Comparative Analysis of Numerical Solutions of Advection-Diffusion Equation

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Abstract. The advection diffusion equation is one of the most popular and convenient equations in calculating the transport of energy and materials in flux areas. In this paper, one-dimensional advection-diffusion equation is solved using the finite difference, fourth order finite difference, finite volume, and differential quadrature methods in explicit condition. The quantitative comparative analysis involved two hypothetical cases and one experimental study. The results of the numerical solutions for the hypothetical cases are compared against the analytical solution. The experimental data are also simulated by the methods. The comparative analysis results revealed that the differential quadrature method performs as good as the analytical solution for the hypothetical cases. All the methods but the finite difference showed comparable performance in simulating the experimental data.

Keywords: Advection-diffusion equation, Numerical methods, Explicit solution

1. INTRODUCTION

The solution of advection diffusion equation (ADE) is necessary in a variety of fields, including but not limited to the transport of heat, sediment, ground water and surface flow pollutant. Many researchers like, Harleman and Rumer [1], Guvanasen and Volker [2], Marshall et al. [3], Banks and Ali [4], Lai and Jurinak [5], Al-Niami and Rushton [6], and Jaiswal et al. [7], tried to find analytical solution of ADE. Most of the solutions by these researchers have been obtained by using the Laplace transformation technique. In this field, many researchers like Raje and Kapoor [8] beside development of numerical solutions had many experimental studies.

Calhoun and LeVeque [9] presented a finite volume algorithm for a fully conservative, high-resolution ADE in irregular geometries. In order to model the fact that some cells are only partially available for the fluid phase, they used capacity functions. Guo and Wang [10] derived the finite difference methods (FDM) by second- and third-order accuracy to solve the convection-diffusion equation and applied a counter-error mechanism to reduce numerical dispersion. Younes and Ackerer [11] proposed a solution method by using the Eulerian-Lagrangian localized adjoint method on unstructured meshes and non-
uniform time stepping. Tian and Dai [12] developed a high-order compact exponential FDM for solving one- and two-dimensional (1D and 2D) steady-state cases of the equation. Hongxing [13] applied finite volume element method for solving the transport in 2Ds. In discretization, he used quasi-uniform triangular elements and piecewise linear element method. Ponsoda et al. [14] introduced a modified space-time conservation element while Kaya [15] solved the equation by differential quadrature method (DQM). Gopaul et al. [16] investigated three methods for solving the 1D case: 1) The Krylov subspace method, 2) Restrictive Taylor’s approximation and 3) Chebyshev pseudospectral collocation. Revelli and Rudolfi [17] gave the generalized collocation method for the linear and nonlinear models. Hermeline [18] proposed a new version finite volume method (FVM) for approximating convection diffusion equations. Karatay and Bayramoglu [19] have extended the Crank-Nicholson difference scheme to solve the time-fractional advection-dispersion equation. Savovic and Djordjevich [20] used explicit scheme of FDM to discretize the 1D ADE with variable coefficients in semi-infinite media. In this research, they assumed initial solute concentration that was a decreasing function of distance and uniform pulse-type input condition. Kaya and Gharehbaghi [21] numerically investigated the performance of several numerical techniques by ADE. In this research, the implicit approach of DQM showed the best results. Korkmaz and Dağ [22] proposed the fourth and fifth degree of B-spline DQM to solve the ADE. To evaluate the developed methods, two initial-boundary value problems modeling the transportation of a concentration and distribution of an initial pulse were used. Gao and Sun [23] suggested a high-order accurate three-point combined compact difference scheme with the L1 formula to solve a class of time-fractional ADEs. The suggested method by them was \((2−γ)th\) order accurate in time and at least fifth-order accurate in space for the constant coefficient time-fractional ADEs subject to periodic boundary conditions (\(γ\) was the order of time-fractional derivative in the governing equation). Gharehbaghi [24] employed explicit and implicit forms of DQM to solve the 1D time-dependent ADE with variable coefficients in semi-infinite domain for two dispersion problems: (i) solute dispersion along steady flow through inhomogeneous domain, and (ii) solute dispersion along temporally dependent unsteady flow through inhomogeneous domain. Both of the approaches used in this research were presented good agreement with analytical solutions.

