

RESEARCH ARTICLE

Numerical simulation of below ground nitrate dynamics in soil columns subjected to reclaimed water

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Abstract: A mathematical model was developed to simulate nitrate mass transport and transformations in soil during continuous application of reclaimed water in a laboratory scale soil column. The coupled material balance equations for both ammonia nitrogen (NH₃-N) and nitrate nitrogen (NO₃-N) within the total soil volume were solved to simulate the NO₃-N concentrations with time along the soil depth. The model is one-dimensional and based on the Galerkin technique of the Finite Element Method. It incorporates convection-dispersion processes of NH₃-N and NO₃-N, nitrification, denitrification and adsorption of ammonium on to soil grains. The adsorption of ammonium was assumed to be represented by the linear form of the Freundlich isotherm. The accuracy and validity of the developed model was examined by comparing simulated data with the experimental data. Optimization of the first order rate constants for nitrification (k₁) and denitrification (k₂) was conducted by varying both k₁ and k₂ within a wide range until the simulated NO₃-N concentrations fitted properly with the corresponding measured values. Optimum k₁ and k₂ were found to be 0.188 d⁻¹ and 0.0248 d⁻¹, respectively. A sensitivity analysis of the kinetics of nitrate dynamics showed that the concentration of belowground nitrate is largely affected by the flow velocity (v), D, k₁ and k₂.

Introduction

Reclaimed water is receiving more attention as a reliable source of water. As a solution for irrigation water scarcity which is a severe problem in the world, reclaimed water can be used with proper engineering practices. However, there are limitations to the extensive use of reclaimed water in irrigation due to the adverse effects on the environment and to public health.

Dayanthi, 2007 describes a soil column experiment which had been conducted to evaluate the nitrate pollution due to the reclaimed water irrigation in Okinawa, Japan. Highly mobile nitrate nitrogen (NO₃-N) can percolate through soil and contaminate the ground water. It causes the deterioration of

ground water quality. Therefore, it is essential to concentrate on nitrogen dynamics in the soil due to the reclaimed water irrigation.

Modeling plays a vital role in estimating the NO₃-N concentration that may result in the ground water. Both analytical and numerical techniques are used to simulate the subsurface transport of chemicals. Though numerical models require a significant database, they are close to actual conditions. To date, a number of researches have been conducted to evaluate belowground nitrate dynamics using laboratory scale soil column experiments followed by mathematical model developments, (McLaren (1969a, 1969b, 1970, 1971), Cho (1971) and Misra et al. (1974). However, there are very few researches in which laboratory soil column studies are coupled with reclaimed water irrigation. In this article, a development of a numerical model using the Galerkin Technique of Finite Element Method to predict the

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nitrate dynamics in the aforementioned soil column experiment conducted by Dayanathi, 2007 is presented. The developed model has been used to estimate the apparent rate constants for the nitrification and denitrification. A sensitivity analysis has been carried out to investigate the degrees of contribution of several parameters on nitrate dynamics in the model.

Materials and Methods

Data Collection

The role of a database is vital since the target is to develop a numerical model for nitrogen dynamics in soil. Experimental data of the soil column

experiments conducted by Dayanathi (2007) were collected. Fig. 1 is the schematic diagram of the laboratory scale soil column.

The column has been filled with limestone up to 85 cm height. It has been continuously irrigated with simulated reclaimed water at an application rate of 11mL/h. Secondary treated wastewater prior to chlorination has been used to prepare the simulated reclaimed water. Anhydrous ammonium chloride (NH₄Cl) has been added to increase NH₃-N concentration to approximately 18 mg/L. The duration of the experimental run of the column with limestone has been 150 days. The collected data contain NH₃-N and NO₃--N concentrations at several depths of the soil column. The parameters in Table 1 were extracted from Dayanathi (2007).

