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The Effect of Decaying Diffusion And Exponential Advection Parameters On Water Quality In Aquifer

Dr. George Ochieng Ogongo

Faculty of Biological and Physical Sciences, Tom Mboya University Collage, P.O BOX 199-40300, Homabay, Kenya.

Abstract
The paper studies the effect of decaying diffusion parameter and exponential advection parameter on the quality of water in aquifer. Taylor series expansion is used to generate the finite difference scheme of Alternating Direction Explicit (ADE) scheme and Alternating Direction Implicit (ADI) scheme. The two schemes are found to be consistent and stable with the model equations.

Keywords: *(3+1) Dimensional Advection Diffusion Equation, Partial Differential Equations (PDE'S), Alternating Direction Explicit (ADE) scheme, Alternating Direction Implicit (ADI) scheme.*

Mathematics Subject Classification: Primary 65N30, 65M12, 65M06; Secondary 65D05, 65M22, 65M60

Introduction

Use of Advection – Diffusion equation in various fields of science like transport of heat, sediment, ground water and surface flow pollutants are fully sufficient for researchers to show interest in solving this equation. Many researchers like Bear [1] tried to propose analytical solutions for these type of equations, but in recent years researchers like Beny [2] have shown more interest thereby introducing numerical solutions to these kind of equations. As noted earlier, most of the researchers showed interest to present numerical solutions for Advection – Diffusion Equation instead of analytical solutions.

Brief review of work done by attention to the data was done by Young and et al [66] who developed an algorithm to solve fully conservative, high resolution Advection – Diffusion Equation in irregular geometries. In this algorithm they developed Finite Volume Method to solve this equation.Bobenko [3] in order to numerically integrate the semi – discrete equation arising arising after the spatial discretization of Advection – Reaction – Diffusion Equation applied two variable step linearly implicit Runge – Kutta methods of order 3 amd 4 equations.

Chapra [5] used the Euclerian – Lagrangian localized adjoin method on non – uniform time steps and unstructured meshes to solve the Advection – Diffusion Equation. Doyo [9] tried to develop an algorithm by second and third order accuracy with finite with finite – difference method to solve the convection – diffusion equation. In this algorithm they used to counter error mechanism to reduce numerical dispersion. One of the researchers that tried to solve Advection – Diffusion Equation in implicit condition is Douglas [8]. He solved the equation with Finite Difference Method by using the upwind and Crank – Nicolson schemes.

First,we derive the finite difference forms of ADE and ADI methods for the given model equation and then present an algorithm for each method.

The model equation

The research examines the Alternating Direction Explicit (ADE) scheme and Alternating Direction Implicit (ADI) scheme for solving the (3+1) Dimensional Advection-Diffusion equation:

$$f_1(x,y,z,t)\frac{\partial^2 C}{\partial x^2}+f_2(x,y,z,t)\frac{\partial^2 C}{\partial y^2}+f_3(x,y,z,t)\frac{\partial^2 C}{\partial z^2}+f_4(x,y,z,t)\frac{\partial^2 C}{\partial x\partial y}+f_5(x,y,z,t)\frac{\partial C}{\partial x}+f_6(x,y,z,t)\frac{\partial C}{\partial y}=C_t \quad (1)$$

which is used to model physical process of Advection-Diffusion in a (3+1) Dimensional system such as one involving contaminant concentration in aquifer. The coefficients$f_1(x,y,z,t), f_2(x,y,z,t), f_3(x,y,z,t) f_4(x,y,z,t)$ represent the diffusion parameters (diffusivity) and $f_5(x,y,z,t)$ *and* $f_6(x,y,z,t)$ are the advection parameters (velocity). The equation is parabolic and is derived from the principle of conservation of mass using Fick's law of conservation in fluid flow problems as presented by (Morton 1971).The Alternating Direction Explicit(ADE) scheme developed for the equation is given by:-

$$4qC_{i,j,k}^{n+1} = 4C_{i+1,j,k}^{n} - 24C_{i,j,k}^{n} + 4C_{i-1,j,k}^{n} + 4C_{i,j+1,k}^{n} + 4C_{i,j-1,k}^{n} + 4C_{i,j,k+1}^{n}4C_{i,j,k-1}^{n} + C_{i+1,j+1,k}^{n} - C_{i+1,j-1,k}^{n} - C_{i-1,j+1,k}^{n} + C_{i-1,j-1,k}^{n} + 2qC_{i+1,j,k}^{n} + 2qC_{i,j+1,k}^{n} \qquad (2)$$