As summarized above, different studies employed different numerical methods, and therefore there is no single study to the best knowledge of the authors that compares the performance of the numerical methods in explicit conditions against the analytical and experimental data sets. The key purpose of this article is to provide a numerical model to compare the performance of some traditional techniques (e.g., FDM, FVM) with one of the almost new developed numerical methods (DQM) in explicit conditions.

2. NUMERICAL SOLUTIONS of ADVECTION-DIFFUSION EQUATION (ADE)

The 1D unsteady ADE is given by

\[
\frac{\partial f}{\partial t} + A \frac{\partial f}{\partial x} = \frac{\partial}{\partial x} \left( D \frac{\partial f}{\partial x} \right)
\]

(1)

where; \(f\) refers to unknown component that change according to physical problem (concentration, flow rate, depth, mass, heat, etc.), \(x\) is space and \(t\) is time independent variables. \(A\) is advection coefficient, which can be velocity in the case of pollutant transport and \(D\) is the diffusion coefficient.

There are several type of boundary conditions, depends to the type of problem, could apply by users. In this essay, authors selected Cell-face type boundary conditions that applied in the inlet and outlet node points.

The initial and boundary conditions for Eq. (1) can be stated as follows:
This problem is solved by different numerical methods that are briefly described in the next section. All of the methods that applied in this essay used explicit scheme. Therefore, these methods must be able to satisfy stability condition. In this research, authors applied Courant number for testing the stability condition. In ADE two types of Courant number must be considered:

\[ C_{adv} = \frac{\Delta t |\nabla|}{\delta x} \leq 1, \quad C_{dif} = \frac{\Delta t |\nabla|}{\delta x^2} \leq 1 \]  

(3)

where \( C_{adv} \) is Courant number of advection and \( C_{dif} \) Courant number of diffusion. Moreover, in order to test the transportiveness property of a fluid flow authors determined the value of Peclet number. This number defined as a ratio of advection coefficient to the diffusion ones:

\[ P_e = \frac{\Delta x}{D/\delta x} \]  

(4)

where \( \delta x \) is the characteristic length or width of cell. The meaning of this number is given as below:

- If \( P_e \) approaches to zero \( (P_e \rightarrow 0) \) it means convection and pure diffusion
- If \( P_e \) approaches to infinite \( (P_e \rightarrow \infty) \) it means diffusion and pure convection

### 2.1. Finite Difference Method (FDM)

In this method, we used the forward difference scheme for the first derivative and the central difference scheme for the second derivative (Wu [25]).

**Forward difference scheme**

\[ \frac{\partial u}{\partial x} = \frac{u_i+1 - u_i}{\Delta x} \]  

(5)

**Central difference scheme**

\[ \frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} \]  

(6)

The final form of the numerical solution by FDM is given below:

\[ u_i^{t+1} = \Delta t \left(-A \frac{u_{i+1} - u_i}{\Delta x} + D \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2}\right) + u_i^t \]  

(7)

### 2.2. Fourth Order Finite Difference Method (FOFDM)

In order to catch the high order accuracy of numerical discretization, it could be selected more grid points in the difference formulation. Thus, in this method, to obtain a more accurate solution, a five-point symmetric difference scheme is employed as follows:

Derivation of first-order accurate in time

\[ \frac{\partial u}{\partial t} = \frac{u_i^{t+1} - u_i^t}{\Delta t} \]  

(8)

and the first and second derivations of five-point symmetric difference scheme are

\[ \left(\frac{\partial u}{\partial t}\right)_i = \frac{u_{i-1} - 8u_{i-1} + 8u_{i+1} - u_{i+2}}{12\Delta x} + o(\Delta x^4), \]  