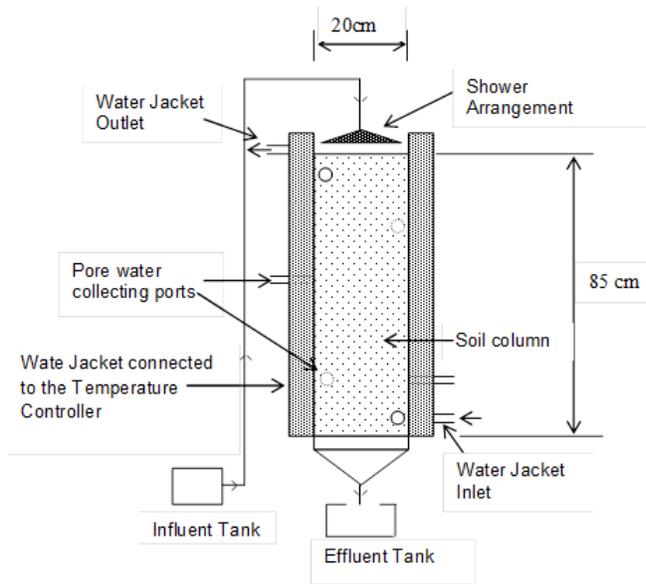


Fig. 1 Schematic Diagram of the Laboratory Scale Soil Column

Table 1: Required Parameters for the Model Development

Parameters	Value	Reference
D_1 and D_2	1.4 cm ² /d	Odenchantz et.al. (1990)
K_d	2 cm ³ /g	Gusman et.al. (1999)
θ	0.62	Measured (Dayanathi, 2007)
θ_w	0.375	Measured (Dayanathi, 2007)

ρ_b	1.378 g/cm ³	Measured(Dayanthi, 2007)
R	3.79	Calculated(Dayanthi, 2007)
v	2.033 cm/d	Calculated using average effluent rate(Dayanthi, 2007)
C_1^0	18 mg/L	Measured(Dayanthi, 2007)
C_2^0	3 mg/L	Measured(Dayanthi, 2007)

Model Development

Contaminant transport in porous media is influenced by advection, molecular diffusion, hydrodynamic dispersion, sorption and transformation processes (Nazaroff et al., 2001). When the sorption of NH₄⁺ is interpreted by the linear form of Freundlich isotherm and first order kinetics are assumed for both nitrification and denitrification, the material balance equations for NH₃-N and NO₃--N that incorporate the advection, dispersion, sorption and transformation can be given by equations Eq. (1) and Eq. (2), respectively (Dayanthy, 2007).

Where,

C1 - Concentration of NH₃-N (mg/L)

C2 - Concentration of NO₃--N (mg/L)

D1, D2 - Apparent molecular diffusion coefficient for NH₄⁺ & NO₃⁻ (cm²/d)

k1, k2 - First order rate constant of nitrification & denitrification (d⁻¹)

R - Retardation factor

v - Interstitial pore water velocity (cm/d)

x -Length along the soil column (cm)

t -Time (d)

Numerical solutions (concentrations of NH₃-N and NO₃--N) for Eq. (1) and Eq. (2) were obtained by using the weighted residual method of Galerkin technique of the Finite Element Method (Leon et. al., 1999). The dependent variable C (= C1, C2) was approximated by a finite series of the form of Eq. (3), where C_j are the nodal values of independent

variables at time t and Φ_j are the shape functions. N is the number of nodes in the solution domain. Since this approximated series do not give the exact solutions, it results a residual, R'. By substituting into Eq. (1) and Eq. (2), R' can be obtained. It should be minimized to obtain accurate results. It can be done by introducing weighting functions orthogonal to R' as indicated by Eq. (4),

where Φ_i are the weighting functions. The Galerkin method results when the weighting function is chosen to be the shape function as defined in Eq. (3). Then R' was obtained by substituting Eq. (3) into Eq. (1) or (2), to be orthogonal to the selected weighted functions. Eq. (5) and (6) result when Eq. (1) and (2) are incorporated into Eq. (4).

Time derivative was approximated by the backward difference time approximation method. Then the final solutions were obtained from an equation similar to the form of Eq. (7). Here, C_{t+1} represents the concentration of NH₃-N and NO₃--N at a particular depth at time t+1.

This equation was solved with the support of Matlab 7.0 software (The MathWorks Inc., Natick, MA). The model was calibrated in terms of k1 and k2, by applying it to the experimental results of the soil column. Transient and steady state NO₃--N concentrations at depths, 15 cm, 35 cm, 45 cm, 55 cm and 85 cm, were computed for each 0.01 d⁻¹ increment of k1 from 0.01 to 0.7 d⁻¹ and k2 from 0.001-0.1 d⁻¹. Then, the optimum k1 and k2 were obtained for each depth using the sum of squares of error between each estimated and measured NO₃--N concentration. When applying the model to optimize the rate constants at each depth, it was considered that the control volume was from the soil surface to each depth. Then, the optimized k1 and k2 per each depth were averaged out.

