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Derivation of (3+1) Dimensional Model Equation With a Mixed Derivative for Predicting Underground Water Quality

Dr. George Ochieng Ogongo

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

Abstract

The paper examines derivation of Advection-Diffusion equation with a mixed Derivative using law of Conservation, Product rule of calculus and Dercy's law .Advection-Diffusion parameters have been assigned on the basis of whether they are Decaying or Exponential.Taylor series expansion is used to generate the Equation. Control volume on control surface is used to simplify the analysis.

Key words: (3+1) Dimensional Advection-Diffusion Equation, Partial Differential Equations (PDE'S),Law of Conservation, Dercy's Law, Taylor Series, Control Volume.

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 deriving this equation. Many researchers like Bear [1] tried to propose analytical solutions for these types of equations, but in recent years researchers like Beny [2] have shown more interest thereby introducing numerical solutions to these kinds 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 Carnahan [4] 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.

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, Dehghan[7]. 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:

$$C(x, y, z, t_0) = Sin(x + y + z) \quad (1)$$

$$C(x, y, z, t_0) = 0 \quad (2)$$

In general, there are three boundary conditions for Advection-Diffusion equations, Dehghan[7]: 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:

The Fundamental equation

Consider a unit volume of saturated porous media. Such a volume is called a control volume. The boundaries of the element are called control surfaces. The law of conservation of mass for a steady state flow requires that the rate at which fluid is entering the control volume is equal to the rate at which fluid is leaving the control volume for a steady flow.

$$\text{Net rate of flow} = \text{Inflow} - \text{Outflow} = 0 \quad (3)$$

For purposes of analysis, consider the rate at which groundwater enters the control volume per unit surface area to consist of three components namely ρV_x, ρV_y, ρV_z, where ρ is the density of water and V_x is the velocity of water perpendicular to the x axis, V_y is the velocity of water perpendicular to the y axis and V_z is the velocity of water perpendicular to the z axis. These are the apparent velocities of ground water flow entering the control volume through control surfaces perpendicular to the x, y and z coordinate axes. Mass flow rate is the mass of a substance which passes through a media per unit of time. Sometimes, mass flow rate is termed as mass flux or mass current. The flow rate is defined by the limit as explained by Drazin[10],

$$m = \lim_{\Delta t \to 0} = \frac{\Delta m}{\Delta t} = \frac{dm}{dt} \quad (4)$$

ie the flow of mass m through a surface per unit time. Since mass is a scalar quantity, the mass flow rate (time derivative of mass) is also a scaler quantity. The change in mass is the amount that flows after crossing the boundary for some time duration, not the initial amount of mass at the boundary minus the final amount at the boundary, since the change in the mass flowing through the area would be zero for steady flow. Mass flow rate can be calculated by the Douglas [8]

$$m = \rho V \tag{5}$$

(i) ρ = *Density of water*

(ii) V = *Volume flow rate*

Using Taylor series approximation, the rate at which ground water leaves the control volume in the *x*-direction can be written as

$$(\rho V_x + \Delta x) = \rho V_x + \frac{\partial}{\partial x}(\rho V_x)\Delta x + \frac{1}{2}\frac{\partial^2}{\partial x^2}(\rho V_x)\Delta x^2 + \frac{1}{6}\frac{\partial^3}{\partial x^3}(\rho V_x)\Delta x^3 + \frac{1}{24}\frac{\partial^4}{\partial x^4}(\rho V_x)\Delta x^4 + \cdots \tag{6}$$

If we make the size of the control volume small and neglect higher order terms (*ie those involving* ∂^2, ∂^3 *etc*) and because we have chosen a unit control volume ($\Delta x = \Delta y = \Delta z = 1$), the rate at which ground

water leaves the control volume is $\rho V_x + \frac{\partial}{\partial x}(\rho V_x)$. The net rate of inflow in the *x*-direction will be given by

Net rate of inflow in the *x*- direction=Rate of inflow in the *x*-direction-Rate of outflow in the *x*-direction

$$\rho V_x - \left[\rho V_x + \frac{\partial}{\partial x}(\rho V_x)\right] = \frac{-\partial}{\partial x}(\rho V_x) \tag{7}$$

The net rate of inflow in the *y*-direction is then given as,

Net rate of inflow in the *y*-direction=Rate of inflow in the *y*-direction-Rate of outflow in the *y*-direction

$$\rho V_y - \left[\rho V_y + \frac{\partial}{\partial y}(\rho V_y)\right] = \frac{-\partial}{\partial y}(\rho V_y) \tag{8}$$

The net rate of inflow in the *z*-direction is then given as, Net rate of inflow in the *z*- direction=Rate of inflow in the *z*-direction-Rate of outflow in the *z*-direction

$$\rho V_z - \left[\rho V_z + \frac{\partial}{\partial z}(\rho V_z)\right] = \frac{-\partial}{\partial z}(\rho V_z) \tag{9}$$

Because the net rate of inflow for the entire control volume must be equal to zero if the law of conservation of mass is to be satisfied, we can then write,

$$\frac{-\partial}{\partial x}(\rho V_x) - \frac{\partial}{\partial y}\left(\rho V_y\right) - \frac{\partial}{\partial z}(\rho V_z) = 0 \tag{10}$$