(9)

\[ \left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{-u_{i-1} + 16u_{i-1} - 30u_{i+1} + 16u_{i+2} - u_{i+3}}{12\Delta x^2} + o(\Delta x^4), \]  

(10)

By substituting equations (8, 9 and 10) in ADE, the final form of this equation yields

\[ u_i^{t+1} = \Delta t \left(-A \frac{u_{i-1} - 8u_{i-1} + 8u_{i+1} - u_{i+2}}{12\Delta x} + D \frac{-u_{i-1} + 16u_{i-1} - 30u_{i+1} + 16u_{i+2} - u_{i+3}}{12\Delta x^2}\right) + u_i^t \]  

(11)
2.3. Finite Volume Method (FVM)

In this method, the central difference scheme is used:

\[ u_e = \frac{u_{p} + u_{w}}{2} \]  
\[ u_w = \frac{u_{p} + u_{w}}{2} \]  

“The key step of the finite volume method is the integration of the governing equation over a control volume to yield a discretized equation at its nodal point \( P \)” [26].

\[ \int_{t}^{t+\Delta t} \int_{CV} \partial_t u \, dV \, dt + \int_{t}^{t+\Delta t} \int_{CV} \frac{\partial u}{\partial x} \, A \, dV \, dt = \int_{t}^{t+\Delta t} \int_{CV} \frac{\partial^2 u}{\partial x^2} \, dV \, dt \]

\[ (u_p^{n+1} - u_p^n) \Delta V = -A \Delta t \left( L_e \frac{u_p^n + u_e^n}{2} - L_w \frac{u_p^n + u_w^n}{2} \right) + D \Delta t \left( \frac{u_p^n - u_n}{\Delta x_p} \right) - \left( \frac{u_p^n - u_n}{\Delta x_p} \right) \]  

Where node \( P \) is the place where the variable of interest is computed by using values at the east (\( e \)) and west (\( w \)) interfaces. The distance between the nodal points is \( \partial x \), and \( L \) is the cross sectional area of face of the control volume. Because the cross sectional areas in east and west are same so it can be written \( L_e = L_w = L \) and by divide the left- and right-hand sides of the equation (14) and by some manipulation, finally the numerical solution of ADE by FVM is given as below

\[ u_p^{n+1} = -\frac{A \Delta t}{2\Delta x} \left( u_p^n - u_w^n \right) + \frac{D \Delta t}{\Delta x^2} \left( \left( u_p^n - u_p^n \right) - \left( u_p^n - u_w^n \right) \right) + u_p^n \]  

The scheme is schematically presented in Fig.1.

![Schematic representation of finite volume scheme](image)

**Figure 1.** Schematic representation of finite volume scheme [26, 27]

2.4. Differential Quadrature Method (DQM)

This numerical method was proposed by Bellman and Casti [28]. The main idea of this method comes from Gauss Quadrature method. Its basic idea is to approximate a definite integral with a weighted sum of integrand values at a group of nodes in the form:

\[ \int_{a}^{b} f(x) \, dx \approx \sum_{j=1}^{N} w_j f(x_j) \]  

Where \( x_j (j=1,2,...,N) \) are nodes and \( w_j \) are weighting coefficients. They are determined by solving a system of linear equations [29]:

\[ a_{ij} = \frac{1}{(x_j-x_0)^{N-1}} \prod_{k=1}^{N} \frac{x_j-x_k}{x_i-x_k} \quad i, j = 1, 2, ..., N, \quad i \neq j \]  

\[ a_{ii} = -\sum_{j=1}^{N} a_{ij} \quad i = 1, 2, ..., N \]  