In order to investigate the degree of contribution of each input parameter in the model, a sensitivity analysis was carried out for D , v , k_1 and k_2 . The range, for which each parameter was varied,

Results

Evaluation of the Model

The average k_1 and k_2 in the soil column were 0.188d^{-1} and 0.0248d^{-1} . Fig. 2 shows the variation of both the measured and simulated $\text{NO}_3\text{-N}$ concentrations vs. time for the depths 15 cm, 35 cm, 45 cm, 55 cm and 85 cm. The simulated $\text{NO}_3\text{-N}$ concentrations correlate well with the measured values at the depths of 15 cm, 35 cm, 45 cm and 55 cm. The correlation coefficients between measured and simulated data for the depths of 35 cm, 45 cm and 55 cm were more than 0.7. In the case of 85 cm depth, the simulated values underestimate the measured values. This may have been caused by a variety of factors. In deriving model equations, the physical and biochemical factors and interrelations that cause nitrogen dynamics were made concise to a few processes and the linear form of variations. However, the nitrogen dynamics depend on many more factors than those considered for this model.

Conclusion

Modelling nitrate dynamics using laboratory scale soil columns may help investigate the precautionary measures to prevent nitrate pollution due to the reclaimed water irrigation. In this study, the Galerkin technique of the Finite Element Method was used to simulate nitrate dynamics in a soil column

The developed model can predict nitrate concentration in the ground below with some limitations. Therefore, it is possible to use it as a decision making tool to prevent ground water pollution by nitrates due to the application of not only reclaimed water but also any other influent. Using the developed model, precautionary measures such as altering the rate and frequency of irrigation, and degree of pre treatment for reclaimed water, can be decided.

In this study, microbial transformation processes were represented by first order kinetics. However it

depended on the existing range as well as the applicability of the value in the model so that the model did not compute indefinite answers.

Further, these interrelations are normally non-linear. Therefore, linearization of these non-linear interrelations may have affected the model-output significantly.

Sensitivity Analysis

Fig.3 shows the sensitivity of the model parameters such as D , v , k_1 and k_2 . Fig. 3a indicates that the time for the steady state to occur and the peak $\text{NO}_3\text{-N}$ concentration decrease with the increase of the interstitial flow velocity. This behavior can be verified by the actual condition that high flow velocities let less time for a complete nitrification to take place, resulting less peak $\text{NO}_3\text{-N}$ concentration. According to Fig. 3b, when k_1 is varied from $0.03\text{-}0.15\text{d}^{-1}$, $\text{NO}_3\text{-N}$ concentration increases. On the contrary, variation of k_2 from $0.001\text{-}0.05\text{d}^{-1}$ decreases $\text{NO}_3\text{-N}$ concentration (Fig. 3c). In reality, nitrification increases the $\text{NO}_3\text{-N}$ concentration while denitrification decreases it. Therefore, there is a great correlation between the simulated data and actual conditions.

continuously irrigated with reclaimed water for 150 days. The average nitrification and denitrification rate constants were 0.188d^{-1} and 0.0248d^{-1} , respectively. A sensitivity analysis on the model parameters showed that the concentration of belowground nitrate is largely affected by the flow velocity, the diffusion coefficient, and nitrification and denitrification rate constants.

may vary with reality. In addition, adsorption of ammonium was represented by means of the linear form of the Freundlich isotherm. If it is possible to incorporate these by non linear interrelations, it may give better predictions. Further, the numerical calculations were based on linear shape functions. Applying non-linear shape functions may improve the predictability of the model. Therefore, as further studies, it is suggested to consider non-linear kinetics for microbial transformations and ammonium adsorption with non-linear shape functions in the numerical calculations.

