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Comparative Analysis of Laplace Transform and Finite Difference Modeling and Simulation of Solute Transport in Soil. (Case Study: Nitrate Solute Transport in Homogeneous Soil)

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Abstract

Analytical Laplace transform and numerical finite difference methods were used to solve solute transport model (conversion dispersion equation) for a simplified homogeneous soil and simulation of the transport were done using Matlab programming language. Nitrate solute was used for the study. The study compared the simulation results that were generated by both the Laplace transform and the finite difference methods. Spatial and Temporal simulation of nitrate transport comparing both analytical and numerical solutions were presented. The errors in the spatial and temporal numerical solution were simulated. A three dimensional simulation of the nitrate concentration, depth and time for both the Laplace transform and the finite difference method were also presented. The results showed that finite difference numerical method gave a good approximation of the Laplace transform analytical method which provide exact solution. Although there were errors associated with the numerical solution, the output of the numerical solution do not sharply deviate from that of the analytical solution. The errors associated with the finite difference numerical solution were mainly as a result of truncation of the Taylor series expression.

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Finite difference numerical method can be used to model solute transport in heterogeneous soil which is a more complex process that cannot be accomplished with analytical method with a reasonable level of accuracy. Modeling of solute transport in soil is essential for management of nutrients supply to plants and water resource.

Keyword: Laplace Transform; Finite Difference; Model; Simulation; Solute.

1. Introduction

Different kinds of solutes can be found in the soil and they include nutrients, salts, pesticides, naturally occurring chemicals and other applied chemicals. A lot of these solutes are of great benefit as they give plants and soil organisms' food and protection against diseases. However, when these solutes move out of their desired zones in the soil into ground and surface water sources, they can cause a substantial agronomic, environmental, economic consequences [1]. Huge cost are usually associated with solutes that move off site as a result of over application of agrichemicals, ineffective treatment of targeted pests (weeds, insects or diseases) or the remediation of contaminated water sources [2]. Hence, knowledge and understanding of solute transport in soil and how to minimize off-site contamination is required to be able to effectively use chemicals and protect the quality of water resources. Studying transport of solute in soils is necessary to improving crop production and assessing its impact on the environment [3].

Mathematical models are critical for any attempt to effectively understand and estimate site specific subsurface water flow and solute transport processes. Mathematical modelling helps to analyze the existing situation, allows forecasting, and to evaluate the effects of nutrients transport on surrounding water quality. Models are helpful tools for designing, testing and implementing soil, water, and crop management practices that minimize soil and water pollution [4]. There are two methods to mathematically model a system and these are analytical methods and numerical methods. The analytical methods provide exact solution to mathematical problems, however, analytical methods cannot be used to model complex situations. The numerical methods provide approximate solution to mathematical problems but they can be used to model very complex situations. Soil is a heterogeneous medium and hence transport phenomena within it is very complex, as a result only numerical approach can be used to model solute transport within the soil without oversimplifying the soil medium. Since numerical approach provides approximate solution, this paper assessed the margin of error of Finite Difference numerical method as compared with Laplace Transform analytical methods when both approaches are used to model nitrate solute transport in a simplified homogeneous soil.

1.1 Laplace Transform analytical method

Laplace transform method uses algebra to solve differential equations. The Laplace transform $\mathcal{L}$ is defined by:

$$\mathcal{L}[f(t)](s) \equiv \int_0^\infty f(t)e^{-st}\,dt \qquad \text{...1.1}$$

Where $f(t)$ is defined for $t \geq 0$ [5]

Laplace transforms are used to simplify the governing equations for solute transport. The transform eliminate one independent variable, usually time, and also convert the original transport equation from a partial to an ordinary differential equation. A governing Convection Dispersion Equation (CDE) in the Laplace domain is obtained with the Laplace transform and the equation in this form is much simpler to solve analytically than the original equation. The Laplace Transform of the solute concentration with respect to time is defined as

$$L[c(z,t)] = \bar{c}\,(z,s) = \int_0^\infty c(z,t)e^{-st}\,dt \qquad 1.2$$

Where s is the Laplace transform variable.

Analytical solution in the Laplace space must be subsequently inverted to the real space using either a Table of Laplace transforms or by applying inversion theorems and the solution is expressed as an error function or complimentary error function [6].

1.2 Finite Difference

The finite difference method consists of approximation of the differential operator by replacing the derivatives in the equation using differential quotients. The domain of interest is partitioned in space and time, and approximate solutions are computed at the space or time points. Time and space are both divided into small increments Δt and Δz or (Δx and Δz) known as step size as shown in Figure 1.1. Temporal and spatial derivatives are approximated by Taylor series expansion. The accuracy of the approximation is determined by the scheme selected and the mesh sizes of the spatial and temporal domains [6].

