Δh is the difference between analytical and numerical results for different points and R is the number of data.

The RMS error values for non-uniform mesh size of 5, 11, 21, and 41 using a semi-implicit Crank-Nicholson scheme is compared with analytical solutions as in [18]. The RMS error values can be seen in Table 2 Which indicate there are a good agreement between numerical and analytical results. Table 2 shows the results for solute concentration at $\delta=8$ corresponding to Fig. 3a. It can be concluded that numerical results obtained from DQM are very close to the analytical results. Also, when the mesh sizes increase, the RMS error values will reduce.

Table 2. RMS values for solute concentration in Fig. 3a at $\delta = 8$

Distance (m)	Analytical result	Mesh size			
		N=5	N= 11	N= 21	N=41
0.2	0.7571	0.7417	0.755	0.7559	0.7575
0.4	0.4037	0.3679	0.3969	0.404	0.404
0.5	0.1693	0.1619	0.1698	0.1702	0.1702
0.6	0.1391	0.1302	0.1368	0.1377	0.1377
0.8	0.0716	0.0665	0.0698	0.0704	0.0704
RMS		0.0183	0.0034	0.0010	0.0009

5.2 Problem 2

In this problem it is assumed that the two layers initially have a zero solute concentration and concentration at the inlet boundary is set to C_0 and at outlet boundary solute concentration gradient is equal to zero. Six types of problem analogous to prior section are assumed to show the effect of various parameters on contaminant transport.

For the four series (depicted in Figs. 4a to 4d), one of the dimensionless relative parameters is varied while the rest are kept constant. In these four cases the Darcy velocity is equal to $4\times10^{-9}\, m/s$, the thickness of the porous media is $H = 1m$ and the time of the process is considered 2 years.

In Fig. 4a effect of the effective dispersion coefficient (D^*) is probed with $\rho = \varphi = \theta = 1$. The results show that all curves with different values of $\delta = 0.5,\ 1,\ 2,\ 4,\ 8$ cross each other at one point.

In Fig. 4b, the impact of retardation factor is investigated considering the different values for ρ while $\delta = \varphi = \theta = 1$. In the third case $\delta = \rho = \theta = 1$ is assumed to determine the variation of the porosity on transport process between the two layers. It can be seen that the interface condition is independent of porosity (Fig. 4c).

The next case has been depicted in Fig. 4d with $\delta = 2$, $\rho = 0.5$, $\phi = 1.5$ for various values of $\delta = 1,\ 1/3,\ 3$ to demonstrate the effect of two layer thickness on solute transport. In the next case, Darcy velocity and its effect on solute transport is investigated. The parameters $\delta = 2$, $\rho = 0.5$, $\varphi = 1.5$, $\theta = 1$ and $H = 1m$ are used in this case and results have been shown in Fig. 4e. The last case with properties equal to prior case except that in this case $v = 4\times10^{-9}\, m/s$ are assumed at different times. The outcomes are depicted in Fig 4f.

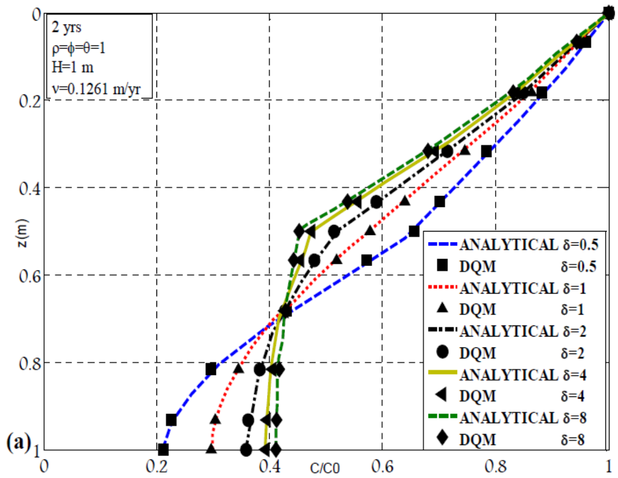

Fig. 4a. Solute concentration profiles in problem 2 with various δ

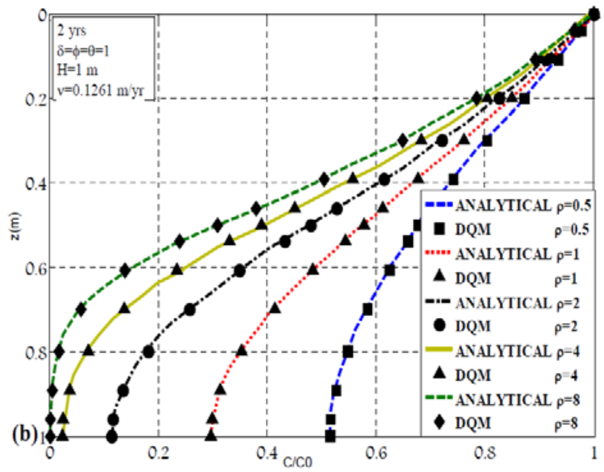

Fig. 4b. Solute concentration profiles in problem 2 with various ρ

A very good agreement is concluded. Normally, selecting the different number of grid points will affect the accuracy of the results. The RMS error values in the case of $\rho = 0.5$ (depicted in Fig. 4b) are given in Table 3 (as an example). It can be concluded that the DQM with a rather smaller number of grid points can produce very good results and negligible RMS error values may occur in DQM results.

