Finite Volume Method-Adams-Bashford Difference for Contaminant Transport Equation

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ABSTRACT
Groundwater quality has recently received a lot of concern as a water resource problem. Contaminant's transport is best described by a mathematical model. In this paper, we study the contaminant transport phenomenon using an advection-diffusion equation. The contaminant transport equation is solved numerically, we apply the finite volume method. Here we use Adams-Bashforth Difference to extrapolate advective terms from previous time step in an explicit manner and handles diffusive terms implicitly using Crank-Nicolson second order scheme. Our numerical model is validated by comparing the numerical results with the existing analytical solution. Further, we conclude that the methods can best approximate the exact solution when using a small Courant number and spatial grid partition.

Keywords: Contaminant transport, Advection-diffusion equation, Adams-Bashforth Difference.

1. Background Information

Groundwater is the invaluable natural resource supporting life on the surface of the earth. Surface and subsurface water covers approximately 75% of our planet earth and out of these a large percentage is salty. Only about 4%-5% of the earth surface water is fresh. The commonest problem of groundwater resources is not only about quantity problem but also quality problem. Groundwater quality is of importance as to surface water quality. Usually, the problems affecting surface water is reported periodically, due it's easiness in measurement in comparison to groundwater quality measurement (Freeze & Cherry, 1979). Contaminant is always on dynamic condition, it means that the contaminant interact to soil particles until equilibrium condition

The solution of advection diffusion equation (ADE) is applicable to the transport of heat, sediment transport, ground water and surface flow contaminants just to mention a few. Quite a number of researchers have tried to solve ADE analytically, for example 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]. Most of these researchers obtained the solution by employing the Laplace transformation methods. (Rao et al., 2011) in the Basaltic Terrain, undertook a field case study in India. The study improved an understanding of the contaminant movement in the regional aquifer system. Raje and Kapoor [8] carried out experimental studies and came up with numerical solutions.

Tian and Dai [12] came up with a high-order compact exponential FDM for solving 1D and 2D steady-state cases of the ADE equation. Savovic and Djordjevich [20] employed FDM explicit scheme to discretize the 1D ADE with variable coefficients in semi-infinite media. In their work, assumption was an initial solute concentration that was a decreasing function of distance and uniform pulse-type input condition. Hongxing [13] used finite volume element method to solve the transport equation in 2Ds. He discretized the equation by using quasi-uniform triangular elements and piecewise linear element method. The finite element method has also been used by [9] in construction of the advection-diffusion equation's numerical model Ponsoda et al. [14] used a modified space-time conservation element and Kaya [15] used differential quadrature method in solving the equation. Kaya and Gharehbaghi [21] investigated numerically the performance of several numerical techniques by ADE. the modified finite difference schemes like the compact finite difference was used by [2] and the combination of high-order finite-difference with 4th-order Runge-Kutta in [3]. [4] used the Runge-Kutta method itself in solving the advection-reaction-diffusion equation. Other numerical methods have been also applied to simulate the transport phenomenon [13]. However, among the various methods, the finite volume method is preferred in solving transport as it conserved the fluid quantity. This study will discuss the numerical simulations using finite volume method by employing Adams-Bashforth Difference where it extrapolates advective terms from previous time step in an explicit manner and handles diffusive terms implicitly using Crank-Nicolson and compare the results with the fourth, and sixth-order explicit finite difference method (FTCS).

2.GOVERNING EQUATION

The advection-diffusion transport equation in one dimensional case without source terms is as follows:

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} - \mathrm{D}\frac{\partial^2 \mathrm{C}}{\partial \mathrm{x}^2} = 0, \qquad 0 \le x \le L,\ 0 < t \le T \tag{1}$$

Initial conditions: $C(x, 0) = C_0(x)$ (2)

Boundary conditions: $C(0, t) = g_0(t), C(L, t) = g_L(t)$ (3)

where t -time, x -space coordinate, D -diffusion coefficient, $C(x,\, t)$ -concentration, $U(x,\, t)$ - water flow velocity, and L channel length respectively. $C_0, g_0,\ and\ g_L$ are prescribed functions, while C is the unknown function. Notice that $D > 0$ and $U > 0$ are positive constants signifying the diffusion and advection processes, respectively.

