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Mathematical Modelling and Simulation of Nitrate Leaching into Groundwater

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Abstract: Nitrate leaching into groundwater is a complicated process that involves a number of different biochemical transformations. These biochemical transformations include immobilisation, mineralization, nitrification, volatilization, crop absorption, and nitrate leaching into groundwater. Groundwater nitrate contamination is a developing challenge that requires precise analytical and numerical solutions. Various approaches to measuring nitrate leaching have been developed from a range of measurement and modelling techniques, but all suffer from one limitation or another due to the complexities, challenges and assumptions made in quantifying nitrate leaching in groundwater. This calls for new approaches in which nitrate leaching can be analysed to gain a better understanding of nitrate fate and transport processes for the proper management of groundwater. The advection-dispersion equations are updated in this research work to simulate nitrogen leaching in soils with variable depth, duration, volumetric water content, and porosity. Graphical representations of numerical simulations of the concentration of nitrate in the soil at varying depths and times can be achieved with the help of MATLAB software. According to the findings of the study, the proportion of soil porosity to soil water volume is directly proportional to the amount of nitrate that leaches into the groundwater. Therefore, it is recommended that measures be taken to reduce the potential for groundwater contamination. These measures include reducing the amount of nitrogen used, avoiding overwatering, and developing a test that helps farmers measure the amount that is already present in the groundwater.

Keywords: Mathematical Modelling, Nitrate, Modelling, Leaching, Advection-Dispersion, Groundwater

1. Introduction

Nitrate is the most prevalent pollutant in groundwater [1]. High concentrations of nitrates in groundwater exceed the World Health Organisation (WHO) criteria of 10 mg / L NO_3 due to the excessive application of nitrogen fertilisers to agricultural land. Nitrates exceeding this threshold are known to cause serious health effects, such as methemoglobinemia in infants, gastric lymphoma in adults, and miscarriages in pregnant women [29]. In addition, there are documented long-term adverse health effects, such as insulin-dependent diabetes, thyroid problems, and an increased risk of non-Hodgkin lymphoma (NHL) [2]. In addition to causing soil acidification and increased algal growth in water, excessive nitrate depletes dissolved oxygen, ultimately resulting in the death of fish and other aquatic life [3].

The interaction between land use practises, ground nitrogen loading, groundwater recharge, soil nitrogen dynamics, and soil characteristics makes it difficult to precisely quantify nitrate leaching into groundwater. To account for transient and spatially variable nitrate leaching into groundwater during regional-scale analysis and modelling, it is necessary to comprehend the interaction between the aforementioned factors. [4]. Due to spatial and temporal variations in soil, climate, and management practises, as well as assumptions made in modelling processes and related to models, the nitrate leaching modelling procedure is subject to several uncertainties. Inadequate regional-scale data and the assumption that heterogeneous media behave similarly to homogeneous media, both of which differ in scale and from heterogeneous media, also contribute to these uncertainties. It also comes from a lack of reliable data [5].

Mathematical models are useful for nitrate leaching research due to their predictive capacity in the study of leaching. The models provide a cost-effective method to determine the impact of management alternatives on groundwater quality and are transportable as a result of their adaptability to different situations, which is achieved by modifying the model parameters. In addition, they allow for a greater understanding of the interdependence of relevant parameters and the identification of input parameters that are especially sensitive [32, 33]. Models that simulate nitrogen processes in soils and evaluate the environmental impact of nitrogen management are now recognised as indispensable for improving cropping techniques and cropping systems [6]. To prevent groundwater contamination, a comprehensive understanding of the leaching processes of nitrates is required.

The advection-dispersion equation has piqued the interest of environmentalists, hydrologists, civil engineers, and mathematical modellers due to the growing concern for a safe hydro environment for life on Earth [7]. The advection-dispersion equation has been used to model tracer dispersion in porous media, pollutant transport in rivers and streams, dispersion of dissolved materials in estuaries and coastal seas, dispersion of contaminants in shallow lakes, and long-distance transport of atmospheric pollutants [8].

Despite the fact that there are a number of one-dimensional models, such as the soil and water assessment tools (SWAT) model, the modular flow model (MODFLOW), and the modular three-dimensional multi-species transport model (MT3DMS), which simulate water flow and solute transport, crop uptake of water and nutrients, and the biological and chemical transformation of nitrogen in soil, there is a lack of three-dimensional models that can simulate these processes. However, accurate and efficient mathematical models are still necessary [9].

Due to the complex and frequently non-linear physical, chemical, and biological processes that affect the fate and transport process in soil, nitrate leaching must be measured in a variety of situations to generate sufficient data for policy formation [10]. Analytical and quasi-analytic approaches are still applicable for the analysis of a variety of contaminant transport processes, especially when insufficient data exist to justify the use of a comprehensive numerical model [11].

One of the most influential factors on the movement of nitrate from the soil to groundwater is the soil's volumetric water content. Water infiltration causes percolation of nitrate ions through the soil profile. If precipitation exceeds evaporation, nitrate can leach into the groundwater. However, the water content is low and evapotranspiration potential exceeds annual precipitation; the concentration of nitrate will be high due to the diminished dilution effect [12]. The impact of soil water on the interaction between surface water and groundwater is essential for crop growth and farm planning. Moreover, it influences the mitigation of flood risk and productivity [13].