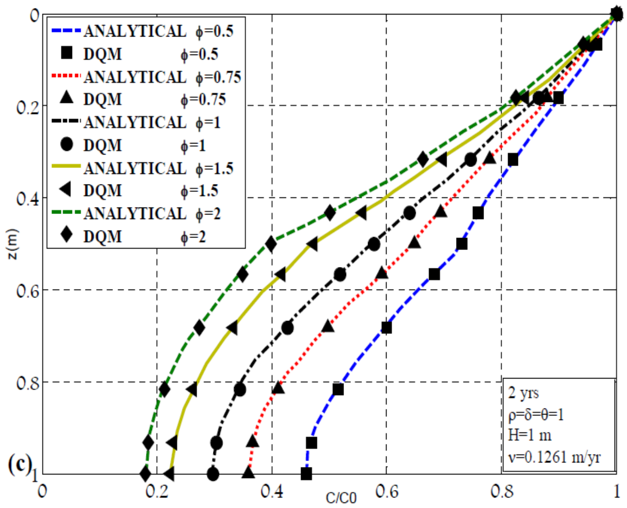

Fig. 4c. Solute concentration profiles in problem 2 with various ϕ

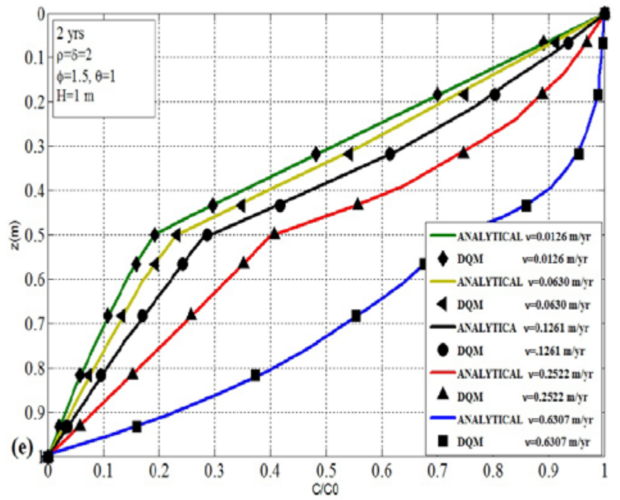

Fig. 4e. Solute concentration profiles in problem 2 with various ν

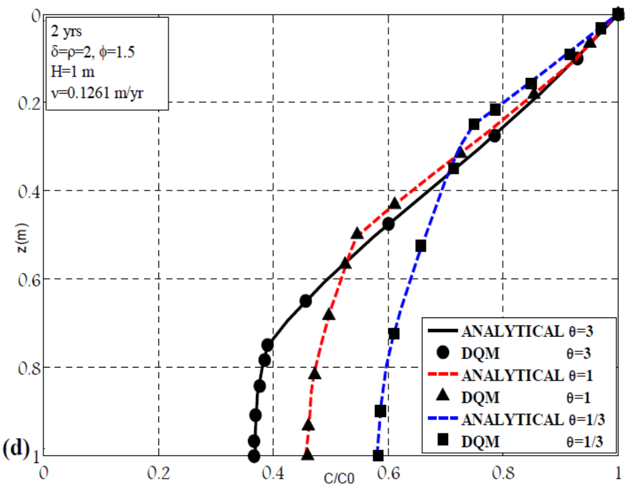

Fig. 4d. Solute concentration profiles in problem 2 with various θ

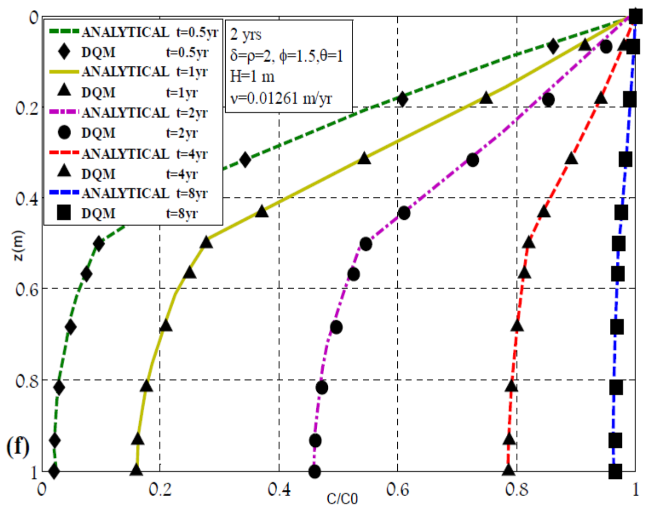

Fig. 4f. Solute concentration profiles in problem 2 at various times

Table 3. RMS values solute concentration in Fig. 4b with $\rho = 0.5$

Distance (m)	Analytical result	Mesh size			
		N=5	N= 11	N= 21	N=41
0.2	0.8694	0.8718	0.874	0.874	0.874
0.4	0.7292	0.7502	0.7381	0.7381	0.737
0.5	0.6697	0.6907	0.6786	0.6786	0.6786
0.6	0.6307	0.6477	0.6298	0.6298	0.629
0.8	0.5477	0.576	0.5501	0.5501	0.5491
RMS		0.0198	0.0079	0.0058	0.0057

