IOSR Journal of Mathematics (IOSR-JM)
e-ISSN: 2278-5728, p-ISSN: 2319-765X. Volume 14, Issue 4 Ver. II (Jul - Aug 2018), PP 18-26
www.iosrjournals.org

Modeling the Impact of Soil Porosity on Nitrate Leaching To Groundwater Using the Advection Dispersion Equation

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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 has developed 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 transformed to a second order ordinary differential equation by Laplace and solved. Simulations showing the variation of soil porosity is presented using the MATLAB software. The study has shown that nitrate leaching to groundwater is directly proportional to soil porosity such that more porous soil will allow more nitrate to reach to the groundwater within a short time leading to faster contamination of groundwater. The results is useful to farmers, policy makers, researchers and the general public for the purpose of understanding movement of nitrates through the soil and also provide science-based input into best alternative mathematical model which can be used to analyse leaching of nitrate into groundwater.*

Keywords— *Nitrate, Modeling, Advection-Dispersion, Leaching, Groundwater, Soil Porosity*

Date of Submission: 17-07-2018 Date of acceptance: 02-08-2018

I. 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 al- low 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.

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). This necessitates the formulation of a mathematical model that simulates nitrate leaching from the surface to groundwater by incorporating soil porosity in the transport equation

II. Model Development

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

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

(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:

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

(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:

$$v(1-\theta)\frac{\partial c}{\partial x}$$

(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:

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

(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:

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

(5)

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

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

(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:

$$R = (1 + \rho kd) \quad (7)$$

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 $kd = 0$ (Martinus *et al.*, 2013). Introducing retardation factor R in equation 6 and substituting the value of bulk density with 0 yields:

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

(8)

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

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

(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 Solution of the Modified Advection-Dispersion Equation

By introducing dimensionless variable in equation 9 such that: $\varphi = R(1-\theta)$, $\omega = D(1-\theta)$, $\sigma = \frac{v}{(1-\theta)}$, $\lambda = \mu(1-\theta)$. Equation 9 can be written as:

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

By dividing equation 26 by φ and letting $\psi = \frac{\omega}{\varphi}$, $\varepsilon = \frac{\sigma}{\varphi}$ and assuming that sink is inversely proportional to the dispersion coefficient then $\eta = \frac{\lambda}{\varphi}$. Then equation 10 can be written as:

$$\frac{\partial C}{\partial t} = \psi \frac{\partial^2 C}{\partial x^2} - \varepsilon \frac{\partial C}{\partial x} - \eta C \quad (11)$$

By introducing $\psi(x,t) = \psi_0 f_1(x,t)$, $\varepsilon(x,t) = \varepsilon_0 f_2(x,t)$, and $\eta(x,t) = \eta_0 f_1(x,t)$. Equation 11 can be written as:

$$\frac{\partial C}{\partial t} = \frac{\partial C}{\partial x}\left(\psi_0 f_1(x,t)\frac{\partial C}{\partial x} - \varepsilon_0 f_2(x,t)C\right) - \eta_0 C/f_1(x,t) \quad (12)$$

Where ψ_0, ε_0 and η_0 are constants. Introducing a new independent variable X by a transformation $\frac{dX}{dx} = -\frac{1}{f_1(x,t)}$ (Dilip *et al.*, 2009). Equation 12 can be written as:

$$f_1(x,t)\frac{\partial C}{\partial t} = \frac{\partial C}{\partial X}\left(\psi_0 \frac{\partial C}{\partial X} - \varepsilon_0 f_2(x,t)C\right) - \eta_0 C \quad (13)$$

Equation 13 is a partial differential equation which 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 time variable t. $f(mt)$ is chosen such that for $m = 0$ or $t = 0$, $m = 0$ $f(mt) = 1$. Therefore, $f(mt)$ is non-dimensional variable. Then the independent varable X can be written as: $X = \frac{x}{f(mt)}$. Substituting $f(mt)$ in equation 13 yields:

$$f(mt)\frac{\partial C}{\partial t} = \frac{\partial C}{\partial X}\left(\psi_0\frac{\partial C}{\partial X} - \varepsilon_0 C\right) - \eta_0 C \qquad (14)$$

Introducing a new time variable using the following transformation $T = \int_0^t \frac{dt}{f(mt)}$ (Crank, 1975), Equation 12 can be written in terms of the new time (T) variable as:

$$\frac{\partial C}{\partial T} = \frac{\partial C}{\partial X}\left(\psi_0\frac{\partial C}{\partial X} - \varepsilon_0 C\right) - \eta_0 C$$

(15)