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In order to calculate the location of the estimate points; various methods can be used. Generally, these methods can be classified under two groups: (1) Equal intervals and (2) Non-equal intervals. For non-equal intervals, many researchers suggest various methods like Chebyshev or normalization of the routes of Legendre polynomial. In this study; Chebyshev node definition is applied to solve the ADE as:

$$b_{ij} = 2 \left[ c_{ij} a_{i-1} - \frac{a_{ij}}{x_{j+1} - x_i} \right] \quad i, j = 1, 2, \ldots, N, \quad i \neq j \quad (18a)$$

$$b_{ii} = - \sum_{j=1}^{N} b_{ij} \quad i = 1, 2, \ldots, N \quad (18b)$$

$$x_i = x_1 + \frac{1}{2} (1 - \cos \frac{i-1}{N-1} \pi)(x_n-x_1) \quad i = 1, 2, \ldots, N, \quad (19)$$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -A \sum_{j=1}^{N} a_{ij} u_j^{n} - \Delta t + D \sum_{j=1}^{N} b_{ij} u_j^{n} - \Delta t, \quad (20)$$

$$u_i^n = -\Delta t \cdot A \sum_{j=1}^{N} a_{ij} u_j^{n} - \Delta t + \Delta t \cdot D \sum_{j=1}^{N} b_{ij} u_j^{n} + u_j^{n} - \Delta t, \quad (21)$$

3. COMPARATIVE ANALYSIS of THE NUMERICAL METHODS

In order to solve the numerical methods, two hypothetical cases and one experimental study have been applied. It is worth pointing out that the required codes written in MATLAB. The feature of computer, that authors used to solve these four numerical methods, was RAM 4GB and CPU 2.40GHz.

3.1. Hypothetical Case 1:

Hypothetical Case 1 was taken from Dehghan [30]. The initial and boundary conditions for this case are given as follows:

$$u(x, 0) = \exp \left(-\frac{(x+0.5)^2}{0.00125}\right), \quad (22a)$$

$$u(0, t) = \frac{0.015}{\sqrt{0.000525 + 0.02t}} \exp \left(-\frac{(0.5-t)^2}{(0.00125 + 0.04t)}\right), \quad (22b)$$

$$u(1, t) = \frac{0.015}{\sqrt{0.000525 + 0.02t}} \exp \left(-\frac{(1.5-t)^2}{(0.00125 + 0.04t)}\right), \quad (22c)$$

The exact solution for the case 1 is given as:

$$u(x, t) = \frac{0.015}{\sqrt{0.000525 + 0.02t}} \exp \left(-\frac{(x+0.5-t)^2}{(0.00125 + 0.04t)}\right), \quad (23)$$

where $A=1.0$ and $D=0.01$.

In Figures 2a, and 2b the illustration of errors for the four numerical methods (FDM, FOFDM, FVM and DQM) are presented, according to the analytical solution. The values of errors are calculated by:

$$E = \frac{(E_n - E_a)/E_{\max}}{} \quad (24)$$

where $E$ refers to calculated error, $E_n$ refers to values of numerical methods, $E_a$ refers to value of analytical solution and $E_{\max}$ refers to maximum value of numerical methods. Meanwhile, to assess the performance of numerical techniques the values of root mean square errors (RMSE) are determined by the following equation:

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (u_{\text{Numerical solution}} - u_{\text{Exact solution}})^2} \quad (25)$$

The absolute values of maximum errors and RMSEs are calculated for three nodal points and three time steps, as presented in Table 1a. Moreover, in order to illustrate the stability condition the values of
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Courant Numbers calculated and given in Table 1b. Finally, in order to test the transportiveness property of a fluid flow, Peclet number calculated and given in Table 1c.

Figure 2a. Errors between DQM, FOFDM, FVM, DQM and Exact Solution Results at 60 node points and 60000 time steps.