and the Alternating Direction Implicit (ADI) scheme developed for the equation is given by:-

$$4qC_{i,j,k}^{n+1} + 4C_{i-1,j,k}^{n+1} - 8C_{i,j,k}^{n+1} - 4C_{i+1,j,k}^{n+1} = 4qC_{i,j,k}^{n} - 16C_{i,j,k}^{n} + 4C_{i,j+1,k}^{n} + 4C_{i,j-1,k}^{n} + 4C_{i,j,k+1}^{n} + 4C_{i,j,k-1}^{n} + C_{i+1,j+1,k}^{n} - C_{i+1,j-1,k}^{n} - C_{i-1,j+1,k}^{n} + C_{i-1,j-1,k}^{n} + 2qC_{i+1,j,k}^{n} - 2qC_{i-1,j,k}^{n} + 2qC_{i,j+1,k}^{n} - 2qC_{i,j-1,k}^{n}$$
(3)

Properties of numerical schemes

Many techniques are available for numerical simulation work and in order to quantify how well a particular numerical technique performs in generating a solution to a problem, there are four fundamental criteria that can be applied to compare and contrast different methods. The concepts are accuracy, consistency, stability and convergence. The method of Finite Difference Method is one of the most valuable methods of approximating numerical solution of Partial Differential Equations (PDEs). Before numerical computations are made, these four important properties of finite difference equations must be considered.

(a) **Accuracy**: Is a measure of how well the discrete solution represents the exact solution of the problem. Two quantities exist to measure this, the local or truncation error, which measures how well the difference equations match the differential equations, and the global error which reacts to the overall error in the solution. This is not possible to find unless the exact solution is known.

(b) **Stability**: A finite difference scheme is stable if the error made at one time step of the calculation do not cause the errors to be magnified as the computations are continued. A neutrally stable scheme is one in which errors remain constant as the computation are carried forward. If the errors decay are eventually damp out, the numerical scheme is said to be stable. If on the contrary, the errors grow with time the numerical scheme is said to be unstable.

(c) **Consistency**: When a truncation error goes to zero, a finite difference equation is said to be consistent or compatible with a partial differential equation. Consistency requires that the original equations can be recovered from the algebraic equations. Obviously this is a minimum requirement for any discretization.

(d) **Convergence**: A solution of a set of algebraic equations is convergent if the approximate solution approaches the exact solution of the Partial Differential Equations (PDEs) for each value of the independent variable. For example, as the mesh sizes approaches zero, the grid spacing and time step also goes to zero.

Lax had proved that under appropriate conditions a consistent scheme is convergent if and only if it is stable. According to $Lax - Richtmyer\ Equivalence\ Theorem$ which states that "given a properly posed linear initial value problem and a finite difference approximation to it that satisfies the consistency condition, stability is the necessary and sufficient condition for convergence"

Initial and Boundary condition

Limit conditions are important in solving the (3+1) dimension advection-diffusion contaminant concentration equation. They are decided by actual geographical information and initial contaminant concentration of the boundaries. There are mainly two approaches to obtain the initial conditions, Griths and Mitchel[27]. One is to set the real approximate pollutant concentration as initial condition and the other is to set zero concentration as initial condition. The latter is viewed as the ideal circumstance. The expression for initial conditions of the equation can therefore be given as:

$$C(x, y, z, t_0) = Sin(x + y + z) \qquad (4)$$

$$C(x, y, z, t_0) = 0 \qquad (5)$$

In general, there are three boundary conditions for Advection-Diffusion equations, Griths and Mitchel[27]: Dirichlet condition (the concentration boundary), Neuman condition (the concentration gradient boundary) and Cauchy condition (the concentration boundary and the concentration gradient boundary specified at the same time). Considering the calculation efficiency we will choose the ideal boundary condition ie the Dirichlet condition, giving the boundary condition as:

$$C(x,y,z,t) = C(10,y,z,t) = 0, 0 \le x \le 10 \quad (6)$$

$$C(x,y,z,t) = C(x,2,z,t) = 0, 0 \le y \le 2 \quad (7)$$

$$C(x,y,z,t) = C(x,y,2,t) = 0, 0 \le x \le 2 \quad (8)$$

Substituting $\boldsymbol{e^x}$ for $\boldsymbol{f_1(x,y,z,t)}, \boldsymbol{f_2(x,y,z,t)}, \boldsymbol{f_3(x,y,z,t)}$ and $\boldsymbol{f_4(x,y,z,t)}$ and $\boldsymbol{e^{-x}}$ for $\boldsymbol{f_5(x,y,z,t)}$and $\boldsymbol{f_6(x,y,z,t)}$ while we let $\boldsymbol{x = 1}$ on $\boldsymbol{e}$ superscript in equation (1) would yield:

When $n = 0$, the systems of linear algebraic equations will be written in matrix-vector form as:

$$\begin{bmatrix} -1.118 & 0.00587 & \cdots & 0 & \cdots & 0 \\ 0.00587 & -1.118 & 0.00587 & \vdots & 0 & \vdots \\ \vdots & 0.00587 & \ddots & \ddots & \vdots & 0 \\ 0 & \cdots & \ddots & \ddots & 0.00587 & \vdots \\ \vdots & \cdots & 0 & 0.00587 & -1.118 & 0.00587 \\ 0 & \cdots & 0 & \cdots & 0.00587 & -1.118 \end{bmatrix} \times \begin{bmatrix} C_{1,1,1}^1 \\ C_{2,1,1}^1 \\ C_{3,1,1}^1 \\ C_{4,1,1}^1 \\ C_{5,1,1}^1 \\ C_{6,1,1}^1 \\ C_{7,1,1}^1 \\ C_{8,1,1}^1 \\ C_{9,1,1}^1 \\ C_{10,1,1}^1 \end{bmatrix} = \begin{bmatrix} -0.0656000 \\ 0.6400000 \\ 0.7070000 \\ 0.1240000 \\ -0.6110000 \\ -0.7940000 \\ -0.2280000 \\ 0.4960000 \\ 0.7640000 \\ 0.3520000 \end{bmatrix} \quad (9)$$

When $n = 1$, the systems of linear algebraic equations will be written in matrix-vector form as:

$$\begin{bmatrix} -1.118 & 0.00587 & \cdots & 0 & \cdots & 0 \\ 0.00587 & -1.118 & 0.00587 & \vdots & 0 & \vdots \\ \vdots & 0.00587 & \ddots & \ddots & \vdots & 0 \\ 0 & \cdots & \ddots & \ddots & 0.00587 & \vdots \\ \vdots & \cdots & 0 & 0.00587 & -1.118 & 0.00587 \\ 0 & \cdots & 0 & \cdots & 0.00587 & -1.118 \end{bmatrix} \times \begin{bmatrix} C_{1,1,1}^2 \\ C_{2,1,1}^2 \\ C_{3,1,1}^2 \\ C_{4,1,1}^2 \\ C_{5,1,1}^2 \\ C_{6,1,1}^2 \\ C_{7,1,1}^2 \\ C_{8,1,1}^2 \\ C_{9,1,1}^2 \\ C_{10,1,1}^2 \end{bmatrix} = \begin{bmatrix} 0.0154000 \\ -0.5310000 \\ -0.5130000 \\ -0.0228000 \\ 0.5170000 \\ 0.5860000 \\ 0.1050000 \\ -0.4330000 \\ -0.5770000 \\ -0.2280000 \end{bmatrix} \quad (10)$$