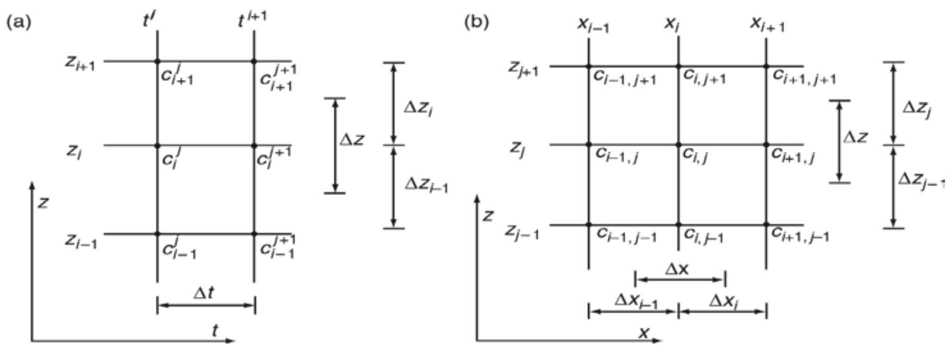

Figure 1.1: Spatial and temporal finite difference discretization [6]

1.3 Solute Transport

Solute transport in soil results from convection of the dissolved substances, molecular or ionic diffusion and mechanical dispersion but the transport process is generally assumed to be convection-dominated process. Other factors including soil matrix-solute interaction and decay phenomena may affect transport of solute in soils.

1.3.1 Convection (Mass) Flow

Convection is passive movement of dissolved constituents of solute with water flowing through the soil, whereby solute and the water move at the same average rate. It is also known as Darcian flow [7]. Convection describes the bulk movement of solute particles along the mean direction of fluid flow at a rate equal to the average interstitial fluid velocity. Convection does not consider microscopic processes but follows the bulk Darcian flow vectors, and is therefore described as the transport along path lines [8]. The velocity at which solutes move through soil matrix is known as pore water velocity, and is described by the ratio of Darcian velocity and moisture content. In general pore water velocity accounts for straight line of length of path traversed in the soil in a given time [9]. The solute flux density, Jc for convective transport is defined;

$$Jc = qC \qquad 1.3$$

C = dissolved solute concentration,

The water flux density, q is expressed as

$$q = v\theta \qquad 1.4$$

v = pore water velocity,

1.3.2 Diffusion

Diffusion is a spontaneous process where solute ions and molecules move from locations of higher to lower concentration as a result of thermal random motion of dissolved ions and molecules. Diffusion is an active process and tends to decrease existing concentration gradients and move the process towards homogeneity rather rapidly [9]. Rates of molecular diffusion are independent of soil water velocity, and diffusion occurs even in the absence of fluid movement [8]. Diffusion flux spreads solute through a concentration gradient. Diffusion is a dominant transport mechanism when convection is insignificant, and is usually a negligible transport mechanism when convection process is very high.

Fick's law defines the diffusive transport as:

$$J_{diff} = -\theta D_{diff} \frac{\partial C}{\partial z} \qquad 1.5$$

J_{diff} = solute flux density for diffusion, z = soil depth

D_{diff} = diffusion coefficient in soils.

$$D_{diff} = D_o\theta\varepsilon \qquad 1.6$$

D_o = diffusion coefficient in pure water, ε = tortuosity

1.3.3 Dispersion

Dispersion is the mixing and spreading of solutes along and transverse to the direction of flow in response to local variations in interstitial fluid velocities. Dispersive transport of solute occurs due to the uneven distribution of water flow velocities within and between different soil pores. Dispersion is a passive process. Macroscopically, dispersion is similar to diffusion; however it occurs only during water movement and not driven by concentration gradients [9]. The dispersion that occurs along the direction of flow path is called longitudinal dispersion and that in the direction normal to flow is known as transverse dispersion. Dispersion process and diffusion process are considered to be additive at macroscopic level.

The dispersive transport is described by an equation similar to diffusion as:

$$J_{dis} = -\theta D_{dis} \frac{\partial C}{\partial z} \quad \text{1.7}$$

J_{dis} = solute flux for dispersion, D_{dis} = dispersion coefficient.

Dispersion is assumed to be a function of fluid velocity as:

$$D_{dis} = \lambda v^n \quad \text{1.8}$$

λ = dispersivity, n = empirical constant (generally assumed to be 1).