It establishes the maximum amount of water the soil can store at a given time. The particle size distribution and the presence of preferential flow paths determine the soil's porosity. Soils have different retentive properties based on their texture and organic matter content. Due to the greater proportion of gravitational pores, coarse soils are typically more susceptible to leaching than clay soils [14, 27]

It is widely acknowledged that the best indicator of soil structure quality is soil porosity. The ability to quantify the pore space in terms of shape, size, continuity, orientation, and arrangement of pores in the soil permits us to define the complexity of the soil structure and comprehend its anthropogenic modifications. Understanding the retention and movement of water in soil necessitates an accurate comprehension of the pore system. Moreover, it permits the evaluation of the impact of agricultural activities and the quantification of a number of aspects of soil degradation [15, 31]. In addition, sandy soils are homogeneous, allowing water to freely permeate the soil matrix. Consequently, soil porosity affects nitrate leaching, so nitrate leaching will be high in loose, porous soil [5, 27].

Nitrate contamination of groundwater is a growing concern requiring precise analytical and numerical solutions. This requires the development of a mathematical model that simulates nitrate leaching from the surface to groundwater.

2. Model Formulation

The Advection-Dispersion equation is derived from the law of mass conservation by taking into account the accumulation and depletion of the solute in a control volume over time as a result of flux divergence, possible nitrate reactions, addition and depletion of nitrate during leaching, and possible nitrate reactions [16].

Consider a solute that enters a volume element over time in the cross-sectional region A extending from x to $x + L$, where L is the length of the volume element that the solute covers over time t. Create a continuity equation by equating the difference between the mass of the solute entering a volume element and the mass of the solute leaving the volume element with the rate of accumulation of mass of the solute inside the volume element, assuming that the densities and viscosities of all fluids within the volume element are identical and no matter is lost or added within the volume element [16].

The net influx is composed of dispersion and advection-related terms. The dispersion coefficient is assumed to be concentration-independent [11, 31]. Then, the mass balance for a control volume in which transport occurs in the positive x direction within time t is given by the following equation 1:

$$V\frac{\partial C}{\partial t} = A(J_1 - J_2) \tag{1}$$

Where V is the volume of particles entering the volume element (L^3), C is the concentration (ML^{-3}), t is time (T), A is the area (L^2), J is the flux ($ML^{-2}T^{-1}$) which is changing in the x- direction from J_1 to J_2 with a gradient $\frac{\partial J}{\partial x}$ such that:

$$J_2 = J_1 + \frac{\partial J}{\partial x} \cdot \Delta x \tag{2}$$

Substituting Equation 2 into Equation 1 and solving yields the following.

$$\frac{\partial C}{\partial t} = -\frac{\partial J}{\partial x} \tag{3}$$

Where

$$J = J_{Adv} + J_{Disp} \tag{4}$$

Here, flux J_{Adv} represents the dispersive flux and J_{Disp} represents the advective flux, which is derived separately. Therefore, Equation 3 can be written as follows:

$$\frac{\partial C}{\partial t} = -\frac{\partial (J_{Adv} + J_{Disp})}{\partial x} \tag{5}$$

2.1. The Advective Flux

During a time interval Δt, advection is regarded as occurring in one direction [17]. Let Δx represent the distance travelled by a particle during Δt. Assume that the particle moves only in the positive x direction; the rate of advection-induced solute transport is determined by the product of the concentration of solute C and the leaching rate [18]. Therefore, the number of particles moving from one region to another within the control volume element can be represented as:

$$Q = C \cdot \Delta x \cdot A \tag{6}$$

where Q represents the number of particles that pass from one region to another during the time interval Δt. The result of dividing equation 6 by $A.\Delta t$ is:

$$\frac{Q}{A.\Delta t} = \frac{C \cdot \Delta x}{\Delta t} = J_{Adv} \tag{7}$$

Taking the limit as $(\Delta t \longrightarrow 0)$, then equation 7 can be written as:

$$\frac{\partial x}{\partial t} \cdot C = \lim_{\Delta t \longrightarrow 0} \left(\frac{C \cdot \Delta x}{\Delta t} \right) = J_{Adv} \tag{8}$$

This is the number of particles that pass from one region to another in unit time per unit area (Flux). Equation 8 can also be written as

$$\frac{\partial x}{\partial t} \cdot C = J_{Adv} \tag{9}$$

Equation 9 represents the advective flux.

2.2. Dispersive Flux

The generalised form of Fick's law of diffusion describes the rate of solute transport via mechanical dispersion [19]. $\hat{A}$ During a time interval Δt, dispersion occurs in both the positive x and negative x directions. Let Δx represent the distance a particle can travel in Δt of time. Assume that the particles will move in a positive x direction and a negative x direction during the interval Δt and that the probability that a particle will move in a positive x direction or a negative x direction is the same for all particles [13]. Then, the number of particles passing from region one of the volume element to region two in time Δt is calculated as follows:

$$\frac{Q}{\partial t} = \frac{1}{2} \frac{C \cdot \Delta x . A \frac{\partial C}{\partial x} \Delta x}{\Delta t} \tag{10}$$

Dividing equation 10 by A and letting $D = -\frac{1}{2} \frac{(\Delta x)^2}{\Delta t}$ yield the following result.

$$-D \frac{\partial C}{\partial x} = J_{Disp} \tag{11}$$

Equation 11 represents the dispersive flux. Putting equations 9 and 11 in equation 12 yields:

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x} \left(\frac{\partial x}{\partial t} C - D \frac{\partial C}{\partial x} \right) \tag{12}$$

Since the velocity v is given by $\frac{\partial x}{\partial t} = (v)$ in the x-direction, equation 11 can be written as:

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x} \left(vC - D \frac{\partial C}{\partial x} \right) \tag{13}$$

Expanding Equation 13 yields:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} \tag{14}$$

Equation 14 is the general one-dimensional diffusion equation.