Figure 2b. Errors between DQM, FOFDM, FVM, DQM and Exact Solution Results at 80 node points and 60000 time steps.
Table 1a. The absolute values of maximum errors and RMSEs

<table>
<thead>
<tr>
<th>Node points</th>
<th>Time Steps</th>
<th>FDM</th>
<th>RMSE of FDM</th>
<th>Required Time (second)</th>
<th>FOFD</th>
<th>RMSE of FOFD</th>
<th>Required Time (second)</th>
<th>FVM</th>
<th>RMSE of FVM</th>
<th>Required Time (second)</th>
<th>DQM</th>
<th>RMSE of DQM</th>
<th>Required Time (second)</th>
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<tr>
<td>60</td>
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<td>0.054146</td>
<td>0.0218455</td>
<td>0.94023</td>
<td>0.005391</td>
<td>0.0041988</td>
<td>1.028461</td>
<td>0.002197</td>
<td>0.000941</td>
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Table 1b. Courant Number.

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<th>Cadv</th>
<th>Cdif</th>
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Table 1c. Peclet Number.

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<th>80</th>
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<tbody>
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<td>Peclet Number</td>
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<td>8000</td>
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As seen in Figures 2a, 2b and in Tables 1a, 1b, and 1c the FDM performs poorly. DQM gives the best results followed by the numerical solutions by FVM and FOFD. Because of the explicit solution and the main concept of DQM (in any step of solution, the value at a point is under effect by all of other nodal points), this method seems more sensitive to the time steps than other numerical methods. By comparing the values in Table 1a, it can be seen that the results of DQM for the least sensitive of calculations (60 nodal points and 40000 time steps) are better than the numerical results of other methods in the maximum sensitive of calculations (80 nodal points and 60000 time steps). Among others, the DQM method requires more CPU time for the solution. This is because; DQM considers all the weighting coefficients of all the nodes simultaneously at each time step. FVM is the most effective in terms of the CPU time.

3.2. Hypothetical Case 2:

Hypothetical Case 2 was also taken from Dehghan [31], where the initial and boundary conditions are given as follows:

\[ u(x, 0) = \exp \left[ -\frac{(x-2)^2}{8} \right] \quad (26a) \]

\[ u(1, \tau) = \sqrt{\frac{2\tau}{10+\tau}} \exp \left[ -\frac{(5+4\tau)^2}{10(\tau+20)} \right] \quad (26b) \]
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\[ u(0, t) = \sqrt{\frac{28}{20+\tau}} \exp \left[ \frac{2((5+2\tau)^2)}{5(\tau+20)} \right] \]  

(26c)

The exact solution for the case 2 is given as:

\[ u(x, t) = \sqrt{\frac{28}{20+\tau}} \exp \left[ \frac{(x-2-0.8\tau)^2}{0.4(\tau+20)} \right] \]  

(27)

where \( A=0.8 \) and \( D=0.1 \).

The errors of FDM, FOFDM, FVM and DQM for two different nodal points and time steps (10x2000 and 30x10000) are presented in Fig.3a and 3b. The absolute value of maximum errors and RMSEs for various nodal points and time steps are summarized in Table 2a. Also the values of calculated Courant numbers and Peclet Numbers are yields in Tables 2b and 2c.

Figure 3a. Errors between DQM, FOFDM, FVM, DQM and Exact Solution Results at 10 node points and 2000 time steps.
As seen in Figures 3a, 3b and Tables 2a, 2b, and 2c DQM performs better than the others. The DQM is followed by FVM and FOFDM while FDM shows poor performance. In this hypothetical case the time domain divided into small number, so there is not any remarkable different in the values of required time but still DQM needs more required time in compare with another method. Even for the minimum number of nodal points and maximum time steps (10x2000), DQM shows better results than other numerical methods (see Table 2a).

