Journal of Progressive Research in Mathematics(JPRM)
ISSN: 2395-0218

SCITECH
RESEARCH ORGANISATION

Volume 14, Issue 2
Published online: October 03, 2018|

Journal of Progressive Research in Mathematics
www.scitecresearch.com/journals

Stability Analysis Of The Modified Advection-Dispersion Model For Nitrate Leaching Into Groundwater

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Abstract

Nitrogen is a vital nutrient that enhances plant growth which has motivated the intensive use of nitrogen based fertilizers to boost crop productivity. However, Pollution by nitrate is a globally growing problem due to the population growth, increase in the demand for food and inappropriate Nitrogen application. The complexities and challenges in quantifying nitrate leaching have led to development of a range of measurement and modeling techniques. However, most of them are not widely applied due to their inaccuracy. This calls for new approaches in which nitrate leaching can be analysed in order to give better understanding of nitrate fate and transport process for proper management of groundwater. This study presents a mathematical model to analyse nitrate leaching into groundwater from the advection-dispersion equation. The advection-dispersion equation is modified by incorporating soil porosity and volumetric water content of the soil. The stability of the model has been performed by the Von Neumann stability condition after performing descritization using the Cranck-Nicolson scheme and finite difference scheme. The model is conditionally stable for all ranges of angle(κ), when Von Neumann stability condition is applied for both the Cranck-Nicolson scheme and finite difference scheme. The results provide science-based input into best alternative mathematical model which can be used to analyse leaching of nitrate into groundwater.

Keywords: Nitrate, Stability Analysis, Advection-Dispersion, Von-neuman, Groundwater.

1 Introduction

Nitrate is the most widespread of all groundwater contaminants (Su *et al.*, 2013). Excessive nitrogen (N) fertilizers application in agricultural land can result in excessive nitrate concentrations in the groundwater above the World Health Organization (WHO) limit established of 10 mg/L of N-NO-3. Above this limit, nitrates are known to have negative health impacts such as methemoglobinemia in infants, gastric lymphoma in adults, miscarriages among pregnant women, insulin-dependent diabetes mellitus, thyroid disease and increased risk for Non-Hodgkin Lymphoma (NHL) (Judith *et al.*, 2013; Marinov *et al.*, 2014).

Excess nitrate can also lead to soil acidification and increase in alga growth in water which can rob the water of dissolved oxygen and eventually kill fish and other aquatic life (Ombaka *et al*., 2012).

Nitrogen is a vital nutrient that enhances plant growth. This has motivated the intensive use of nitrogen-based fertilizers to boost up the productivity of crops in many regions of the world. Nitrogen in soil undergoes many biochemical transformations such as immobilization, mineralization, nitrification, denitrification, volatilization, crop uptake and leaching to groundwater.

Nitrate can reach both surface water and groundwater as a consequence of activity from non-point source which includes fertilizer and manure applications, dissolved nitrogen in precipitation, irrigation flows, atmospheric deposition from point source which include waste water treatment and from oxidation of nitrogenous waste products in human and animal excreta, including septic tanks and industrial pollutants (Ombaka *et al*., 2012; WHO, 2011).

Mathematical models are useful for the study of nitrate leaching because of their predictive capability. The models are portable due to their adaptability to different situations after adjusting the model parameters accordingly. They also allow better understanding of the inter-dependency of the relevant parameters and permits identification of sensitive input parameters. Models that simulate nitrogen processes in soils and evaluate environmental impact associated with nitrogen management are now recognized as being critical for improving cropping technique and cropping systems (Greenwood *et al*., 2010). Prevention of groundwater contamination requires a good understanding of the processes involved in nitrate leaching.

Volumetric water content in soil is one of the most important factors affecting the movement of nitrate in soil to groundwater. The water infiltrates the soil causing nitrate ions to move down through the soil profile by percolation. If precipitation exceeds evapotranspiration, nitrate can leach to groundwater. But where the amounts of water content are low and potential evapotranspiration exceeds annual precipitation, the concentration of nitrate will be high because the dilution effect is reduced (Leskosek, 1994). Soil porosity is the total soil volume that is taken up by the pore space and it determines the maximum amount of water that soil can store at a given time. The particle size distribution and the occurrence of preferential flow paths are the factors which determine the Porosity of the soil. Soils have varied retentive properties depending on their texture and organic matter content. Due to the higher proportion of gravitational pores, coarse soils are usually more vulnerable to leaching than clay soils (Wu *et al*., 1997). Sandy soils are also fairly homogeneous hence water moves freely through the soil matrix. Therefore nitrate leaching is affected by soil porosity, such that leaching of nitrate will be high in loose porous soil.