If we assume that the ground water density ρ is a constant(ie the fluid is incompressible), we can use product rule to evaluate a typical term in equation (7), (8) and (9) to have

$$\frac{-\partial}{\partial x}(\rho V_x) = -\left[\rho\frac{\partial V_x}{\partial x} + V_x\frac{\partial \rho}{\partial x}\right] = -\rho\frac{\partial V_x}{\partial x} \tag{11}$$

$$\frac{-\partial}{\partial y}\left(\rho V_y\right) = -\left[\rho\frac{\partial V_y}{\partial y} + V_y\frac{\partial \rho}{\partial y}\right] = -\rho\frac{\partial V_y}{\partial y} \tag{12}$$

$$\frac{-\partial}{\partial z}(\rho V_z) = -\left[\rho\frac{\partial V_z}{\partial z} + V_z\frac{\partial \rho}{\partial z}\right] = -\rho\frac{\partial V_z}{\partial z} \tag{13}$$

Because the ground water density appears outside the derivative, it cancels from the three equations. Now,

$$-\frac{\partial V_x}{\partial x} - \frac{\partial V_y}{\partial y} - \frac{\partial V_z}{\partial z} = 0 \tag{14}$$

The apparent ground water velocities are given by Darcy's Law as

$$V_x = -K_x\frac{\partial C}{\partial x} \tag{15}$$

$$V_y = -K_y\frac{\partial C}{\partial y} \tag{16}$$

$$V_z = -K_z\frac{\partial C}{\partial z} \tag{17}$$

Where K_x, K_y, and K_z are the advection coefficients and C is the concentration. Substituting equation (15), (16) and (17) into equation (14) respectively we arrive at the saturated flow equation

$$\frac{\partial}{\partial x}\left(-K_x\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(-K_y\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}(-K_z\frac{\partial C}{\partial z}) \tag{18}$$

Because the component of advection coefficient is independent of position for a particular direction, we can further simplify equation (18) using product rule.

$$\frac{\partial}{\partial x}\left(K_x \frac{\partial C}{\partial x}\right) = K_x \frac{\partial^2 C}{\partial x^2} + \frac{\partial C}{\partial x}.\frac{\partial K_x}{\partial x} = K_x \frac{\partial^2 C}{\partial x^2} \quad (19)$$

$$\frac{\partial}{\partial y}\left(K_y \frac{\partial C}{\partial y}\right) = K_y \frac{\partial^2 C}{\partial y^2} + \frac{\partial C}{\partial y}.\frac{\partial K_y}{\partial y} = K_y \frac{\partial^2 C}{\partial y^2} \quad (20)$$

$$\frac{\partial}{\partial z}\left(K_z \frac{\partial C}{\partial z}\right) = K_z \frac{\partial^2 C}{\partial z^2} + \frac{\partial C}{\partial z}.\frac{\partial K_z}{\partial z} = K_z \frac{\partial^2 C}{\partial z^2} \quad (21)$$

Finally if $K_x \neq K_y \neq K_z$ and the media is anisotropic then,

$$K_x \frac{\partial^2 C}{\partial x^2} + K_y \frac{\partial^2 C}{\partial y^2} + K_z \frac{\partial^2 C}{\partial z^2} = f(x, y, z, t) \quad (22)$$

Diffusion at the interface of the x-y plane

As water enters the control volume from *x* into the *y* plane, we can use the product rule of calculus to evaluate a typical term in the equation for diffusion at this interface Bobenko [3]

$$\frac{\partial}{\partial x}\left(K_v.\frac{\partial C}{\partial y}\right) \quad (23)$$

$$K_v \frac{\partial^2 C}{\partial x \partial y} + \frac{\partial C}{\partial y}.\frac{\partial K_v}{\partial x} = K_v \frac{\partial^2 C}{\partial x \partial y} \quad (24)$$

Putting together equation (22) and (24) and also taking into account diffusion on the *x* and *y* plane from Drazin[10]

$$K_x \frac{\partial^2 C}{\partial x^2} + K_y \frac{\partial^2 C}{\partial y^2} + K_z \frac{\partial^2 C}{\partial z^2} + K_v \frac{\partial^2 C}{\partial x \partial y} + M_x \frac{\partial C}{\partial x} + L_y \frac{\partial C}{\partial y} = C_t \quad (25)$$

where K_x, K_y, K_z, K_v, M_x, and L_y are funtions of *x*, *y*, *z* and *t* or can be a constant. Equation (25) can hence be written as

$$f_1(x, y, z, t)\frac{\partial^2 C}{\partial x^2} + f_2(x, y, z, t)\frac{\partial^2 C}{\partial y^2} + f_3(x, y, z, t)\frac{\partial^2 C}{\partial z^2} + f_4(x, y, z, t)\frac{\partial^2 C}{\partial x \partial y} + f_5(x, y, z, t)\frac{\partial C}{\partial x} + f_6(x, y, z, t)\frac{\partial C}{\partial y} = C_t \quad (26)$$

Conclusion

The first four parameters of diffusion will influence diffusivity and the last two parameters are functions of underground fluid transport (Advection).The parameters of diffusion and advection will be assigned to the fundamental equation alternately on the basis of whether they are exponential or decaying. Eventually the equation will examine the influence of alternating exponential and decaying diffusion and advection parameters of the model equation on underground water quality.

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