4. EXPERIMENTAL STUDY

The data of experimental study were taken from Raje and Kapoor [8]. In their experimental research, they used glass beads to represent the porous medium microstructure. The dimension of glass column that shows the porous domain is 18 cm in length and 4.5 cm in diameter. Researchers selected all of the beads in same radius (1.5 mm) to represent the uniform domain. Thus, they could focus on the nonlinear kinetics transformation of chemical material in a porous media flow. The setup of that study is shown in Figure 4.
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Figure 4. Experimental setup for studying reactive transport in a porous medium [8].

The initial and boundary conditions for the experimental study are given as:

Initial concentration $c(x,0) = 0$
Boundary concentration $c(1,t) = 0.25$ mM

where the values of dispersivity $\alpha = 0.33$ cm, seepage velocity $v = 0.07$ cm/s sampling time = 510 s and advection coefficient is $A = v$. It is important to note that in this experimental study, $D$ denote the hydrodynamic dispersion coefficient of the solute and defined by $D = \alpha v$.

The comparison of measurements and numerical solution are given in the Figures 5a and 6b for 30 and 40 node points, respectively. Also, the figures of calculated errors for two cases are presented in Figures 5b and 6b.

According to the results in Figures 5a, b and 6a, b, DQM and FOFDM produced less errors, followed by FVM. The FDM performs poorly.

The required time for calculate these numerical solutions at 40 node points and 15000 time steps are given in Table 3a.

Finally, the values of Courant numbers and RMSEs for testing stability conditions and compare the results are given in table 3b and the values of Peclet Number, in order to test the transportiveness property of a fluid flow, are given in table 3c.
Figure 5a. Results of DQM, FOFDM, FVM, DQM and Measurement at 30 node points and 7500 time steps

Figure 5b. Errors between DQM, FOFDM, FVM, DQM at 30 node points and 7500 time steps and measurement Results
Figure 6a. Results of DQM, FOFD, FVM, DQM and Measurement at 40 node points and 15000 time steps

Figure 6b. Errors between DQM, FOFD, FVM, and DQM at 40 node points and 15000 time steps and measurement results
Table 3a. Table of Required Time for numerical methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Required Time for FDM (second)</th>
<th>Required Time for HighOrderFDM (second)</th>
<th>Required Time for FVM (second)</th>
<th>Required Time for DQM (second)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1.156109</td>
<td>1.094068</td>
<td>1.080752</td>
<td>2.107362</td>
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</tbody>
</table>

Table 3b. Courant Number and values of RMSEs

<table>
<thead>
<tr>
<th>Node points</th>
<th>Time steps</th>
<th>Cadv</th>
<th>Cdf</th>
<th>RMSE of FDM</th>
<th>RMSE of FOFDM</th>
<th>RMSE of FVM</th>
<th>RMSE of DQM</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>7500</td>
<td>0.0013</td>
<td>9.2400e-05</td>
<td>3.36917E-05</td>
<td>7.55322E-06</td>
<td>1.0203E-05</td>
<td>7.86351E-06</td>
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</tbody>
</table>

Table 3c. Peclet Number

<table>
<thead>
<tr>
<th>Node points</th>
<th>Peclet Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>428.5714</td>
</tr>
<tr>
<td>40</td>
<td>571.4286</td>
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</tbody>
</table>

5. CONCLUSIONS

In this paper, the general ADE is solved by four different numerical methods. The comparative analysis was carried out by using two hypothetical cases, one experimental study, and the analytical solution as a benchmark.

The comparative analysis results revealed that DQM is reliable. Results of DQM are more close to those of the analytical solution. Finite volume and fourth order finite difference methods are also found to be reliable (Tables 1a, 2a and 3a). In the experimental study, DQM and FOFDM results are compatible. Yet, the FDM shall be used with caution since it produced poor results for the hypothetical and experimental cases. By considering the required time of these four numerical solutions, it takes more time for the DQM, which can produce good approximation under small spacing step. Overall it can be concluded that, FVM is more efficient numerical solution method for the solution of the advection diffusion equation.

REFERENCES

Comparative Analysis