Dispersion process and diffusion process are considered to be additive at macroscopic level. The two are therefore combined to define a new parameter called the apparent dispersion coefficient or hydrodynamic dispersion coefficient (D)

$$D = D_{diff} + D_{dis} \quad \text{1.9}$$

1.4 Nitrate Solute

Nitrate (NO_3^-) is negatively charged ion. It is very mobile in soils and can easily be lost from the soil with water that moves downward laterally through a soil profile. The surface of the negatively charged clay or organic matter particles repels nitrate rather than been attracted and therefore it can be lost by leaching. Movement of the NO_3^- ion through soil is governed by convection, or mass-flow, with the moving soil solution and by diffusion and dispersion within the soil solution. The widespread appearance of NO_3^- in ground water is a consequence of its high solubility, mobility, and easy displacement by water [10]. Nitrate is a potential pollutant if it reaches surface and ground water supplies.

2. Methodology

The governing equation for the modelling process was the one dimensional convectional dispersion equation (CDE). The CDE was solve using both Laplace transform and finite difference methods and the solutions were implemented in mat- lab programming environment.

2.1 Solute Transport Equation

The convection-dispersion equation (CDE) which is the accepted deterministic solute transport equation describes the time rate of change of solute concentration for a single solute [8]. The CDE is a partial differential equation of parabolic type, derived on the principle of conservation of mass using Fick's law. The analytical/numerical solutions of the CDE along with initial and boundary conditions help to understand the solute concentration profile or distribution behavior through an open medium like air, rivers, lakes and porous medium on the basis for which remedial measures to reduce or eliminate the damages may be implemented [11].

2.1.1 Convection-Dispersion Equation

The classic one dimensional CDE for transport of conservative species without adsorption or decay in a partially saturated porous medium can be written as [7]:

$$\frac{\partial(\theta C)}{\partial t} = \frac{\partial}{\partial z}\left(\theta D\frac{\partial C}{\partial z} - qC\right) \ldots\ldots (2.1)$$

The comprehensive CDE for one-dimensional transport of reactive solutes, subject to reaction terms of adsorption, first-order degradation, and zero-order production is given as [12];

$$\frac{\partial}{\partial t}(\theta C + \rho_b S_s) = \frac{\partial}{\partial z}\left(\theta D\frac{\partial C}{\partial z} - qC\right) - \theta\mu_l C - \rho_b\mu_s S_s + \theta\gamma_l(z) + \rho_b\gamma_S(z \ldots\ldots (2.2)$$

$$S_s = k_d C \ldots\ldots (2.3)$$

Assuming reversible equilibrium adsorption and steady state flow in a homogeneous soil, equation (2.2) reduces to

$$R\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial z^2} - \frac{q}{\theta}\frac{\partial C}{\partial z} - \mu C + \gamma(z) \ldots\ldots (2.4)$$

$$R = 1 + \frac{\rho_{bK_d}}{\theta} \ldots\ldots (2.5)$$

$$\mu = \mu_l + \frac{\rho_{bK_d}\mu_s}{\theta} \ldots\ldots (2.6)$$

$$\gamma(z) = \gamma_l(z) + \frac{\rho_{bK_d}\gamma_s}{\theta} \ldots\ldots (2.7)$$

μ_l, μ_s = First-order decay coefficients for degradation of the solute in the liquid and adsorbed phases respectively.

γ_l *and* γ_S = zero order production terms for the liquid and adsorbed respectively.

R = retardation factor, μ and γ = combined first and zero order rate coefficients respectively.

$$R\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial z^2} - v\frac{\partial C}{\partial z} - \mu C + \gamma(z) \ldots\ldots (2.8)$$

2.2 Assumptions

- Nitrate transport occurs in the vertical direction only.
- The soil is homogeneous and unsaturated.
- Nitrate transport is affected by only convection, and hydrodynamic dispersion (combined dispersion and diffusion) processes. Any other solute process is negligible.
- Nitrate is non-adsorbing solute

2.3 Initial and Boundary Conditions

$$C(z,0) = 0 \qquad 0 \leq z \leq \infty, t = 0 \ldots\ldots (2.9)$$

$$C(0,t) = C_0 \qquad z = 0, t > 0 \ldots\ldots (2.10)$$

$$C(\infty,t) = 0 \qquad z \to \infty, t > 0 \ldots\ldots (2.11)$$

2.4 Laplace Transform Solution of the CDE

Applying the assumptions, equation (2.8) reduces to

$$\frac{\partial \mathrm{c}}{\partial \mathrm{t}} = \mathrm{D}\frac{\partial^2 \mathrm{c}}{\partial \mathrm{z}^2} - \mathrm{v}\frac{\partial \mathrm{c}}{\partial \mathrm{z}} \ldots\ldots (2.12)$$