When $n = 2$, the systems of linear algebraic equations will be written in matrix-vector form as:

$$\begin{bmatrix} -1.118 & 0.00587 & \cdots & 0 & \cdots & 0 \\ 0.00587 & -1.118 & 0.00587 & \vdots & 0 & \vdots \\ \vdots & 0.00587 & \ddots & \ddots & \vdots & 0 \\ 0 & \cdots & \ddots & \ddots & 0.00587 & \vdots \\ \vdots & \cdots & 0 & 0.00587 & -1.118 & 0.00587 \\ 0 & \cdots & 0 & \cdots & 0.00587 & -1.118 \end{bmatrix} \times \begin{bmatrix} C_{1,1,1}^3 \\ C_{2,1,1}^3 \\ C_{3,1,1}^3 \\ C_{4,1,1}^3 \\ C_{5,1,1}^3 \\ C_{6,1,1}^3 \\ C_{7,1,1}^3 \\ C_{8,1,1}^3 \\ C_{9,1,1}^3 \\ C_{10,1,1}^3 \end{bmatrix} = \begin{bmatrix} 0.0172000 \\ 0.4350000 \\ 0.3650000 \\ -0.0386000 \\ -0.4290000 \\ -0.4260000 \\ -0.0246000 \\ 0.3690000 \\ 0.4300000 \\ -0.7960000 \end{bmatrix} \quad (11)$$

When $n = 3$, the systems of linear algebraic equations will be written in matrix-vector form as:

$$\begin{bmatrix} -1.118 & 0.00587 & \cdots & 0 & \cdots & 0 \\ 0.00587 & -1.118 & 0.00587 & \vdots & 0 & \vdots \\ \vdots & 0.00587 & \ddots & \ddots & \vdots & 0 \\ 0 & \cdots & \ddots & \ddots & 0.00587 & \vdots \\ \vdots & \cdots & 0 & 0.00587 & -1.118 & 0.00587 \\ 0 & \cdots & 0 & \cdots & 0.00587 & -1.118 \end{bmatrix} \times \begin{bmatrix} C^4_{1,1,1} \\ C^4_{2,1,1} \\ C^4_{3,1,1} \\ C^4_{4,1,1} \\ C^4_{5,1,1} \\ C^4_{6,1,1} \\ C^4_{7,1,1} \\ C^4_{8,1,1} \\ C^4_{9,1,1} \\ C^4_{10,1,1} \end{bmatrix} = \begin{bmatrix} -0.0368000 \\ -0.0522000 \\ -0.2530000 \\ 0.0726000 \\ 0.3490000 \\ 0.3040000 \\ -0.0244000 \\ -0.3070000 \\ -0.2660000 \\ 0.6330000 \end{bmatrix} \quad (12)$$

Solving the matrix-vector equations (9), (10), (11), (12) for $n = 0, n = 1, n = 2\ and\ n = 3$ respectively using *MATLAB* software, we get the solution results as given in Table 1.0 for ADE scheme. The results in Table 1.0 are represented graphically in 2D and 3D in figure (1.1) and (1.2). It is seen from the results in Table 1.0 that for a given value of $i, C^n_{i,j,k}$ values traces a downward trend in concentration. Also for a given value of n, $C^n_{i,j,k}$ values decrease as i tends to increase. The results reveal that where advection parameter is dominant or exponential and diffusion parameter is decaying, the contaminant concentration will be lower in the entire length of the channel. The finding is consistent with the fact that where the speed of underground water is high, chances are that the contaminant concentration in the aquifer will be low.

Table 1.0: **Effect of Decaying Diffusion and Exponential Advection parameters on contaminant concentration in ADE Scheme**

Grid Point (i,j,k,n)	n=0	n=1	n=2	n=3
(1,1,1,n)	0.0022760	0.00124600	-0.00225600	0.9281
(2,1,1,n)	0.0038690	0.0028232	0.0015032	0.9300
(3,1,1,n)	0.00384240	0.0028603	0.0018450	0.5300
(4,1,1,n)	-0.00249130	-0.0034984	-0.0044980	0.07200
(5,1,1,n)	-0.0021390	-0.0031346	-0.0041360	0.9300
(6,1,1,n)	-0.0015730	-0.0027330	-0.0037310	1.3180
(7,1,1,n)	-0.0012520	-0.0022118	-0.0032770	1.2870
(8,1,1,n)	0.0037650	0.0027628	0.0017610	0.3320
(9,1,1,n)	0.0033740	0.0023746	0.0013730	0.9800
(10,1,1,n)	0.0024205	0.0000490	-0.0054500	0.2400