3. Finite Volume Method

Finite volume uses the central difference scheme to estimate the required point

$$u_e = \frac{u_P + u_E}{2} \tag{4}$$

$$u_w = \frac{u_P + u_W}{2} \tag{5}$$

In Finite volume method, the governing equation is integrated over a control volume to yield a discretized equation at its nodal point 'P'.

Taking integral in equation (1) we obtained

$$\int_t^{t+\Delta t}\left[\int_V \frac{\partial C}{\partial t}\,\partial V + \int_V \nabla.(\,u\,C)\,dV\right]dt = \int_t^{t+\Delta t}\left[\int_V \nabla.(D\,\nabla\,C)\partial V\right]dt \tag{6}$$

The terms in equation (6) are discretized using finite volume method as discussed in the next section.

3.1 Advection terms

The advection term in equation (6) is interpolated linearly between faces E and W about point P using Central Differencing scheme (CD) to obtain

$$\int_w^e U\frac{\partial C}{\partial x}dx \approx\ (u)_e\frac{(C_E + C_P)}{2} - (u)_w\frac{(C_P + C_W)}{2} \tag{7}$$

CD is second accurate even on a non-uniform meshes.

3.2 Viscous terms

The Crank-Nilcoson method is an implicit second order both in time and space and is unconditionally stable. Equation (7) is integrated from t to $t + \Delta t$, where in this scheme, values average of t and $t + \Delta t$ are used. The Crank-Nicolson discretisation for the viscous term can be written as

$$\frac{1}{\Delta \mathrm{t}}\int_{\mathrm{t}}^{\mathrm{t}+\Delta \mathrm{t}} D\left\{\left(\frac{\mathrm{C_E} - \mathrm{C_P}}{(\delta \mathrm{x})_\mathrm{e}}\right) - \left(\frac{\mathrm{C_P} - \mathrm{C_W}}{(\delta \mathrm{x})_\mathrm{w}}\right)\right\}\mathrm{dt} \approx \left\{\left(\mathrm{D}\frac{\mathrm{C}_\mathrm{E}^{\mathrm{n}+1} - \mathrm{C}_\mathrm{P}^{\mathrm{n}+1}}{2\delta \mathrm{x}}\right) - \left(\mathrm{D}\frac{\mathrm{C}_\mathrm{E}^{\mathrm{n}} - \mathrm{C}_\mathrm{P}^{\mathrm{n}}}{2\delta \mathrm{x}}\right) + \left(\mathrm{D}\frac{\mathrm{C}_\mathrm{P}^{\mathrm{n}+1} - \mathrm{C}_\mathrm{W}^{\mathrm{n}+1}}{2\delta \mathrm{x}}\right) - \left(\mathrm{D}\frac{\mathrm{C}_\mathrm{P}^{\mathrm{n}} - \mathrm{C}_\mathrm{W}^{\mathrm{n}}}{2\delta \mathrm{x}}\right)\right\} \tag{8}$$

The Adams-Bashforth Difference extrapolate advective terms from previous time step in an explicit manner and handles diffusive terms implicitly using Crank-Nicolson second order scheme.

The integration of advective terms in equation (8) from time step n to n+1 is approximated by

$$\frac{1}{\Delta t}\int_n^{n+1} u\,Cdt \approx \frac{3}{2}(U\,C)^n - \frac{1}{2}(\,U\,C)^{n-1} \tag{9}$$

The value of the scalar C at the cell face is approximated by using the central differencing scheme, hence the advective term becomes

$$\frac{1}{\Delta t}\int_t^{t+\Delta t}(U((C)_e-(C)_w))\,dt \approx U\left(\frac{3}{2}C_e^n-\frac{1}{2}C_e^{n-1}\right)$$

$$\approx U\left(\frac{3}{4}(C_P^n+C_E^n)-(C_P^n+C_W^n)-\frac{1}{4}((C_P^{n-1}+C_E^{n-1})-(C_P^{n-1}+C_W^{n-1})\right) \qquad (10)$$