In order to generate sufficient data for providing the basis for forming policies, nitrate leaching must be measured under a wide variety of situations , due to complex and often nonlinear physical, chemical and biological processes affecting nitrate fate and transport process in soil (Anderson & Phanikumar, 2011). With the increasing concern of pollution by nitrate to the groundwater, accurate analytical solution useful in validating numerical solutions is required. This necessitates the formulation of a mathematical model that simulates nitrate leaching from the surface to groundwater by incorporating soil porosity and volumetric water content in the transport equation.

2 Model development

A general one-dimensional advection-dispersion equation is derived from the law of conservation of mass as:

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x} \tag{1}$$

Where D is the dispersion coefficient and v is the flow velocity. C is concentration of the dispersing solute along x direction at a time t. We shall modify equation 1 by introducing volumetric water content and soil porosity to simulate nitrate leaching to groundwater. Volumetric water content can be expressed as a ratio, which can range between 0 to 1 (Sobey, 1983). By letting the volumetric water content to be θ such that $(0 < \theta < 1)$ and soil porosity to be ϕ such that $(0 < \phi < 1)$, and introducing $(1-\theta)$ and $(1-\phi)$ in the dispersive flux since dispersion is the spreading out of solute due to variations in water velocity within individual pores and since volumetric water content and soil porosity are the main factors being considered to determine the rate of dispersion in this study, then the second term of equation 1 can be modified as:

$$-D(1-\theta)(1-\phi)\frac{\partial^2 C}{\partial x^2} \tag{2}$$

The volumetric water content in the soil will affect the flow velocity of the dissolved nitrate, such that the last term of equation 1 can be modified as:

$$v(1-\theta)\frac{\partial C}{\partial x} \tag{3}$$

The rate of nitrate leaching to groundwater also depends on soil porosity ϕ, volumetric water content of the porous medium , bulk density of the porous medium and distribution coefficient (Cameron, 1983), From the first term of equation 1 the rate term can be written as:

$$(1-\phi)(1-\theta)\frac{\partial C}{\partial t} = -\rho k_d\frac{\partial C}{\partial t} \tag{4}$$

Where ρ is the bulk density of the porous medium and k_d is the distribution coefficient at equilibrium state. During leaching, nitrate also under goes radioactive decay, biological transformations among other factors which leads to nitrate loss and load in soil which affects the leaching process. Introducing these factors in equation 4, rate of leaching of nitrate can be rewritten as:

$$(1-\phi)(1-\theta)\frac{\partial C}{\partial t} = -\rho k_d\frac{\partial C}{\partial t} - \mu(\rho k_d C + (1-\theta)(1-\phi)C) \tag{5}$$

Where μ represents source and sink factors. From the aforementioned modifications equation 1 can written as:

$$\begin{aligned}(1-\phi)(1-\theta)\frac{\partial C}{\partial t} = D(1-\phi)(1-\theta)\frac{\partial^2 C}{\partial x^2} - v(1-\theta)\frac{\partial C}{\partial x} - \frac{\partial C}{\partial t}\rho k_d \\ - \mu(\rho k_d C + (1-\phi)(1-\theta)C)\end{aligned} \tag{6}$$

When solutes flows through porous medium they interact with the solid phase, which can lead to sorption or desorption of nitrate. The net process is called Retardation (R). Where:

$$R = (1+\rho k_d) \tag{7}$$

Retardation generally depends on the solute, water chemistry and geochemical make of the porous medium and it can slow down leaching process of nitrate (Mikotajkaw, 2003). Sorption of nitrate reduces the apparent advective and dispersive fluxes. This sorption is negligible in nitrate since bulk density of nitrate $k_d = 0$ (Martinus *et al.*, 2013). Introducing retardation factor R in equation 6 and substituting the value of bulk density with 0 yields:

$$(1-\phi)(1-\theta)R\frac{\partial C}{\partial t} = D(1-\phi)(1-\theta)\frac{\partial^2 C}{\partial x^2} - v(1-\theta)\frac{\partial C}{\partial x} - \mu((1-\phi)(1-\theta)C) \tag{8}$$

Dividing equation 8 by $(1-\phi)$ yield:

$$(1-\theta)R\frac{\partial C}{\partial t} = D(1-\theta)\frac{\partial^2 C}{\partial x^2} - \frac{v}{(1-\phi)}\frac{\partial C}{\partial x} - \mu(1-\theta)C \tag{9}$$

Equation 9 is the modified advection-dispersion equation that is used to simulate nitrate leaching to 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 soil porosity ranging from $(0 < \phi < 1)$ and R is retardation factor.