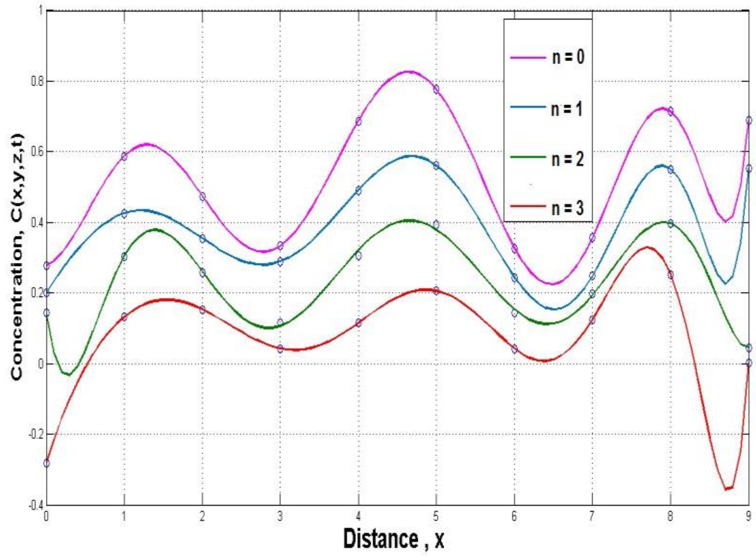

Figure 1.1: 2D Plot of (3+1) Advection-Diffusion Equation, ADI Scheme for varying n

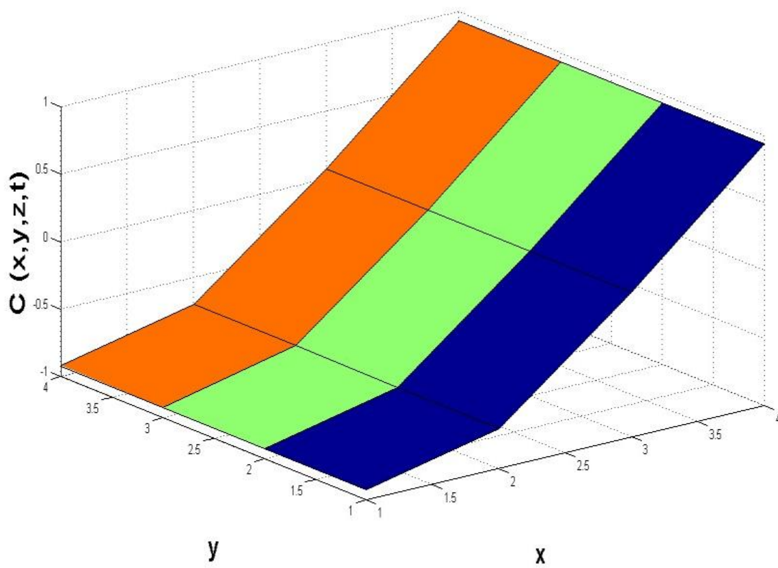

Figure 1.2: 3D Plot of(3+1)Advection-Diffusion Equation,ADI Scheme for varying n

Comparison of Numerical Results

The numerical computational results obtained for solutions of (3+1) dimensional Advection-Diffusion Equation for varying Diffusion (Decaying) and Advection (Exponential) parameters, compared between ADE and ADI. The comparison seen in these results between ADE and ADI are very close and that the error between the two schemes when compared are very small.

Comparison of (3+1) Dimensional Advection-Diffusion Equation for Decaying Diffusion and Exponential Advection parameter for ADE and ADI at n=3

x	1	2	3	4	5	6	7	8	9	10
ADE	0.9300	0.9400	0.5400	0.0700	0.9500	1.3280	1.2970	0.3400	0.9900	0.2500
ADI	0.9281	0.9300	0.5300	0.0720	0.9300	1.3180	1.2870	0.3320	0.9800	0.2400
Absolute Error	0.0099	0.0100	0.0100	0.00200	0.0200	0.0100	0.010	0.0080	0.0100	0.0100

Conclusion

In both Alternating Direction Explicit (ADE) Scheme and Alternating Direction Implicit (ADI) scheme, when the diffusion parameter is decaying and the Advection parameter is exponential, concentration in the entire length of the x- plane tends to zero and below showing high water quality in the aquifer (low or lack of contaminant concentration).

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