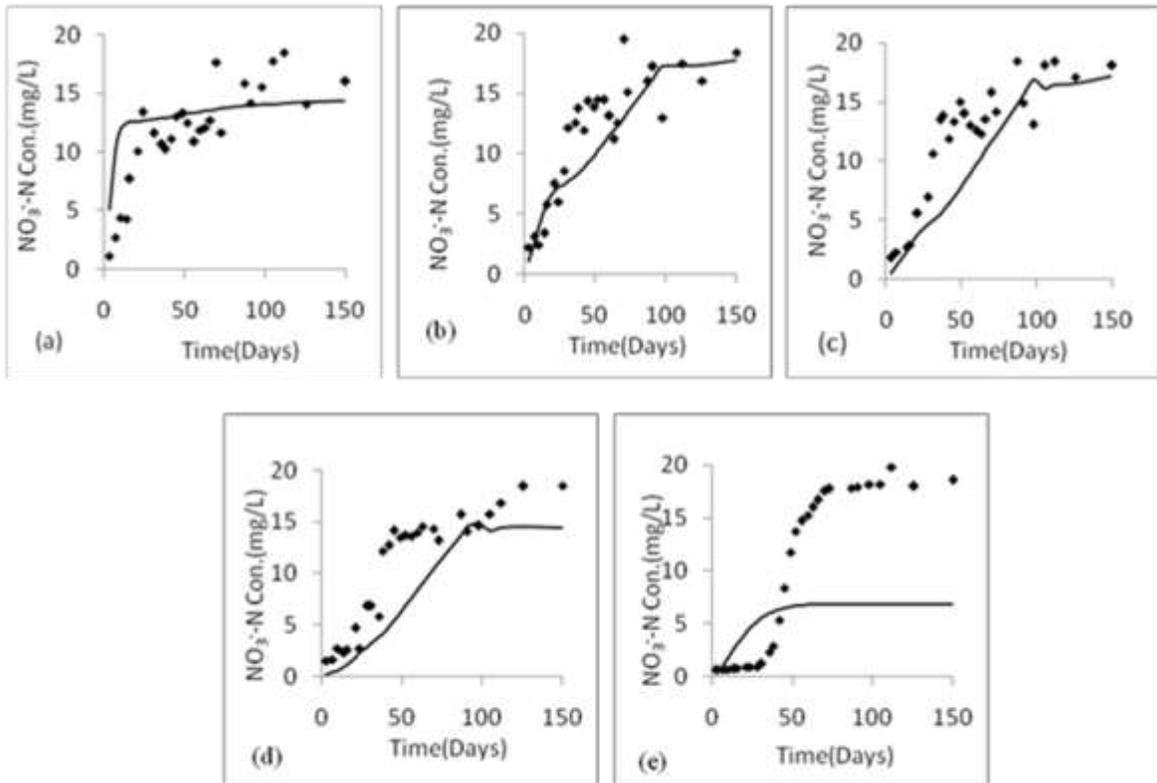


Fig. 2 The Graphs of Modeled (lines) and Measured (Diamond) NO_3-N Concentrations at Depths of (a) 15cm, (b) 35cm, (c) 45cm, (d) 55cm, and (e) 85cm with Time

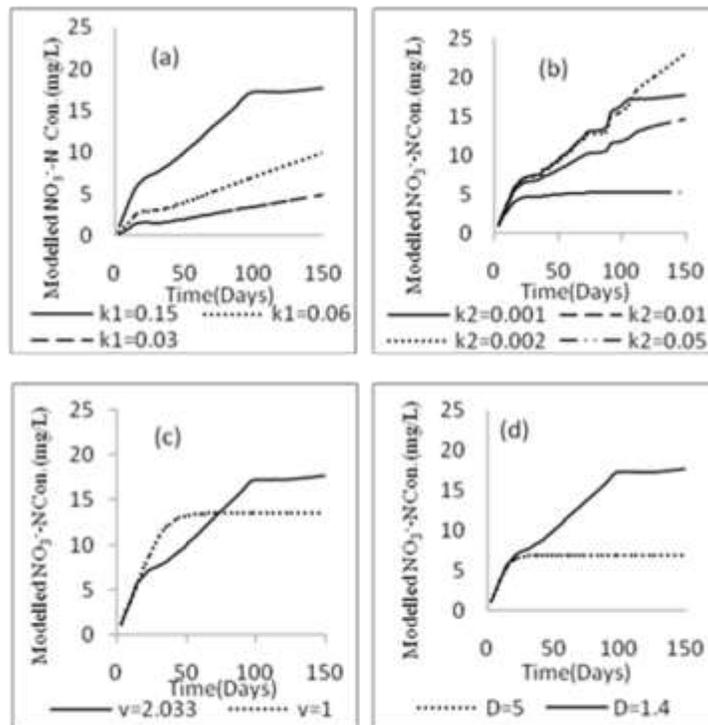


Fig. 3 Sensitivity Analysis on the Developed Model (a) k_1 (b) k_2 (c) v (d) D

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