2.3. Modification of Advection-Dispersion Equation

The soil's volumetric water content is determined by the soil's texture, structure, amount of organic matter, depth to impervious layers such as hard walls or bedrock, the amount of water already present in the soil, and the soil's temperature. Nitrate dispersion is contingent upon the soil's water content and permeability [13]. Volumetric water content can be expressed as a ratio, which can range from 0 to 1 [20].

By letting the volumetric water content be θ; such that $(0 < \theta < 1)$ and the soil porosity be ϕ, such that $(0 < \phi < 1)$; and introducing $(1 - \theta)$ and $(1 - \phi)$ in the dispersive flux, since the dispersion is the spread of the solute due to variations in water velocity within individual pores; and since the volumetric water content, and soil porosity are the main factors considered to determine the dispersion rate in this study, Equation 11 can be modified as:

$$-D(1 - \theta)(1 - \phi) \frac{\partial C}{\partial x} = J_{Disp} \tag{15}$$

Therefore, the final term of Equation 14 can be modelled as follows:

$$v(1 - \theta) \frac{\partial C}{\partial x} \tag{16}$$

The rate of nitrate leaching into groundwater also depends on the soil's porosity ϕ, the volumetric water content of the porous medium, the porous medium's bulk density, and its distribution coefficient [5]. The rate term can be derived from the first term of Equation 12 as:

$$(1-\phi)(1-\theta)\frac{\partial C}{\partial t} = -\rho k_d \frac{\partial C}{\partial t} \tag{17}$$

Where ρ is the bulk density of the porous medium and k_d is the distribution coefficient in the equilibrium state. During leaching, nitrate undergoes radioactive decay, biological transformations, and other processes that result in the loss of nitrate and soil load, which impacts the leaching process. By incorporating these variables into Equation 17, the rate of nitrate leaching can be rewritten as follows:

$$(1-\phi)(1-\theta)\frac{\partial C}{\partial t} = -\rho k_d \frac{\partial C}{\partial t} - \mu(\rho k_d C + (1-\theta)(1-\phi)C) \tag{18}$$

Where μ represents the sources and sink factors.
Combining equation 15,16,17 and 18 yields:

$$(1-\phi)(1-\theta)\frac{\partial C}{\partial t} = D(1-\phi)(1-\theta)\frac{\partial^2 C}{\partial x^2} - v(1-\theta)\frac{\partial C}{\partial x} - \frac{\partial C}{\partial t}\rho k_d - \mu(\rho k_d C + (1-\phi)(1-\theta)C) \tag{19}$$

When solutes move through a porous medium, they interact with the solid phase, leading to sorption or desorption of nitrate. The overall process is known as Retardation (R). Where

$$R = (1+\rho k_d) \tag{20}$$

Depending on the solute, the chemistry of the water, and the geochemical composition of the porous medium, retardation can slow the nitrate leaching process [21]. The sorption of nitrate decreases the apparent advective and dispersive fluxes. This sorption is negligible in nitrate due to its high bulk density $k_d = 0$ [16]. Introducing the retardation factor R in Equation 19 and substituting the value of the bulk density with 0 yields the following.

$$(1-\phi)(1-\theta)R\frac{\partial C}{\partial t} = D(1-\phi)(1-\theta)\frac{\partial^2 C}{\partial x^2} - v(1-\theta)\frac{\partial C}{\partial x} - \mu((1-\phi)(1-\theta)C) \tag{21}$$

Dividing equation 21 by $(1-\phi)$ yields the following.

$$(1-\theta)R\frac{\partial C}{\partial t} = D(1-\theta)\frac{\partial^2 C}{\partial x^2} - \frac{v}{(1-\phi)}\frac{\partial C}{\partial x} - \mu(1-\theta)C \tag{22}$$

Equation 22 is the modified advection-dispersion equation that is used to simulate the leaching of nitrates into groundwater. Where C is the concentration of nitrate (g/m^3), D is the longitudinal dispersivity (m), μ is the linear decay coefficient, x is the depth of leaching of nitrate (m), θ is the volumetric water content ranging from $(0 < \theta < 1)$, ϕ is the soil porosity ranging from $(0 < \phi < 1)$ and R is the retardation factor.

2.4. *Solution of the Modified Advection-Dispersion Equation*

The use of analytical methods to solve the advection-dispersion equation necessitates the approximation of some of the processes underlying nitrate leaching [22, 26]. This approximation utilises constant values for flow velocity u and dispersion coefficient D with respect to time and position under the assumption that nitrate production and degradation are limited to zero- or first-order processes [16].

Analytical solution of the modified advection-dispersion equation necessitates consideration of initial and boundary conditions. This study examines the initial condition for constant nitrate concentration C_i; which can be written as $C(x,0) = C_i$ [7]. For nitrate leaching, Equation 25's mixed type of boundary condition is considered and assumed to be a time-dependent concentration.

$$-\omega\frac{\partial C}{\partial x} + \sigma C|_{x=0} = \left\{\sigma C_0 \quad \text{if } 0 < t \leq t_0\right. \tag{23}$$

where C_0 and C_i are prescribed functions, while C is an unknown function that will be solved. Since the soil medium is considered to be of semi-infinite porous medium, the boundary condition becomes $\frac{\partial C}{\partial x}(\infty, t) = 0$ [17]. The Laplace transform, as illustrated in Definition 1, converts the advection dispersion equation into an ordinary differential equation that can be easily solved [23].

Definition 2.1. Consider a real function $F(t)$, *Laplace Transform* of $F(t), \mathcal{L}[F(t)] = \overline{F}(s)$ as defined as:

$$\mathcal{L}[F(t)] = f(s) = \int_0^\infty e^{(st)}F(t)dt$$

Where s is a complex variable. F(t) is called the original function and $f(s)$ is called the image function [24].