For diffusive terms we employ the Crank-Nicolson Scheme as given in equation (8). Substituting equations (8) and (9) in (1) to obtain

$$\frac{1}{\Delta t}\int_t^{t+\Delta t}\boldsymbol{D}\left\{\left(\frac{C_E-C_P}{(\delta x)_e}\right)-\left(\frac{C_P-C_W}{(\delta x)_w}\right)\right\}dt \approx \left(\mathbf{D}\frac{C_E^{n+1}-C_P^{n+1}}{2\delta x_e}\right)-\left(\mathbf{D}\frac{C_P^n-C_W^n}{2\delta x_w}\right)\frac{\Delta x}{\Delta t}(C_P^{n+1}-C_P^n)=\frac{1}{2}\boldsymbol{D}\left((C_E^{n+1}-2C_P^{n+1}+C_W^{n+1})-(C_E^n-2C_P^n+C_W^n)\right) \qquad (11)$$

Integrating the transient term in time

$$\frac{1}{\Delta t}\int_t^{t+\Delta t}\frac{\partial(C)}{\partial t}\Delta x\,dt=\frac{\Delta x}{\Delta t}(C_P^{n+1}-C_P^n) \qquad (12)$$

Using the finite volume discretization (10), (11) and (12) in (1) to obtain the discretized transport equation

$$\frac{1}{\Delta t}(C_P^{n+1}-C_P^n)=\frac{1}{2\Delta x}\mathbf{D}\left((C_E^{n+1}-2C_P^{n+1}+C_W^{n+1})-(C_E^n-2C_P^n+C_W^n)\right)-\left[U\left(\frac{3}{4}(C_E^n-C_W^n)-\frac{1}{4}((C_E^{n-1}-C_W^{n-1})\right)\right] \qquad (13)$$

We let $r=\frac{D\Delta t}{\Delta x}$ and substituting in (13)

$$C_p^{n+1}-r(C_E^{n+1}+C_W^{n+1})=C_P^n+r(C_E^n-C_W^n)+U\left(\frac{3}{4}(C_E^n-C_W^n)\right)-\frac{1}{4}(C_E^{n-1}-C_W^{n-1})\right) \quad (14)$$

$$C_p^{n+1}-r(C_E^{n+1}+C_W^{n+1})=C_P^n+\left(r+\frac{3}{4}U\right)C_E^n-\left(r+\frac{3}{4}U\right)C_W^n-\frac{1}{4}U(C_E^{n-1}-C_W^{n-1}) \quad (15)$$

Points P, E and W can be rewritten as P=i, E= i+1 and W=i-1 hence equation (15) becomes

$$C_i^{n+1}-r(C_{i+1}^{n+1}+C_{i-1}^{n+1})=C_i^n+\left(r+\frac{3}{4}U\right)C_{i+1}^n-\left(r+\frac{3}{4}U\right)C_{i-1}^n-\frac{1}{4}U(C_{i+1}^{n-1}-C_{i-1}^{n-1}) \quad (16)$$

4. Numerical Illustrations

Let us consider the advection-diffusion equation with the initial and boundary conditions. The numerical results are compared with the exact solutions. The technique is applied to solve the ADE with $C0(x)$, $f0(t)$, $fL(t)$, and$g(t)$ prescribed. To test the performance of the proposed method, absolute error, $L2$ and $L\infty$ error norms are used as follows: Two examples for which the exact solutions are known are used to verify the proposed numerical method.

$$L_\infty=\left|C_i^{exact}-C_i^{numerical}\right|$$

$$L_\infty=max_i\left|C_i^{exact}-C_i^{numerical}\right|$$

$$L_2=\sqrt{\sum_{i=1}^{N}\left|C_i^{exact}-C_i^{numerical}\right|^2}$$

Here, we consider two cases to observe contaminant spreading

Case 1. Consider a channel of length L=100m. Flow velocity and diffusion coefficient are taken to be U = 0.01m/s and D = 0.002m2/s respectively. The Cr numbers are selected as 0.01, 0.1, and 0.6 for the present work. Exact solution of the current problem is as follows [18]

$$C(x,t)=\frac{1}{2}erfc\left(\frac{x-Ut}{2\sqrt{Dt}}\right)+\frac{1}{2}exp\left(\frac{Ux}{D}\right)erfc\left(\frac{x+Ut}{2\sqrt{Dt}}\right)$$

where erfc(x) is the complementary error function. The boundary conditions of the contaminant concentration are:

$$C(0,t)=1$$

$$-D\left(\frac{\partial C}{\partial x}\right)(L,t)=0$$

The initial conditions are obtained from the exact solution.