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

$$C(X,T) = C_i \quad , \quad X = 0, \quad T > 0$$

(16)

$$-\psi_0\frac{\partial C}{\partial X} - \varepsilon_0 C|_{x=0} = \{\varepsilon_0 C \; if \; 0 < T \le T_0 \qquad (17)$$

$$\frac{\partial C}{\partial X}(X,T) = 0, X \to \infty, T = 0 \qquad (18)$$

Introducing a new dependent variable by the following transformation:

$$C(X,T) = E(X,T)exp\left\{\frac{\varepsilon_0 X}{2\psi_0} - \left(\frac{\varepsilon_0^2}{4\psi_0} + \eta_0\right)\right\}$$

(19)

Equation 16, 17, 18 and 19 reduces to:

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

(20)

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

(21)

$$-\psi_0\frac{\partial E}{\partial X} + \frac{\varepsilon_0}{2}E = \varepsilon_0 C_0 \, exp\,(\alpha T), \;\; X = 0, \;\; 0 < T \le T_0 \qquad (22)$$

Where $\alpha = \sqrt{\left(\frac{\varepsilon_0^2}{4\psi_0} + \eta_0\right)}$

Applying Laplace transform on equation 20, 21, and 22 yields:

$$s\bar{E} = \psi_0\frac{\partial^2\bar{E}}{\partial X^2}$$

(23)

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

(24)

$$-\psi_0\frac{\partial\bar{E}}{\partial X} + \frac{\varepsilon_0}{2}\bar{E} = \frac{\varepsilon_0 C_0}{(s-\alpha)}, \;\; X = 0$$

(25)

The general solution of equation 23 can be written as:

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

(26)

Where $C_1 = C_3 = \frac{\varepsilon_0 C_0}{\sqrt{\psi_0}(s-\alpha)(\sqrt{s}+\beta)}$, $C_2 = \frac{\varepsilon_0 C_i}{(s+\varepsilon_0)\sqrt{\psi_0}(s-\alpha)(\sqrt{s}+\beta)}$, $C_4 = \frac{C_0}{(s+\varepsilon_0)}$, $\beta = \sqrt{\left(\frac{\varepsilon_0{}^2}{4\psi_0}\right)}$. The inverse Laplace transform of equation 26 can be solved term by term after applying the initial and boundary conditions. The first term of equation 26 can be written as:

$$\overline{E_1}(X,s) = \frac{\varepsilon_0 C_0}{\sqrt{\psi_0}(s-\alpha)(\sqrt{s}+\beta)} \exp\left(-X\sqrt{\frac{s}{\psi_0}}\right)$$

(27)

According to Carslaw and Jaeger (1959), the inverse Laplace transform of the first term of equation 27 yields:

$$E(X,T) = \frac{\varepsilon_0 C_0}{2\sqrt{\psi_0}\{\sqrt{\alpha}+\sqrt{(\beta^2\psi_0)}\}} exp\left\{\frac{\{\alpha\sqrt{\psi_0}T - X\alpha\}}{\sqrt{\psi_0}}\right\} erfc\left\{\frac{X-\sqrt{4(\alpha\psi_0)T}}{2\sqrt{(\psi_0 T)}}\right\} + \frac{\varepsilon_0 C_0}{2\sqrt{\psi_0}\{\sqrt{\alpha}+\sqrt{(\beta^2\psi_0)}\}} exp\left\{\frac{\{\sqrt{\alpha}\sqrt{\psi_0}T - X\sqrt{\alpha}\}}{\sqrt{\psi_0}}\right\} erfc\left\{\frac{X+\sqrt{4(\alpha\psi_0)T}}{2\sqrt{(\psi_0 T)}}\right\} + \frac{\varepsilon_0 C_0 \psi_0 \beta}{\sqrt{\psi_0}\{\beta^2\psi_0 - \alpha\}} exp\{\beta X - \beta^2\psi_0 T\} erfc\left\{\frac{X-\psi_0\beta T}{2\sqrt{(\psi_0 T)}}\right\}$$

(28)

The inverse Laplace transform of the second term of equation 26 leads to complex variable in complex domain (Leij *et al.*, 1991; Lindstrom, *et al.*, 1967), therefore $Ci = 0$ for the leaching of nitrate, then second term of equation 60 yields zero (Gardenas *et al.*, 2005; Van Genuchten, 1981. The inverse Laplace transform of the third term of equation 26 is zero on the interval of $0 < t \leq t0$, since as $x \to \infty$, $t0 = 0$ as shown in equation 24 (Abramowitz & Stegun, 1970. According to Carslaw and Jaeger (1959), the inverse Laplace transform of the forth term of equation 26 yields:

$$\overline{E_4}(X,s) = C_0\, exp(-\varepsilon_0 T) \qquad (29)$$

By using transformations 16 and 21, and applying transformation of Crank (1975), on equation 28 and 29 and substituting for α in equation 25, then the inverse Laplace transform of equation 28 can be written in terms of $C(x, T)$ as:

$$C(x,T) = \frac{\varepsilon_0 C_0}{2\sqrt{\psi_0}\left\{\beta+\sqrt{(\beta^2+\eta_0)}\right\}} exp\left\{\frac{\left\{\beta-\sqrt{(\beta^2+\eta_0)}\right\}x}{f(mt)\sqrt{\psi_0}}\right\} erfc\left\{\frac{\frac{x}{f(mt)} - \sqrt{(\varepsilon_0{}^2+4\eta_0\psi_0)T}}{2\sqrt{(\psi_0 T)}}\right\} + \frac{\varepsilon_0 C_0}{2\sqrt{\psi_0}\left\{\beta-\sqrt{(\beta^2+\eta_0)}\right\}} exp\left\{\frac{\left\{\beta+\sqrt{(\beta^2+\eta_0)}\right\}x}{f(mt)\sqrt{\psi_0}}\right\} erfc\left\{\frac{\frac{x}{f(mt)} + \sqrt{(\varepsilon_0{}^2+4\eta_0\psi_0)T}}{2\sqrt{(\psi_0 T)}}\right\} + \frac{\varepsilon_0 C_0}{2\eta_0\psi_0} exp\left\{\frac{\varepsilon_0 x}{\psi_0 f(mt)} - \eta_0 T\right\} erfc\left\{\frac{\frac{x}{f(mt)} + \varepsilon_0 T}{2\sqrt{(\psi_0 T)}}\right\} + C_0 \exp(-\varepsilon_0 T)$$

(30)

By performing back substitution, equation 30 can be written in terms of dimensionless variables in equation 10 as:

$$C(x,t) = \frac{\sigma C_0}{\{\sigma+\upsilon\}} exp\left\{\frac{\{\sigma-\upsilon\}x}{2\omega}\right\} erfc\left\{\frac{\varphi x - \upsilon t}{2\sqrt{(\omega\varphi)}}\right\} + \frac{\sigma C_0}{\{\sigma-\upsilon\}} exp\left\{\frac{\{\sigma+\upsilon\}x}{2\omega}\right\} erfc\left\{\frac{\varphi x + \upsilon t}{2\sqrt{(\omega\varphi)}}\right\} + \frac{\sigma^2 C_0}{2\lambda\psi_0} exp\left\{\frac{\upsilon x}{\omega} - \frac{\lambda t}{\varphi}\right\} erfc\left\{\frac{\varphi x + \sigma t}{2\sqrt{(\varphi\omega t)}}\right\} + C_0\, exp\left(-\frac{\sigma t}{\varphi}\right)$$

(31)

Where: $\upsilon = \sigma\left(1+\frac{4\lambda\omega}{\sigma^2}\right)$. Equation 31 is the analytical solution to the modified advection-dispersion equation which simulates nitrate leaching to groundwater at any given depth x in time t.

III. Numerical Results

In this section numerical simulations showing concentration of nitrate varying soil porosity are illustrated graphically using MATLAB software. The simulation parameters are set to vary within realistic limits for purposes of comparison and analysis. The concentration values of nitrate in soil at different depths are evaluated from the analytical solution described by equation 31 for varying input in a finite domain $0 \leq x \leq 1$ a long longitudinal direction. The unit of distance and time are considered in meters and years respectively. The initial concentration C is considered to be equal $1.0 g/m^3$. The parameter values in table 1 are considered constant and are used in all the simulations.

Parameter Values for Nitrate Leaching to Groundwater

Symbol	Parameter	Value	Source
D	Dispersion coefficient	$85.51 m^2/s$	Raji *et al*., (2014)
u	Flow velocity	$0.424 m/s$	Martinus *et al*., (2013)
R	Retardation factor	1	Martinus *et al*., (2013)
μ	First-order decay	$0.3/day$	Perez Guerrero *et al*., (2013)

Table 1: Parameter values for nitrate leaching to groundwater

An illustration of the concentration of nitrate against time varying soil porosity is shown in figure 1. The figure shows that concentration of nitrate decrease from 1 to almost 0 concentration after some time in all the different range of soil porosity. At a higher soil porosity of 0.6, concentration attains zero faster than when the soil porosity is low 0.1. This shows that soil Porosity affect the rate of leaching of nitrate to groundwater.