Consider equation 24 and dividing across by φ and letting $\psi = \frac{\omega}{\varphi}$, $\Omega = \frac{\sigma}{\varphi}$ and assuming that sink is inversely proportional to the dispersion coefficient then $\eta = \frac{\lambda}{\varphi}$. Then Equation 23 can be written as:

$$\frac{\partial C}{\partial t} = \psi \frac{\partial^2 C}{\partial x^2} - \Omega_0 \frac{\partial C}{\partial x} - \eta C \tag{24}$$

By introducing $\psi(x,t) = \psi_0 f_1(x,t)$, $\Omega_0(x,t) = \Omega_0 f_2(x,t)$ and $\eta(x,t) = \eta_0 / f_1(x,t)$. Equation 24 can be written as:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(\psi_0 f_1(x,t)\frac{\partial C}{\partial x} - \Omega_0 f_2(x,t) C\right) - \eta_0 C / f_1(x,t) \tag{25}$$

Where ψ_0, Ω_0 and η_0 are constants. Introducing a new independent variable X by a transformation $\frac{dX}{dx} = -\frac{1}{f_1(x,t)}$ [7] . Equation 25 can be written as:

$$f_1(x,t)\frac{\partial C}{\partial t} = \frac{\partial}{\partial X}\left(\psi_0 \frac{\partial C}{\partial X} - \Omega_0 f_2(x,t) C\right) - \eta_0 C \tag{26}$$

Equation 26 is a partial differential equation that can be solved analytically using the initial and boundary conditions. Let $f_1(x,t) = f(mt)$ and $f_2(x,t) = 1$. Where m is a resistive coefficient whose dimension is inverse to that of the time variable t. $f(mt)$ is chosen such that for $m = 0$ or $t = 0$, $f(mt) = 1$. Therefore, $f(mt)$ is non-dimensional variable.

Then the independent variable X can be written as:

$$X = \frac{x}{f(mt)} \tag{27}$$

Substituting $f(mt)$ into Equation 26 yields:

$$f(mt)\frac{\partial C}{\partial t} = \frac{\partial}{\partial X}\left(\psi_0 \frac{\partial C}{\partial X} - \Omega_0 C\right) - \eta_0 C \tag{28}$$

Introducing a new time variable using the following transformation $T = \int_0^t \frac{dt}{f(mt)}$[30], Equation 28 can be written in terms of the new time variable (T) as:

$$\frac{\partial C}{\partial T} = \frac{\partial}{\partial X}\left(\psi_0 \frac{\partial C}{\partial X} - \Omega_0 C\right) - \eta_0 C \tag{29}$$

Rewriting the initial and boundary conditions in terms of new space (X) and time (T) variables yields the following:

$$C(X,T) = C_i, X = 0, T > 0 \tag{30}$$

$$-\psi_0 \frac{\partial C}{\partial X} + \Omega_0 C|_{X=0} = \left\{ \Omega_0 C_0 \quad \text{if } 0 < T \le T_0 \right. \tag{31}$$

$$\frac{\partial C}{\partial X}(X,T) = 0, X \to \infty, T = 0 \tag{32}$$

Introduce a new dependent variable by the following transformation:

$$C(X,T) = E(X,T) exp\left\{\frac{\Omega_0 X}{2\psi_0} - \left(\frac{\Omega_0^2}{4\psi_0} + \eta_0\right)\right\} \tag{33}$$

Equation 28, 29, 30 and 31 reduce to:

$$\frac{\partial E}{\partial T} = \psi_0 \frac{\partial^2 E}{\partial X^2} \tag{34}$$

$$\frac{\partial E}{\partial X}(X,T) = 0, X \to \infty, T = 0 \tag{35}$$

$$-\psi_0 \frac{\partial E}{\partial X} + \frac{\Omega_0}{2} E = \Omega_0 C_0 exp(\alpha T), X = 0, 0 < T \le T_0 \tag{36}$$

Where

$$\alpha = \sqrt{\left(\frac{\Omega_0^2}{4\psi_0} + \eta_0\right)}$$

Applying Laplace transform on equation 32, 33 and 34 yields:

$$s\overline{E} = \psi_0 \frac{d^2 \overline{E}}{dX^2} \tag{37}$$

$$\frac{\partial \overline{E}}{\partial X}(X,s) = 0, X \to \infty, T = 0 \tag{38}$$

$$-\psi_0 \frac{\partial \overline{E}}{\partial X} + \frac{\Omega_0}{2}\overline{E} = \frac{\Omega_0 C_0}{(s-\alpha)}, X = 0 \tag{39}$$

The general solution of Equation 40 can be written as:

$$\overline{E}(X,s) = C_1 exp\left(-X\sqrt{\frac{s}{\psi_0}}\right) + C_2 exp\left(X\sqrt{\frac{s}{\psi_0}}\right) + C_3 exp\left(-T_0\sqrt{\frac{s}{\psi_0}}\right) + C_4 \tag{40}$$

Where

$$C_1 = C_3 = \frac{\Omega_0 C_0}{\sqrt{\psi_0}(s-\alpha)(\sqrt{s}+\beta)}$$

$$C_2 = \frac{\Omega_0 C_i}{(s+\Omega_0)\sqrt{\psi_0}(s-\alpha)(\sqrt{s}+\beta)}$$

$$C_4 = \frac{C_0}{s+\Omega_0}$$

$$\beta = \sqrt{\left(\frac{\Omega_0^2}{4\psi_0}\right)}$$

After applying initial and boundary conditions, the inverse Laplace transform of equation 40 can be resolved term-by-term. The initial term of Equation 40 can be expressed as follows:

$$\overline{E_1}(X,s) = \frac{\Omega_0 C_0}{\sqrt{\psi_0}(s-\alpha)(\sqrt{s}+\beta)} exp\left(-X\sqrt{\frac{s}{\psi_0}}\right) \tag{41}$$