Laplace Transform with respect to time is defined as

$$L[c(z,t)] = \bar{c}\,(z,s) = \int_0^\infty c(z,t)e^{-st}\,dt \ldots\ldots (2.13)$$

Applying Laplace transform with respect to time to equation (2.12) gave:

$$L\left[\frac{\partial c}{\partial x}\right] = L\left[D\,\frac{\partial^2 y}{\partial z^2}\right] - L\left[v\,\frac{\partial c}{\partial z}\right] \ldots\ldots (2.14)$$

The Laplace transforms are; [13]

$$L\{f(t)\} = \int_0^\infty f(t)e^{-st}dt = F(s) \ldots\ldots (2.15)$$

$$L\{f'(t)\} = sF(s) - f(0) \ldots\ldots (2.16)$$

$$L\left[\frac{\partial c}{\partial t}\right] = s\bar{c} - c(z,0) \ldots\ldots (2.17)$$

Applying the initial condition, equation (2.17) becomes:

$$L\left[\frac{\partial c}{\partial t}\right] = s\bar{c} - c(z,0) \ldots\ldots (2.18)$$

$$L\left[v\frac{\partial c}{\partial z}\right] = v\int_0^\infty \frac{\partial c}{\partial z} e^{-st} dt \quad (2.19)$$

Since the integral of derivative = derivative of integral, then by exchanging the order of integration and differentiation in eqn. (2.19) becomes:

$$L\left[v\frac{\partial c}{\partial z}\right] = v\frac{\partial c}{\partial z}\int_0^\infty c(z,t)e^{-st}\, dt \quad (2.20)$$

$$L\left[v\frac{\partial c}{\partial z}\right] = v\frac{\partial \bar{c}}{\partial z} \quad (2.21)$$

$$L\left[D\frac{\partial^2 c}{\partial z^2}\right] = D\int_0^\infty \frac{\partial^2 c}{\partial z^2} e^{-st} dt \quad (2.22)$$

$$L\left[D\frac{\partial^2 c}{\partial z^2}\right] = D\frac{\partial^2}{\partial z^2}\int_0^\infty c(z,t)\, e^{-st} dt \quad (2.23)$$

$$L\left[D\frac{\partial^2 c}{\partial z^2}\right] = D\frac{\partial^2 \bar{c}}{\partial z^2} \quad (2.24)$$

Putting eqn. (2.18), (2.21) and (2.24) into eqn. (2.14) yielded:

$$s\bar{c} = D\frac{\partial^2 \bar{c}}{\partial z^2} - v\frac{\partial \bar{c}}{\partial z} \quad (2.25)$$

Taking Laplace transform of the boundary conditions

$$L[c(0,t)] = L[c_0] \quad (2.26)$$

$$\bar{c}\,(0,s) = c_0\int_0^\infty e^{-st} dt = c_0\left[\frac{e^{-st}}{s}\right]_0^\infty = \frac{c_0}{s} \quad (2.27)$$

$$L[(\infty,t)] = L[0] \quad (2.28)$$

$$\int_0^\infty c(\infty,t)e^{-st} dt = 0 \quad (2.29)$$

$$\bar{c}\,(\infty,s) = 0 \quad (2.30)$$

Dividing through equation (2.25) by D and rearranging gives:

$$\frac{\partial^2 \bar{c}}{\partial z^2} - \frac{v}{D}\frac{\partial \bar{c}}{\partial z} - \frac{1}{D}s\bar{c} = 0 \quad (2.31)$$

Which is a second order ordinary differential equation with auxiliary equation

$$m^2 - \frac{v}{D}m - \frac{s}{D} = 0 \quad (2.32)$$

The roots of equation (2.32) were determined from the quadratic formula.

$$m = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \quad (2.33)$$

Hence equation (2.32) had the roots:

$$m = \frac{1}{2}\left(\frac{v}{D} \pm \sqrt{\frac{v^2}{D^2} + \frac{4s}{D}}\right) \quad (2.34)$$

The general solution of equation (2.31) is given as [13]

$$\bar{c} = Aexp\left(\frac{vz}{2D} + \frac{z}{2}\sqrt{\frac{v^2}{D^2} + \frac{4s}{D}}\right) + Bexp\left(\frac{vz}{2D} - \frac{z}{2}\sqrt{\frac{v^2}{D^2} + \frac{4s}{D}}\right) \quad (2.35)$$