2.1 Stability Analysis

The stability analysis of the modified Advection-dispersion equation 9 is done by using Von Neumann stability condition after introducing the following dimensionless variables such that:$\varphi = R(1-\theta)$, $\omega = D(1-\theta)$, $\sigma = \frac{v}{(1-\phi)}$ and $\lambda = \mu(1-\theta)$. Equation 9 can then be written as:

$$\frac{\varphi\partial C}{\partial t} = \omega\frac{\partial^2 C}{\partial x^2} - \sigma\frac{\partial C}{\partial x} - \lambda C \tag{10}$$

The stability of PDE can be investigated by performing Von Neumann stability analysis since it ignores the boundary conditions (Wesseling,1995). To investigate the stability of equation 10 using Von Neumann stability analysis, we substitute the trial function $C_j^n = A\xi^n e^{i\kappa j}$ into the approximate difference scheme to obtain the characteristics equation for the amplification factor ξ then finding the restriction parameters (Recktenwald, 2004). The scheme is Von Neumann stable if $|\xi| \leq 1$ and the scheme is Von Neumann unstable if $|\xi| > 1$. If the characteristics equation has multiple roots, then the roots must be distinct meaning all roots are not equal to one another for the scheme to be stable (Wesseling, 1995).

In this study finite different scheme and Crank Nicolson scheme are used to discretize equation 10 and their results compared as illustrated in the two subsequent subsections.

2.2 Finite Difference Scheme

The finite difference scheme is one of several techniques for obtaining numerical solutions to partial differential equation. Discritizing equation 24 using finite difference scheme yields:

$$\varphi\frac{C_j^{n+1} - C_j^n}{\Delta t} = \omega\frac{C_{j+1}^n - 2C_j^n + C_{j-1}^n}{(\Delta x)^2} - \sigma\frac{C_{j+1}^n - C_{j-1}^n}{2\Delta x} - \lambda C_j^n \tag{11}$$

Multiply equation 11 by $\frac{\Delta t}{\varphi}$ and Letting $\gamma = \omega\frac{\Delta t}{(\varphi\Delta x)^2}$, $\tau = \sigma\frac{\Delta t}{\varphi\Delta x}$ and $\zeta = \varphi\lambda\Delta t$ equation 11 can then be written as:

$$C_j^{n+1} - C_j^n = \gamma(C_{j+1}^n - 2C_j^n + C_{j-1}^n) - \frac{1}{2}\tau(C_{j+1}^n - C_{j-1}^n) - \zeta C_j^n \tag{12}$$

Introducing Von Neumann stability condition to equation 12 by substituting the trial function and dividing through by $A\xi^n e^{i\kappa j}$ yields:

$$\xi = 1 + \gamma(e^{i\kappa} - 2 + e^{-i\kappa}) - \frac{1}{2}\tau(e^{i\kappa} - e^{-i\kappa}) - \zeta \tag{13}$$

Equation 13 can be rearranged as:

$$\xi = (1-2\gamma) + \gamma(e^{i\kappa} + e^{-i\kappa}) - \frac{1}{2}\tau(e^{i\kappa} - e^{-i\kappa}) - \zeta \tag{14}$$

Converting the Exponential function to trigonometric equivalent in equation 14 yields:

$$\xi = (1-2\gamma) + 2\gamma\cos\kappa - \frac{1}{2}\tau i \sin\kappa - \zeta \tag{15}$$

But

$$\cos\kappa = 1 - 2\sin^2\frac{\kappa}{2} \tag{16}$$

Substituting equation 16 into 15 and simplifying yields:

$$\xi = 1 - 4\gamma\sin^2\frac{\kappa}{2} - \frac{1}{2}\tau i \sin\kappa - \zeta \tag{17}$$

For Von Neumann stability condition,$|\ \xi\ | \leq 1$ that is $-1 \leq \xi \leq 1$, Since

$$-1 \leq 1 - 4\gamma\sin^2\frac{\kappa}{2} - \frac{1}{2}\tau i \sin\kappa - \zeta \geq 1 \tag{18}$$

Equation 18 is conditionally stable when using finite difference scheme. The unstable points is when $\kappa = \pi$, otherwise all scheme is stable for all other values of π.