According to [25], the inverse Laplace transform of the first term of equation 41 yields:

$$\begin{aligned} E(X,T) = {} & \frac{\Omega_0 C_0}{2\sqrt{\psi_0}\left\{\sqrt{\alpha}+\sqrt{(\beta^2\psi_0)}\right\}} \exp\left\{\frac{\{\alpha\sqrt{\psi_0}T - X\alpha\}}{\sqrt{\psi_0}}\right\} erfc\left\{\frac{X - \sqrt{4\,(\alpha\psi_0)}T}{2\sqrt{(\psi_0 T)}}\right\} \\ & + \frac{\Omega_0 C_0}{2\sqrt{\psi_0}\left\{\sqrt{\alpha}-\sqrt{(\beta^2\psi_0)}\right\}} \exp\left\{\frac{\{\sqrt{\alpha}\sqrt{\psi_0}T + X\sqrt{\alpha}\}}{\sqrt{\psi_0}}\right\} erfc\left\{\frac{X + \sqrt{4\,(\sqrt{\alpha}\psi_0)}T}{2\sqrt{(\psi_0 T)}}\right\} \\ & + \frac{\Omega_0 C_0 \psi_0 \beta}{\sqrt{\psi_0}\,\{\beta^2\psi_0 - \alpha\}} \exp\left\{\beta X - \beta^2\psi_0 T\right\} erfc\left\{\frac{X + \psi_0\beta T}{2\sqrt{\psi_0 T}}\right\} \end{aligned} \tag{42}$$

The inverse Laplace transform of the second term of equation 60 leads to a complex variable [26, 27]. Therefore, for the leaching of nitrate, $C_i = 0$. Consequently, the second term of equation 43 yields zero [17, 28].

The inverse Laplace transform of the third term of equation 43 is zero on the interval of $0 < t \leq t_0$, since $x \to \infty, t_0 = 0$ as shown in equation 55 [24].

According to [25], the inverse Laplace transform of the fourth term of equation 43 yields the following:

$$E_4(X,T) = C_0 exp(-\Omega_0 T) \tag{43}$$

By using transformations 33, and applying the transformation of [30], on equations 44 and 45 and substituting for α in equation 39, the inverse Laplace transform of equation 45 can be written in terms of $C(x,T)$ as:

$$\begin{aligned} C(x,T) = {} & \frac{\Omega_0 C_0}{2\sqrt{\psi_0}\left\{\beta+\sqrt{(\beta^2+\eta_0)}\right\}} \exp\left\{\frac{\left\{\beta-\sqrt{(\beta^2+\eta_0)}\right\}x}{f(mt)\sqrt{\psi_0}}\right\} erfc\left\{\frac{\frac{x}{f(mt)} - \sqrt{(\Omega_0^2+4\eta_0\psi_0)}T}{2\sqrt{(\psi_0 T)}}\right\} \\ & + \frac{\Omega_0 C_0}{2\sqrt{\psi_0}\left\{\beta-\sqrt{(\beta^2+\eta_0)}\right\}} \exp\left\{\frac{\left\{\beta+\sqrt{(\beta^2+\eta_0)}\right\}x}{f(mt)\sqrt{\psi_0}}\right\} erfc\left\{\frac{\frac{x}{f(mt)} + \sqrt{(\Omega_0^2+4\eta_0\psi_0)}T}{2\sqrt{(\psi_0 T)}}\right\} \\ & + \frac{\Omega_0 C_0}{2\eta_0\psi_0} \exp\left\{\frac{\Omega_0 x}{\psi_0 f(mt)} - \eta_0 T\right\} erfc\left\{\frac{\frac{x}{f(mt)} + \Omega_0 T}{2\sqrt{\psi_0 T}}\right\} + C_0 exp(-\Omega_0 T) \end{aligned} \tag{44}$$

Equation 44 can be rewritten in terms of dimensionless variables in equation 20 via back substitution as:

$$C(x,t) = \frac{\sigma C_0}{\{\sigma+\upsilon\}}\exp\left\{\frac{\{\sigma-\upsilon\}x}{2\omega}\right\}erfc\left\{\frac{\varphi x-\upsilon t}{2(\omega\varphi t)^{\frac{1}{2}}}\right\}+\frac{\sigma C_0}{\{\sigma-\upsilon\}}\exp\left\{\frac{\{\sigma+\upsilon\}x}{2\omega}\right\}erfc\left\{\frac{\varphi x+\upsilon t}{2(\omega\varphi t)^{\frac{1}{2}}}\right\}$$
$$+\frac{\sigma^2 C_0}{2\lambda\omega}\exp\left\{\frac{\upsilon x}{\omega}-\frac{\lambda t}{\varphi}\right\}erfc\left\{\frac{\varphi x+\sigma t}{2(\omega\varphi t)^{\frac{1}{2}}}\right\}+C_0\exp\left(-\frac{\sigma t}{\varphi}\right) \tag{45}$$

Where

$$\upsilon = \sigma\left(1+\frac{4\lambda\omega}{\sigma^2}\right)^{\frac{1}{2}}$$

Equation 45 is the analytical solution to the modified advection-dispersion equation that simulates nitrate leaching into groundwater at any depth x and time t.