Applying the lower boundary condition $[\bar{c}\,(\infty, s) = 0]$means as $z \to \infty$ there would be no concentration, hence A=0, and equation (2.35) reduced to:

$$\bar{c} = Bexp\left(\frac{vz}{2D} - \frac{z}{2}\sqrt{\frac{v^2}{D^2} + \frac{4s}{D}}\right) \quad (2.36)$$

Applying the upper (surface) boundary condition, $\left[\bar{c}(0, s) = \frac{C_0}{s}\right]$ to equation (2.36) yields, $B = \frac{C_0}{s}$ and eqn. (2.36) becomes:

$$\bar{c} = \frac{C_0}{s} exp\left(\frac{vz}{2D} - \frac{z}{2}\sqrt{\frac{v^2}{D^2} + \frac{4s}{D}}\right) \quad (2.37)$$

Rearranging equation (2.37) produced:

$$\frac{\bar{c}}{C_0} = \frac{1}{s} exp\left(\frac{vz}{2D}\right) exp\left(-z\sqrt{\frac{s + \frac{v^2}{4D}}{D}}\right) \quad (2.38)$$

Letting $Q = s + \frac{v^2}{4D} \;\; \rightrightarrows \;\; s = Q - \frac{v^2}{4D}$

$$\frac{\bar{c}}{C_0} = \left(\frac{1}{Q - \frac{v^2}{4D}}\right) exp\left(\frac{vz}{2D}\right) exp\left(-z\left[\frac{Q}{D}\right]^{0.5}\right) \quad (2.39)$$

From Shift theorem [14]

$$L^{-1}[F(s + a)] = e^{-at} L^{-1}[F(s)] \quad (2.40)$$

$$L^{-1}[F(Q)] = L^{-1}\left[F\left(s+\frac{v^2}{4D}\right)\right] = exp\left(-\frac{v^2t}{4D}\right)L^{-1}[F(s)] \quad (2.41)$$

The Laplace inverse of equation (2.39) was written as:

$$\frac{C(z,t)}{C_0} = \exp\left(\frac{vz}{2D}\right) exp\left(-\frac{v^2t}{4D}\right) L^{-1}\left(\frac{1}{Q-\frac{v^2}{4D}} exp\left(-z\left[\frac{Q}{D}\right]^{0.5}\right)\right) \quad (2.42)$$

Carslaw and Jaeger [15] have shown that the inverse Laplace expression on RHS of eqn. (2.42) could be written as:

$$L^{-1}\left(\frac{1}{Q-\frac{v^2}{4D}} exp\left(-z\left[\frac{Q}{D}\right]^{0.5}\right)\right) = \frac{1}{2} exp\left(\frac{v^2t}{4D}\right)\begin{bmatrix} exp\left(-\frac{vz}{2D}\right) erfc\left(\frac{z}{2\sqrt{Dt}} - \sqrt{\frac{v^2t}{4D}}\right) + \\ exp\left(\frac{vz}{2D}\right) erfc\left(\frac{z}{2\sqrt{Dt}} + \sqrt{\frac{v^2t}{4D}}\right)\end{bmatrix} \quad (2.43)$$

Substituting equation (2.43) into equation (2.42) gave

$$\frac{c(z,t)}{c_0} = \frac{1}{2}\exp\left(\frac{vz}{2D}\right) exp\left(-\frac{v^2t}{4D}\right) exp\left(\frac{v^2t}{4D}\right)\begin{bmatrix} exp\left(-\frac{vz}{2D}\right) erfc\left(\frac{z}{2\sqrt{Dt}} - \sqrt{\frac{v^2t}{4D}}\right) + \\ exp\left(\frac{vz}{2D}\right) erfc\left(\frac{z}{2\sqrt{Dt}} + \sqrt{\frac{v^2t}{4D}}\right)\end{bmatrix} \quad (2.44)$$

$$\frac{c(z,t)}{c_0} = \frac{1}{2}\left[exp\left(-\frac{vz}{2D}\right) erfc\left(\frac{z}{2\sqrt{Dt}} - \sqrt{\frac{v^2t}{4D}}\right) + exp\left(\frac{vz}{2D}\right) erfc\left(\frac{z}{2\sqrt{Dt}} + \sqrt{\frac{v^2t}{4D}}\right)\right] \quad (2.45)$$

$$\frac{c(z,t)}{c_0} = \frac{c_0}{2}\left[erfc\left(\frac{z-vt}{2\sqrt{Dt}}\right) + exp\left(\frac{vz}{D}\right) erfc\left(\frac{z+vt}{2\sqrt{Dt}}\right)\right] \quad (2.46$$

2.5 Finite Difference Solution of the CDE

The CDE was also solved numerically by fully implicit (backward in time) finite difference scheme. The model domain was discretized into grid points using space and time steps of 1cm and 1 hour respectively.