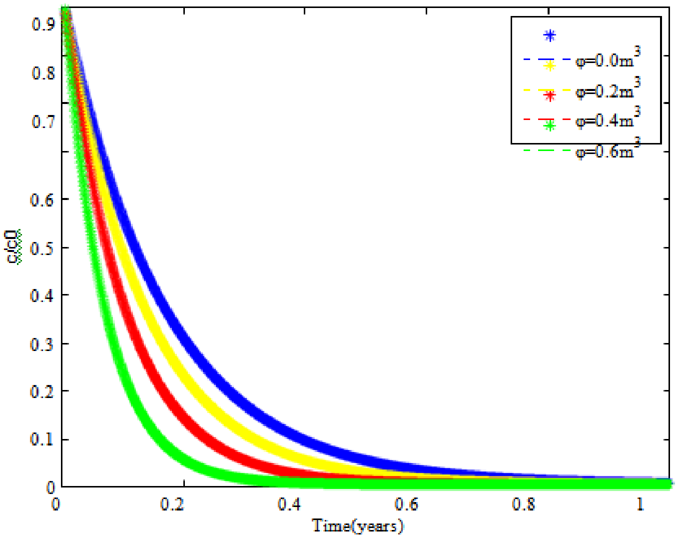

Figure 1: Concentration of nitrate with time varying soil porosity

Figure 2 illustrates concentration of nitrate against soil porosity. From the figure, it is shown that concentration of nitrate increases with increase in soil porosity.

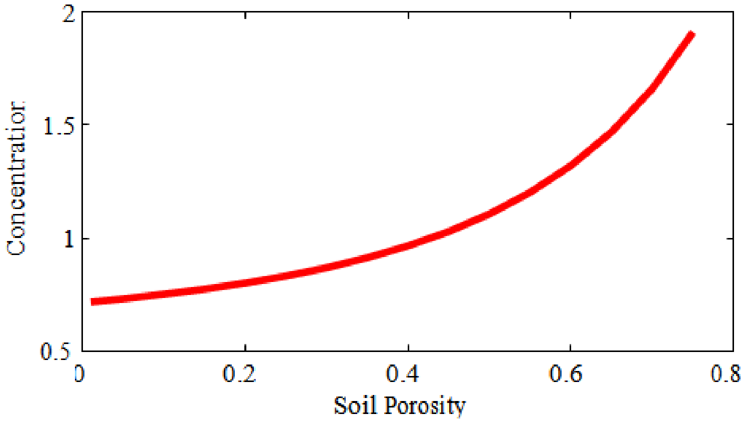

Figure 2: Concentration of nitrate against soil porosity

Figure 3 shows concentration of nitrate against depth varying soil porosity. The figure shows that nitrate concentration decreases with increase in time, the decrease is faster in a higher soil porosity and slower in a lower soil porosity.

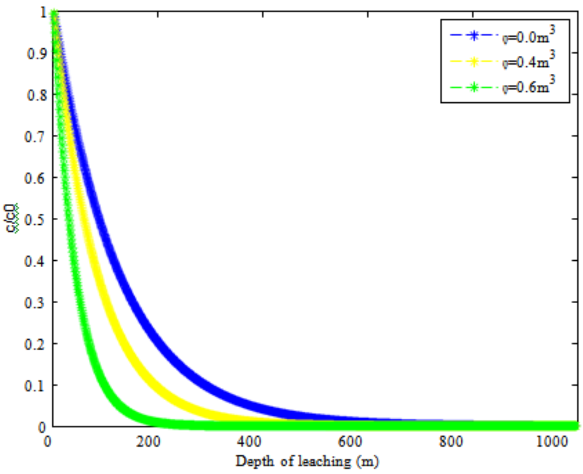

Figure 3: Concentration of nitrate with depth varying soil porosity

IV. Conclusions

This study, principally concerns the modification of the advection-dispersion equation to model nitrate leaching taking into account the impact of soil porosity on nitrate leaching. Figures 1, 2 and 3 illustrate how leaching of nitrate to groundwater depends on soil porosity. From the figures it is clear that leaching of nitrate to groundwater increases with increase in soil porosity. Porous soils have a lower water holding capacity and, therefore, a greater potential to lose nitrate via leaching. Therefore soil porosity affects the rate of water percolation in soil which increases the rate of nitrate leaching to groundwater.

V. Recommendations

This study has demonstrated how soil porosity affects nitrate leaching into groundwater therefore, potential mitigating actions should be put in place to reduce this risk of groundwater pollution which include limiting the amount of nitrogen applied, avoiding over-irrigation, devising a test that enables farmers to measure the amount of nitrogen already in the soil more accurately. 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.

6 Conflicts of interest

There are no conflicts to declare.

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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Jimrise O. Ochwach " Modeling the Impact of Soil Porosity on Nitrate Leaching To Groundwater Using the Advection Dispersion Equation" IOSR Journal of Mathematics (IOSR-JM) 14.4 (2018) PP: 18-26.