3. Model Simulation

In this section, MATLAB software is used to graphically represent numerical simulations of a nitrate concentration that varies with depth, time, volumetric water content, and soil porosity. For the purposes of comparison and analysis, the simulation's parameters are set to vary within realistic limits.

The subsequent subsections depict graphically simulations representing depth-leaching nitrate, the effect of soil porosity on nitrate leaching, and the effect of volumetric water content on nitrate leaching.

3.1. Simulation Parameters

The analytical solution described in equation 46 for varying the input in a finite domain $0 \leq x \leq 1$ with a long longitudinal direction is used to calculate the nitrate concentration values at different depths in the soil. Regarding distance and time, metres and years are used, respectively. The initial concentration C is equal to $1.00g/m^3$. The parameter values listed in Table 1 are considered constant and are implemented in every simulation.

Table 1. *Parameter values for nitrate leaching to groundwate.*

Symbol	Parameter	Value	Source
D	Dispersion coefficient	$85.51m^2/s$	Raji *et al.*, (2014)
C	Concentration	Variable	
u	Flow velocity	$0.424m/s$	Martinus *et al.*, (2013)
R	Retardation factor	1	Martinus *et al.*, (2013)
μ	First-order decay	$0.3/day$	Pérez Guerrero *et al.*, (2013)
ϕ	Soil Porosity	$(0 < \phi < 1)$	Nimmo, (2004)
θ	Volumetric water content	$(0 < \theta < 1)$	Wanjuan Hau *et al.*, (2017)

3.2. Nitrate Leaching with Depth

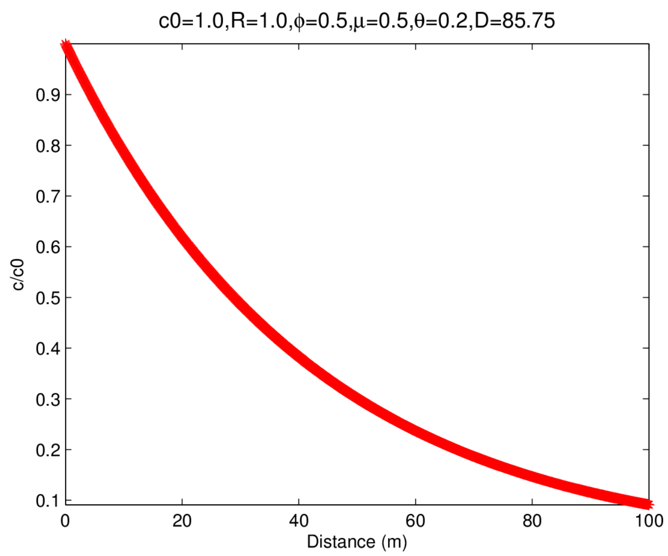

Figure 1. *Concentration of nitrate with depth.*

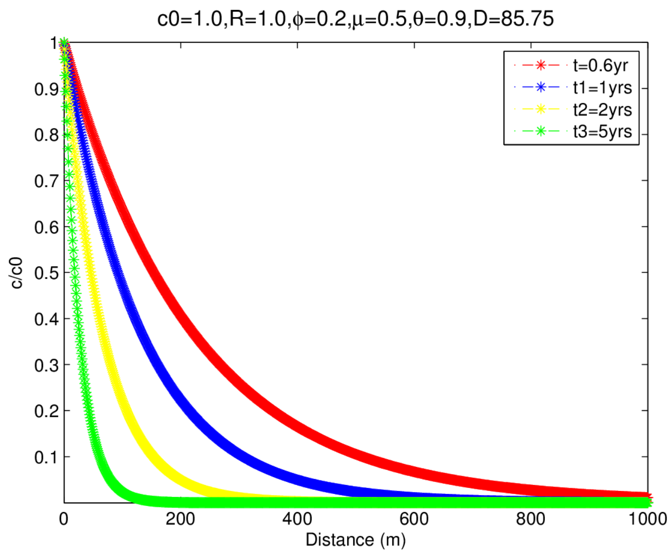

Figure 2. *Concentration of nitrate with depth varying time.*

In this section, numerical simulations of the concentration of nitrate as it varies with depth and time are represented graphically using MATLAB software. For the purposes of comparison and analysis, the simulation's parameters are set to vary within realistic limits.

Figure 1 depicts a simulation depicting the concentration of nitrate versus the depth of leaching. The concentration of nitrates decreases with increasing soil depth, as shown in Figure 1. This suggests that as depth increases, nitrate concentrations decrease due to processes such as plant uptake.

Figure 2 illustrates the depth-dependent concentration of nitrate over time. The graph demonstrates that the nitrate concentration decreases with increasing depth, and after a longer period of time, it approaches zero. After a period of time, the nitrate concentration reaches zero because all nitrate in the soil is believed to have leached into groundwater, leaving a concentration of zero in the soil column.

3.3. Effect of Soil Porosity on Leaching of Nitrate

In this section, numerical simulations illustrating how soil porosity affects the leaching of nitrate into groundwater are graphically represented and discussed using MATLAB software. For the purposes of comparison and analysis, the simulation's parameters are set to vary within realistic limits.

Figure 3 depicts the relationship between the concentration of nitrates and the time-varying porosity of the soil, with the volumetric water content held constant, using the parameters specified in Table 1. In all soil porosity ranges, the concentration of nitrates decreases from 1 to nearly 0 over time, as depicted in Figure 3. When the soil porosity is greater than 0.6, the concentration reaches zero more quickly than when it is less than 0.1. This demonstrates that soil porosity influences the rate of nitrate leaching into groundwater.