Applying the assumptions, equation (2.8) reduces to

$$\frac{\partial \mathrm{c}}{\partial \mathrm{t}} = \mathrm{D}\frac{\partial^2 \mathrm{c}}{\partial \mathrm{z}^2} - \mathrm{v}\frac{\partial \mathrm{c}}{\partial \mathrm{z}} \quad (2.47)$$

Converting the CDE equation (3.24) into a difference equation gives:

$$\frac{\partial c}{\partial t} = \frac{c_i^{j+1} - c_i^j}{\Delta t} \quad (2.48)$$

$$D\frac{\partial^2 c}{\partial z^2} = D\frac{C_{i+1}^{j+1} - 2C_i^{j+1} + C_{i-1}^{j+1}}{(\Delta z)^2} \quad (2.49)$$

$$v\frac{\partial c}{\partial z} = v\frac{C_{i+1}^{j+1} - C_{i-1}^{j+1}}{2\Delta z} \quad (2.50)$$

Substituting equation (3.63), (3.64), and (3.65) into equation (3.24)

$$\frac{C_i^{j+1} - C_i^j}{\Delta t} = D\frac{C_{i+1}^{j+1} - 2C_i^{j+1} - C_{i-1}^{j+1}}{(\Delta z)^2} - v\frac{C_{i+1}^{j+1} - C_{i-1}^{j+1}}{2\Delta z} \quad (2.51)$$

$$C_i^{j+1} - C_i^j = \frac{D(\Delta t)}{(\Delta z)^2}\left(C_{i+1}^{j+1} - 2C_i^{j+1} + C_{i-1}^{j+1}\right) - \frac{v\Delta t}{2\Delta z}\left(C_{i+1}^{j+1} - C_{i-1}^{j+1}\right) \quad (2.52)$$

Let $p = \frac{D\Delta t}{(\Delta z)^2}$, $\quad q = \frac{v\Delta t}{2\Delta z}$

$$C_i^{j+1} - C_i^j = p\left(C_{i+1}^{j+1} - 2C_i^{j+1} + C_{i-1}^{j+1}\right) - q\left(C_{i+1}^{j+1} - C_{i-1}^{j+1}\right) \quad (2.53)$$

$$C_i^{j+1} - C_i^j = pC_{i+1}^{j+1} - 2pC_i^{j+1} + pC_{i-1}^{j+1} - qC_{i+1}^{j+1} + qC_{i-1}^{j+1} \quad (2.54)$$

$$-(p+q)C_{i-1}^{j+1} + (1+2p)C_i^{j+1} + (q-p)C_{i+1}^{j+1} = C_i^j \quad (2.55)$$

When i =1 equation (3.70) reduces to:

$$-(p+q)C_0^{j+1} + (1+2p)C_1^{j+1} + (q-p)C_2^{j+1} = C_1^j \quad (2.56)$$

Applying the boundary condition $C(0,t) = C_0$, $\quad z = 0, t > 0$ equation ( ) becomes

$$(1+2p)C_1^{j+1} + (q-p)C_2^{j+1} = C_1^j + (p+q)C_0^{j+1} \quad (2.57)$$

When $i = 2 \rightarrow n-1$, equation (3.71) remains:

$$-(p+q)C_{i-1}^{j+1} + (1+2p)C_i^{j+1} + (q-p)C_{i+1}^{j+1} = C_i^j \quad (2.58)$$

n = number of grid points

When i = n

$$-(p+q)C_{n-1}^{j+1} + (1+2p)C_n^{j+1} + (q-p)C_{n+1}^{j+1} = C_n^j \quad (2.59)$$

Applying the boundary condition $C(\infty,t) = 0$, $\quad z \rightarrow \infty, t > 0$ equation ( ) becomes

$$-(p+q)C_{n-1}^{j+1} + (1+2p)C_n^{j+1} = C_n^j \quad (2.60)$$

Assuming $x_1 = p + q$, $x_2 = 1 + 2p$ $x_3 = q - p$, the above sets of simultaneous equations can be expressed in a tri-diagonal matrix notation as follows:

$$\begin{bmatrix} x_2 & x_3 & 0 & & & & & \\ -x_1 & x_2 & x_3 & 0 & & & & \\ 0 & -x_1 & x_2 & x_3 & 0 & & & \\ & & \ddots & & & & & \\ & & & \ddots & & & & \\ & & 0 & 0 & -x_1 & x_2 & x_3 & 0 \\ & & & 0 & 0 & -x_1 & x_2 & x_3 \\ & & & 0 & 0 & 0 & -x_1 & x_2 \end{bmatrix} \begin{bmatrix} C_1^{j+1} \\ C_2^{j+1} \\ C_3^{j+1} \\ \downarrow \\ \downarrow \\ C_{n-2}^{j+1} \\ C_{n-1}^{j+1} \\ C_n^{j+1} \end{bmatrix} = \begin{bmatrix} C_1^j + (q+p) C_0^{j+1} \\ C_2^j \\ C_3^j \\ \downarrow \\ \downarrow \\ C_{n-2}^j \\ C_{n-1}^j \\ C_n^j \end{bmatrix} \qquad \text{………..} \; (2.61)$$

3. Result and Discussion

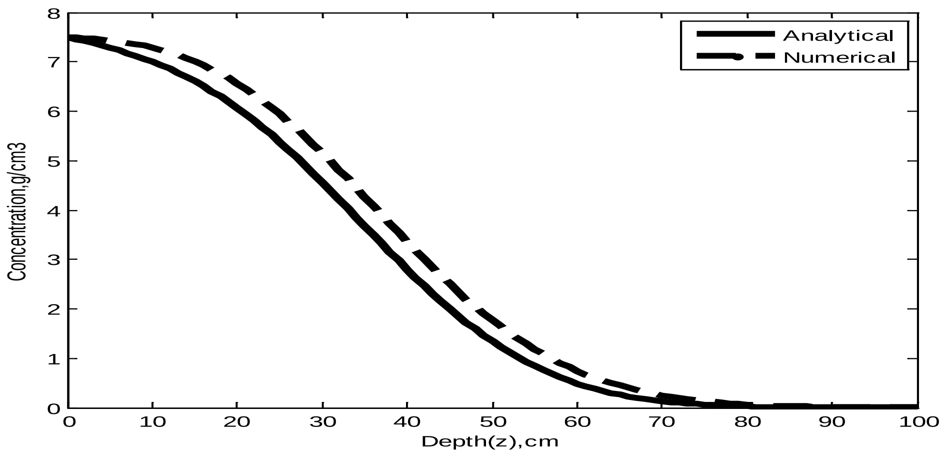

Figure 3.1: Analytical and Numerical simulation of nitrate transport with respect to soil depth

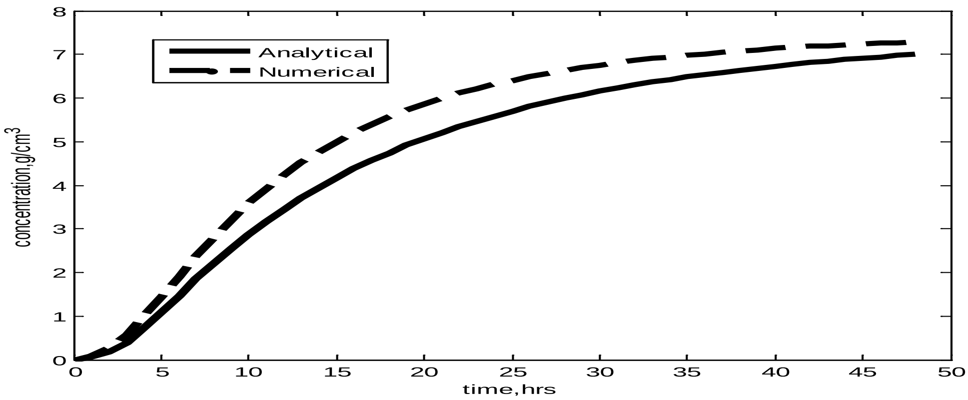

Figure 3.2: Analytical and Numerical simulation of nitrate transport with respect to time