2.3 Crank-Nicolson Scheme

The Crank-Nicolson method is used because it is unconditionally stable and is second-order accurate in time and in space (Awni and Atef, 2007; Micheal, 2005; Khebchareon and Saenton, 2012). The Von Neumann stability condition is used to test the stabilty of equation 10 using Crank-Nicolson scheme after discritization which yields:

$$\begin{aligned} \varphi\frac{C_j^{n+1} - C_j^n}{\Delta t} &= \omega\frac{C_{j+1}^n - 2C_j^n + C_{j-1}^n + C_{j+1}^{n+1} - 2C_j^{n+1} + C_{j-1}^{n+1}}{2(\Delta x)^2} \\ &- \sigma\frac{C_{j+1}^n - C_{j-1}^n + C_{j+1}^{n+1} - C_{j-1}^{n+1}}{4\Delta x} - \lambda(C_j^n + C_j^{n+1}) \end{aligned} \tag{19}$$

Multiply equation 19 by $\frac{\Delta t}{\varphi}$ and Letting $\gamma = \omega\frac{\Delta t}{\varphi(\Delta x)^2}$, $\tau = \sigma\frac{\Delta t}{\varphi\Delta x}$ and $\zeta = \lambda\frac{\Delta t}{\varphi}$ equation 19 can then be written as:

$$\begin{aligned} C_j^{n+1} - C_j^n &= \frac{\gamma}{2}\left[C_{j+1}^n - 2C_j^n + C_{j-1}^n + C_{j+1}^{n+1} - 2C_j^{n+1} + C_{j-1}^{n+1}\right] \\ &- \frac{\tau}{4}\left[C_{j+1}^n - C_{j-1}^n + C_{j+1}^{n+1} - C_{j-1}^{n+1}\right] - \zeta[C_j^n + C_j^{n+1}] \end{aligned} \tag{20}$$

Substituting trial function in equation 20 and dividing through by $A\xi^n e^{i\kappa j}$ yields:

$$\begin{aligned} \xi - 1 &= \frac{\gamma}{2}\left[e^{i\kappa} - 2 + e^{-i\kappa} + \xi e^{i\kappa} - 2\xi + \xi e^{-i\kappa}\right] \\ &- \frac{\tau}{4}\left[e^{i\kappa} - e^{-i\kappa} + \xi e^{i\kappa} - \xi e^{-i\kappa}\right] - \zeta[1+\xi] \end{aligned} \tag{21}$$

Collecting the like terms in equation 19 and substituting $\cos\kappa = \frac{1}{2}\left(e^{i\kappa} + e^{-i\kappa}\right)$ and $\sin\kappa = \frac{1}{2i}\left(e^{i\kappa} - e^{-i\kappa}\right)$ yields:

$$\xi - 1 = \gamma\cos\kappa + \gamma\xi\cos\kappa - \gamma - \xi\gamma - \frac{\tau}{2}i\sin\kappa - \frac{\xi\tau}{2}i\sin\kappa - \zeta - \zeta\xi \tag{22}$$

Collecting like terms and making ξ the subject equation 22 becomes:

$$\xi = \frac{1 + \gamma\cos\kappa - \gamma - \frac{\tau}{2}i\sin\kappa - \zeta}{1 - \gamma\cos\kappa + \gamma + \frac{\tau}{2}i\sin\kappa + \zeta} \tag{23}$$

For Von Neumann stability condition: $|\ \xi\ | \leq 1$ that is $-1 \leq \xi \leq 1$, Since

$$-1 \leq \frac{1 + \gamma\cos\kappa - \gamma - \frac{\tau}{2}i\sin\kappa - \zeta}{1 - \gamma\cos\kappa + \gamma + \frac{\tau}{2}i\sin\kappa + \zeta} \leq 1 \tag{24}$$

Equation 24 satisfy the Von Neumann stability condition within certain values of $|\xi|$, and will always be stable for all values of κ, γ, ζ and τ except when γ, ζ and τ are infinitesimal small.

3 Conclusions

In this study, a deterministic model to study nitrate leaching to groundwater has been developed, from the law of conservation of mass under reasonable assumptions and parameters. The stability of the model has been performed by the Von Neumann stability condition after performing descritization using the Cranck-Nicolson scheme and finite difference scheme. The study has shown that, when using both the finite difference scheme and Crank Nicolson scheme Equation 10 is conditionally stable. Therefore, the modified Advection-Dispersion equation is conditionally stable for all ranges of angle(κ) when Von Neumann stability condition is applied on both Crank Nicolson scheme and Finite different scheme This shows that leaching of nitrate to groundwater takes place longitudinally downwards since advection and dispersion are considered to occur in vertical direction only. Other factors affecting leaching of nitrate like volumetric water content and soil porosity does not affect the directional flow of nitrate to groundwater. The results provide science-based input into best alternative mathematical model which can be used to analyse leaching of nitrate into groundwater.

4 Recommendations

In this study only longitudinal dispersivity of nitrate is considered, however in real situation leaching might also occur in any direction, therefore three dimensional models which incorporates soil porosity and volumetric water content should be considered in future.

5 Conflicts of interest

There are no conflicts to declare.

6 Acknowledgments

We thanks the administrative staff in the department of physical science of Chuka University for their hospitality and assistance in matters related to our research work.

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