5.3 Problem 3

The final problem we studied in this paper is a problem with constant solute flux at the inlet boundary equal to νC_0 and a zero concentration gradient at the outlet boundary as in Eq. (9). The needed parameters to analyze this problem are provided in Table 4.

Table 4. Parameters used in the second problem verification.

Layer	$D^*(m^2/s)$	R_d	n	$h(m)$
Inlet layer	2.315×10^{-8}	1.0	0.4	0.1
Outlet layer	5.787×10^{-8}	1.0	0.25	0.1

In both layers $h = 0.1m$, $R_d = 1$, at inlet layer $D_1^* = 2.315\times10^{-8}$ m/s $n_1 = 0.4$ and at outlet layer

$n_2 = 0.25$, $D_1^* = 5.787 \times 10^{-8}$ m/s and pore-water velocity $1.1574 \times 10^{-6} m/s$ ($10 cm/day$) are assumed. This problem has been probed previously by Leij and van Genuchten and Li and Cleall. The results at various times of $0.2, 0.4, 0.6, 0.8$ *day* are depicted in Fig. 5. The results of the two analytical solutions and DQM show a good match when $t = 0.2$ day but in larger times Leij and van Genuchten as in [3] analytical solution results are less than Li and Cleall work as in [4] and the present work. Indeed, the DQM results are close to the Li and Cleall analytical solution results in Fig 5.

It is seen from Fig 5 that at $t = 0.6$ day and $t = 0.8$ day the solute concentration near the outlet boundary are not correlated with Leij and van Genuchten and Li and Cleall works. In this case, the DQM results are close to Li and Cleall analytical solution.

The RMS error values at $t = 0.2$ *day* are presented in Tables 5. In this case a good agreement can be seen between Leij and van Genuchten and Li and Cleall analytical solutions. So, the DQM results are compared with Leij and van Genuchten and Li and Cleall analytical solutions simultaneously.

Table 5. Leij and van Genuchten and Li and Cleall Analytical and DQM solute concentration represented in Fig. 5 at $t = 0.2$

Distance (m)	Analytical result	Mesh size			
		N=5	N= 11	N= 21	N=41
0.01	0.9370	0.8341	0.9500	0.9358	0.9361
0.06	0.3450	0.4208	0.3427	0.3487	0.3457
0.11	0.0201	0.1364	0.0224	0.0198	0.0198
0.16	0.0025	0.0253	0.0004	0.0006	0.0005
0.19	0.0	0.0004	0.0	0.0044	0.0
RMS		0.0779	0.0060	0.0027	0.001

In the case where $t = 0.6$ day (Fig. 5) there is not a good match between the solute concentration for Leij and van Genuchten and Li and Cleall near the outlet boundary. It is seen that the DQM results are in a good agreement with Li and Cleall analytical solution rather than Leij and van Genuchten . Also, negligible errors occur in DQM and Li and Cleall analytical solution.

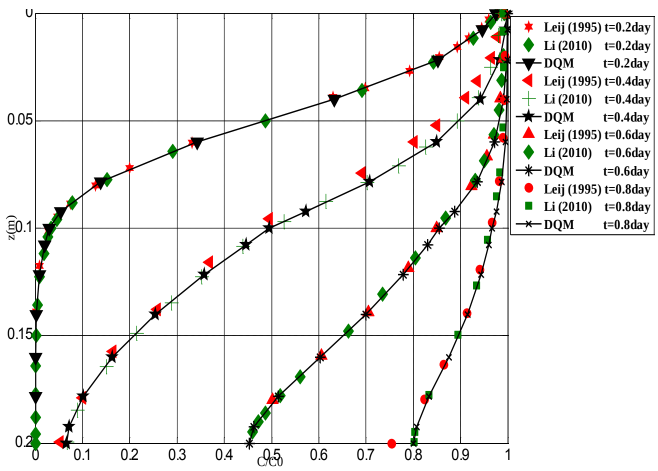

Fig. 5. Solute concentration profiles in problem 3

6. Conclusion

The DQM has been widely used for solving PDE's, recently. However, this method has not been used extensively in solute transport problems and more specifically, in solute transport in layered porous media. In this work, a DQM solution was utilized for solute transport problem in double layered porous media. Three different types of problems were solved and the results were compared with analytical solutions. The comparisons of this work show lower RMS error value, less computational time, rapid convergence than the other numerical methods while a good agreement with the exact results. Furthermore, applying the boundary conditions in conservative numerical methods (FE, FD, FV) accompanies with many difficulties which is not the case for DQM.

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