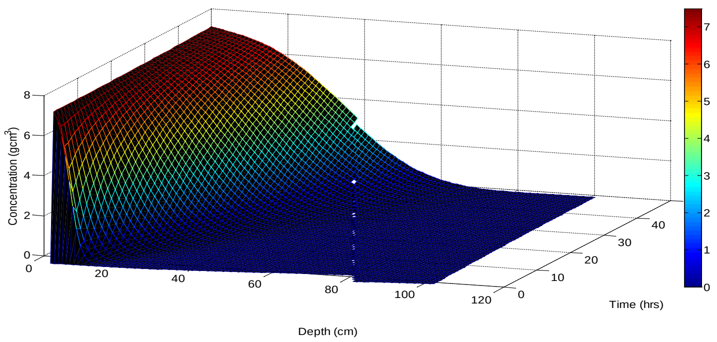

Figure 3.3: analytical simulation of concentration, time and depth

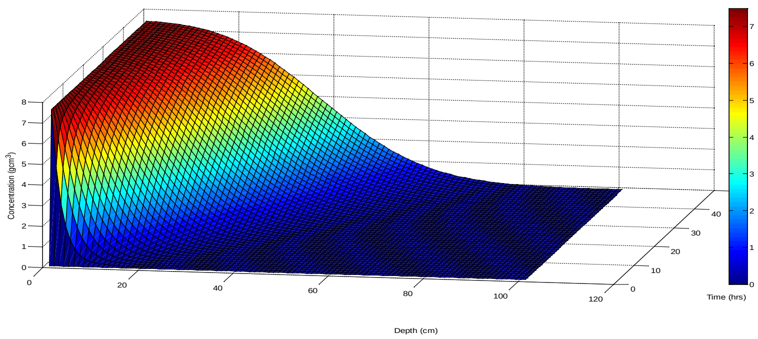

Figure 3.4: 3D numerical simulation of concentration, time and depth

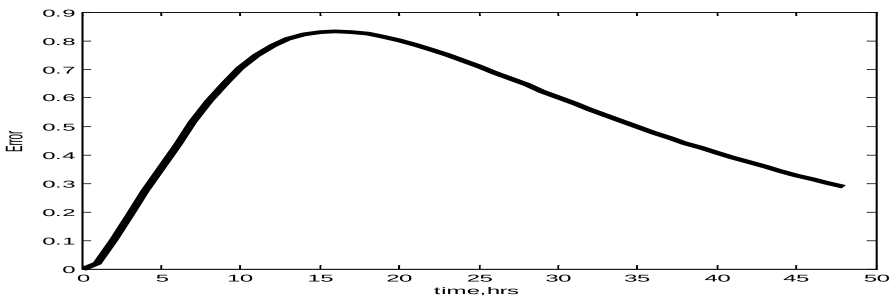

Figure 3.5: Plot of error in temporal numerical model against time

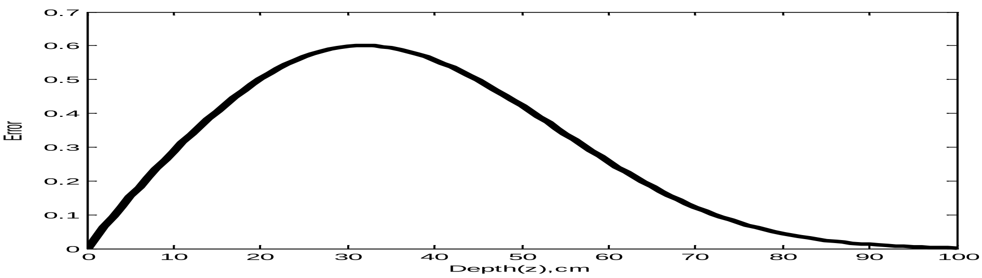

Figure 3.5: Plot of error in spatial numerical model against depth

Figure 3.1 and 3.2 compare the analytical and numerical simulation of nitrate transport in soil with respect to depth and time respectively. Figure 3.3 and Figure 3.4 show three dimensional analytical and numerical simulation of nitrate transport with respect to both depth and time respectively. Figure 3.5 and 3.6 depict the error associated with the numerical simulation with respect to time and depth respectively. The simulations show that although there are errors associated the finite difference numerical method, its results do not deviate sharply from the Laplace transform analytical simulations results. The errors in the finite difference simulations were as a result of truncation of Taylor series and therefore the error is mainly truncation error. The finite difference numerical simulation generated values which were greater than the values generated by the Laplace transform analytical simulation. The errors in both the temporal and spatial simulations initially grew to a point and started declining from that point.

4. Conclusion

Modeling of solute transport in soil is a very complex process, hence the analytical models cannot capture most of the complexities of such process. Analytical models can only describe simplified process which is far from what pertains in reality. Numerical models are able to capture most the complexities of solute transport in soil hence it is very close to what happens in nature. However, numerical models unlike analytical models provide approximate and not exact solutions. There are errors associated with the numerical models. A comparison between Laplace transform model and finite difference model for nitrate solute transport in soil showed that the finite difference model gave a good approximation of the Laplace transform model. There were errors associated with the numerical model but it was mainly as a result of truncation error. The error associated with both the temporal and spatial simulations grew initially to some point and decline from that point onwards. The finite difference numerical model can be used to model the complex solute transport process in soil. However, there will be some errors but these errors will not cause too much difference between the numerical model solution and analytical model solution should it have been possible.

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