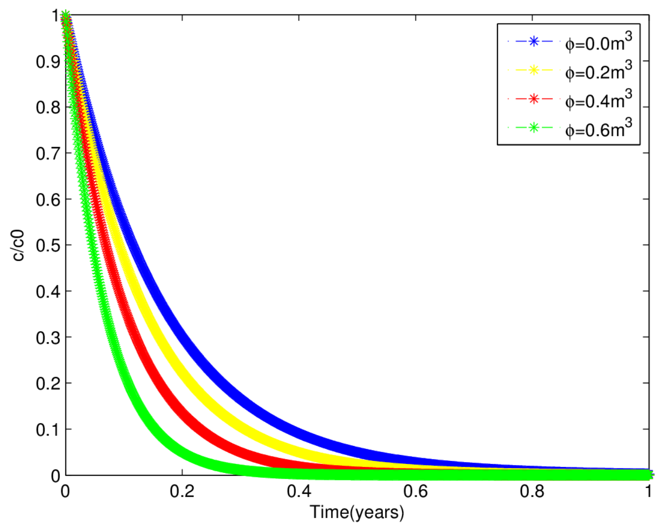

Figure 3. *Concentration of Nitrate with Time-Varying Soil Porosity.*

Figure 4 depicts the concentration of nitrates as a function of soil porosity, while keeping the volumetric water content, soil depth, and time constant, in accordance with Table 1's parameters. The concentration of nitrate increases with increasing soil porosity, as shown in Figure 4. This demonstrates that nitrate leaching is dependent on soil porosity; thus, increasing soil porosity accelerates nitrate leaching into groundwater.

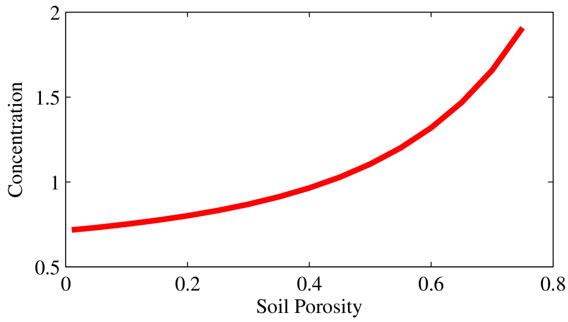

Figure 4. *Concentration of nitrate against soil porosity.*

Graph of Nitrate Concentration versus Depth and Soil Porosity Variation

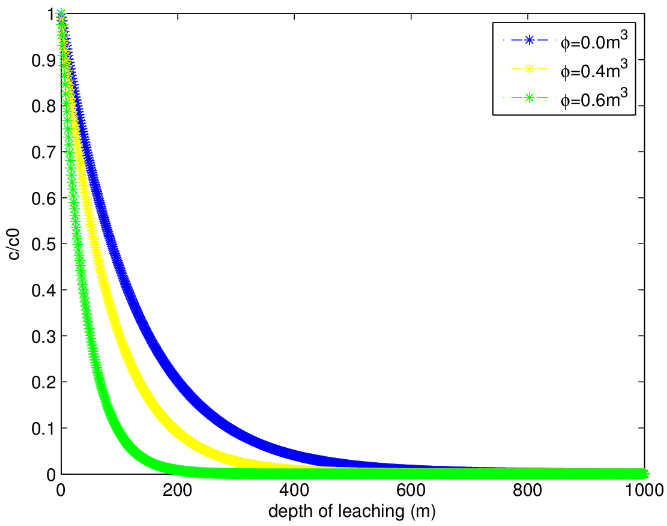

Figure 5. *Nitrate Concentration with Differentiated Soil Porosity.*

Figure 5 depicts the concentration of nitrate in relation to the soil's porosity as it varies with depth, while keeping the soil's volumetric water content constant and utilising the parameters listed in Table 1. Figure 5 demonstrates that the concentration of nitrates decreases with time; the decrease is more rapid in soils with higher porosity and slower in soils with lower porosity. This indicates that nitrate leaches faster from more porous soil than from less porous soil.

The porousness of the soil influences the leaching of nitrate into groundwater, as depicted in Figures 3, 4, and 5. According to the data, nitrate leaching into groundwater increases with an increase in soil porosity, as indicated by the decrease in nitrate concentration at the soil surface. Therefore, porous soils are more likely to lose nitrate through leaching, as they have a lower capacity to retain water. Consequently, soil porosity influences the rate of water percolation in the soil, thereby accelerating the rate of nitrate leaching into groundwater. This means that nitrate leaching into groundwater occurs more rapidly in porous soils than in less porous soils, which is consistent with the findings of [14].

3.4. Effect of Volumetric Water Content on Leaching of Nitrate

In this subsection, numerical simulations showing how volumetric water content affects the leaching of nitrates into groundwater are represented graphically using MATLAB software and are discussed. The simulation parameters are set to vary within realistic limits for comparison and analysis purposes.

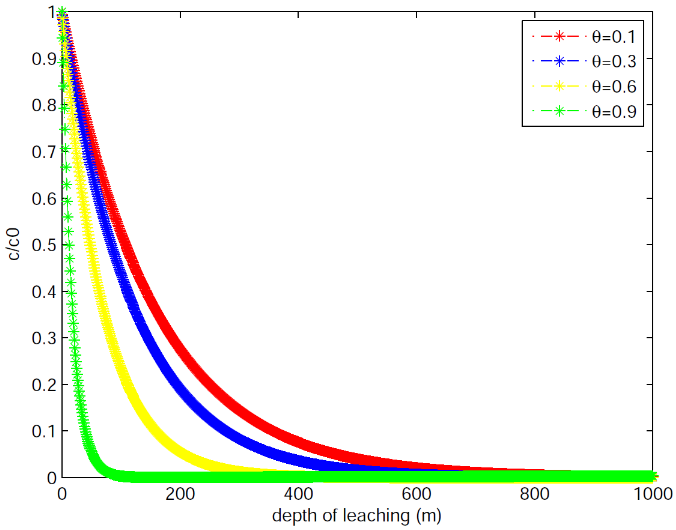

Figure 6. *Concentration of nitrate with depth varying volumetric water content.*