Table 1. The norm error of each finite difference methods using various Cr

Cr	Δx	Δt	L_2	L_∞
0.1	0.1	1	0.002	0.002657
0.01	0.5	0.5	0.0003	0.0009121
0.002	0.5	1	0.0054	0.0043751

Case 2. We Consider a channel of length L = 10 m. The water velocity is U = 0.8 m/s and the diffusion coefficient is D = 0.005 m//s. As written in [4], the obtained exact solution

$$C(x,t) = \frac{1}{\sqrt{(4t+1)}} exp\left[-\frac{(x-1-Ut)^2}{D(4t+1)}\right] \qquad 23$$

And boundary conditions are

$$C(0,t) = \frac{1}{\sqrt{(4t+1)}} exp\left[-\frac{(x-1-Ut)^2}{D(4t+1)}\right]$$

$$C(9,t) = \frac{1}{\sqrt{(4t+1)}} exp\left[-\frac{(8-Ut)^2}{D(4t+1)}\right]$$

The initial conditions are obtained from the exact solution where t=0. In the computation,$\Delta x = 0.5$. the obtained results using numerical method are compared with the exact as shown in table1.

Table 2. The absolute error of finite volume methods at different points

x	exact	FVM	Absolute error
4	2985.6	2963	22.5
4.5	25.5246	28.5	3.0
5	0.2182	0.2390	0.0208
5.5	0.0019	0.0017	0.0002
6	0.0000159	0.0000160	0.0000001

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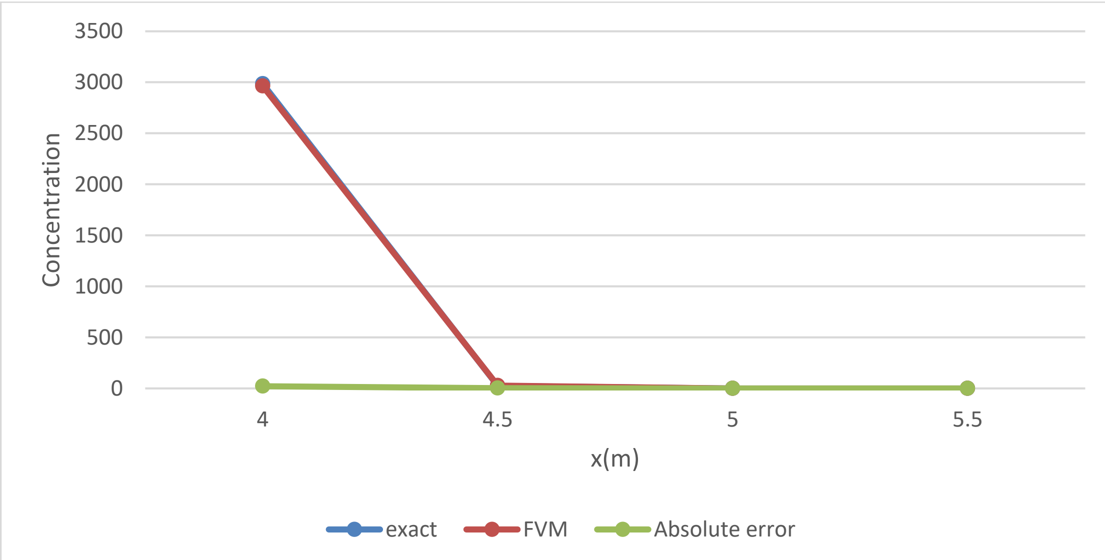

Figure 1:Comparison of exact and the numerical solution

Figure 1 shows result comparison between the numerical using FVM and the exact solution. The graph depicts almost similar pattern suggesting that they are in good agreement. As shown in Table 1, the norm errors of the with Cr=0.01 and spacing of Δx=0.5 are small in comparison to Cr=0.1 and Cr=0.002. But when we change Δt to 1hour and Cr to Cr=0.1 and Cr=0.002 it produces different result as recorded in Table 1.

5. CONCLUSION

We derived the finite volume scheme by employing Adams-Bashforth Difference to extrapolate advective terms from previous time step in an explicit manner and handles diffusive terms implicitly using Crank-Nicolson second order scheme. This scheme best approaches exact solution when small number of Cr and Δx are used. For further study the method can be compared with other numerical methods.

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