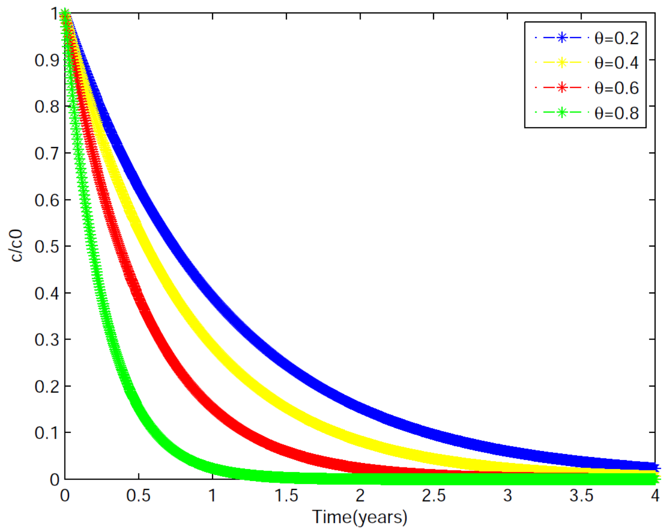

Figure 7. *Concentration of nitrate with time-varying volumetric water content.*

Figure 6 depicts the simulation of the concentration of nitrates as a function of depth with varying volumetric water content, while keeping soil porosity constant at a level less than 0.2 and employing the parameters from Table 1. As shown in Figure 6, the nitrate concentration decreases with increasing soil depth, so that at greater depths, such as 1000 m, there is no nitrate concentration. At a higher volumetric water content of $0.9m^3$, the concentration decreases more quickly than at a lower volumetric water content of $0.1m^3$.

Figure 7 is an illustration of the concentration of nitrate over time with varying volumetric water contents and constant soil porosity, using the parameters listed in Table 1. Figure 7 demonstrates that the nitrate concentration decreases with time, with the rate of decrease being faster for higher volumetric water content ($0.6m^3$) and slower for lower volumetric water content ($0.1m^3$). The concentration of nitrate also decreases more rapidly between 0 and 1 year, eventually reaching zero. This decrease in nitrate concentration in soils with varying volumetric water content may be attributable to the fact that a higher water content in soils results in faster solute transport and, consequently, a greater potential for nitrate loss through leaching. This suggests that volumetric water content increases the rate of nitrate leaching into groundwater. Because all nitrates had leached into the groundwater, the graph remains unchanged.

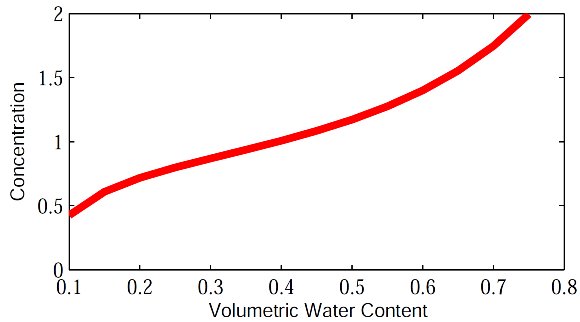

Figure 8. *Concentration of nitrate against volumetric water content.*

Figure 8 depicts a simulation illustrating the concentration of nitrate in relation to the soil's volumetric water content while maintaining the soil's porosity, depth, and time, as well as the parameters specified in Table 1. The graph demonstrates that the rate of nitrate leaching into groundwater is proportional to the volumetric water content, such that an increase in volumetric water content accelerates nitrate leaching.

Figures 6, 7, and 8 illustrate how the volumetric water content of the soil column influences the leaching of nitrate into groundwater. According to the data, an increase in volumetric water content decreases soil nitrate concentration, which increases leaching into groundwater. This indicates that soil with a high volumetric water content transports solutes faster and has a greater potential for nitrate loss through leaching. [3]According to their study, nitrate leaching is greater during the wet season than during the dry season, which is consistent with the findings of this study.

4. Conclusions

This study focuses primarily on the modification of the advection-dispersion equation to model nitrate leaching taking soil porosity and water content by volume into account. MATLAB software was used to simulate the leaching of nitrates into groundwater under varying volumetric water content and soil porosity, and the results were presented graphically. According to the study, the leaching of nitrate in groundwater is directly proportional to the volumetric water content in the soil and the porosity of the soil. Therefore, a more porous soil with a high volumetric water content will allow more nitrate to reach groundwater in a shorter period of time, resulting in faster contamination of groundwater. Leaching of nitrate into groundwater results in high levels of nitrate pollution, particularly in low-income, densely populated peri-urban and rural areas where a large number of people rely on water from boreholes and wells.

5. Recommendations

This study demonstrates that the leaching of nitrate into groundwater is proportional to the soil's permeability and volumetric water content. To reduce this risk of groundwater contamination, possible mitigation measures must be implemented, such as limiting the amount of nitrogen applied, avoiding over-irrigation, and developing a test that allows farmers to measure the amount of nitrogen already present in the soil with greater precision. This study only considers the longitudinal dispersivity of nitrate. In reality, however, leaching could occur in any direction; therefore, future research should incorporate three-dimensional models that incorporate soil porosity and volumetric water content.

Conflict of Interest

The authors declare that they have no competing interests.

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