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Simulation of Water and Nitrogen Dynamics in Soils During Wastewater Applications by Using a Finite-Element Model

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Abstract. A mathematical model was developed to simulate water movement, mass transport, and nitrogen transformations in soils during wastewater applications. The model is one-dimensional and based on the Galerkin finite-element method. The submodel of mass transport of nitrogen incorporates the convection-dispersion processes of ammonium and nitrate nitrogen, nitrification, denitrification, ammonium exchange and uptake of ammonium and nitrate ions. The accuracy and validity of the proposed model was examined by comparison with an explicit-implicit finite-difference model results. The model was used for simulation of water and nitrogen dynamics during wastewater application in homogeneous and multi-layered soils under different N concentration, rate, duration and scheduling of application.

Key words. Land treatment, water flow, nitrogen transport, mathematical model, finite elements method, unsaturated-saturated conditions.

1. Introduction

Application of sewage water to land is a good method of preventing pollution of water resources and also enables wastewater to be reused. Sewage water applied to land can be used immediately for crop production, it can be renovated by infiltration and movement in the soil and it can cause groundwater and surface water contamination.

Nitrogen is one of the main nutrients contributing to eutrophication of surface water and when excess nitrogen reaches the groundwater and surface impoundments, it can be a health and water quality hazard. The nitrogen load of wastewater can be eliminated by the application to land, where a significant part of the nitrogen is removed by the nitrification, denitrification, and root uptake processes. The extent of this removal is affected by numerous physical, chemical, and biological processes in the soil and by the dynamic state of the soil moisture.

A method of application of wastewater to land is the low-rate or irrigation system. With the low-rate systems, the application of wastewater takes place by irrigation of land where crops are grown. Water and nitrogen are taken up by plant roots to satisfy growth needs and removed from the field in the harvested plant material

(Lance, 1975). Denitrification is another significant mechanism of nitrogen removal during the anaerobic periods of wetting.

Knowledge of nitrogen mass transport and transformations in soils, when nitrogen is applied by fertilizer or by wastewater, nitrogen, or organic, is obtained by mathematical modeling and computer simulation (Tanji, 1982). Many nitrogen simulation models have been developed during recent years (Gureghian *et al.*, 1979; Johnsson *et al.*, 1987; Kaluarachchi and Parker, 1988; Lotse *et al.*, 1992. Few papers, however, have tried to develop models describing nitrogen transport and transformations in soil from the viewpoint of land treatment of wastewater. Selim and Iskandar (1981) presented such a model based on the finite difference method and validated the model for slow infiltration. The mathematical models significantly improve the quantitative understanding of nitrogen cycling processes and can be valuable tools in designing environmentally and economically sustainable land treatment systems.

In this paper, a mathematical model is developed to simulate water movement, mass transport and nitrogen transformations in variably saturated soils under transient flow conditions. The model is one-dimensional and is based on the Galerkin finite-element method. It is used for simulation of water and nitrogen dynamics during nitrogen content wastewater application in homogeneous and multi-layered soils under different ammonium concentrations in wastewater, rate, duration, and scheduling of application.

2. Model Description

2.1. WATER FLOW IN VARIABLY SATURATED SOIL

The one-dimensional vertical flow of water in variably saturated porous media with water uptake by plant roots is described by the equation

$$L_w(h) = \frac{\partial}{\partial z}\left(K\frac{\partial h}{\partial z} - K\right) - C_h\frac{\partial h}{\partial t} + Sw = 0\,, \tag{1}$$

where h is the pressure head, K is the hydraulic conductivity, C_h is the specific moisture capacity, Sw is the sink term for root water extraction, z is the vertical coordinate (positive down), and t is the time. In the present mathematical model the macroscopic approach of water uptake by plants is described by the Molz and Remson (1970) model, as modified by Selim and Iskandar (1981). This model is represented as

$$Sw(z,h) = T\,R(z)\,K(h)\,/\int_0^d R(z)\,K(h)\,\mathrm{d}z\,, \tag{2}$$

where d is the maximum depth of root zone in the soil, T is the evapotranspiration rate per unit area of soil surface, and $R(z)$ is the root distribution as a function of depth in the soil profile. The model was successfully used when high soil water contents (low suctions) were maintained in the soil root zone, such as in land treatment-slow infiltration systems.

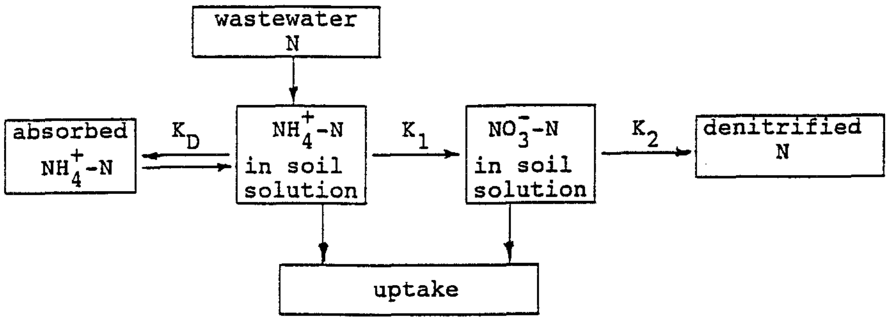

Fig. 1. The simplified model of nitrogen transformations in the soil.

2.2. SOIL NITROGEN TRANSPORT AND TRANSFORMATIONS

The main chemical and biological reactions of nitrogen transformation in the soil when sewage effluent is applied are nitrification, denitrification, uptake of ammonium and nitrate by plants, and adsorption of NH_4–N on the soil cation exchange sites (Antonopoulos, 1991) (Figure 1).

The one-dimensional vertical mass transport and transformations of NH_4–N and NO_3–N under transient flow and variably saturated soil conditions, are described by the equations.

$$L_A(C) = \frac{\partial \Theta C}{\partial t} + \frac{\partial \rho S}{\partial t} - \frac{\partial}{\partial z}\left(\Theta D \frac{\partial C}{\partial z}\right) + \frac{\partial q C}{\partial z} + \Phi_1 - Q_{am} = 0\,, \tag{3}$$

$$L_N(Y) = \frac{\partial \Theta Y}{\partial t} - \frac{\partial}{\partial z}\left(\Theta D \frac{\partial Y}{\partial z}\right) + \frac{\partial q Y}{\partial z} + \Phi_2 - Q_{ni} = 0\,, \tag{4}$$

where C and Y are the concentrations of NH_4–N and NO_3–N in the soil solution, respectively, D is the dispersion coefficient, Θ is the volumetric moisture content, q is the Darcy velocity, ρ is the bulk density, S is the amount of NH_4–N in the absorbed phase per unit mass of soil, Φ_i are the rates of NH_4–N and NO_3–N transformations per unit soil volume and Q_{am} and Q_{ni} are the rates of plant uptake of NH_4–N and NO_3–N per unit soil volume, respectively.

The transformation terms Φ_i describe the nitrification of NH_4–N and the denitrification of NO_3–N which are approached by first-order kinetic-type reactions

$$\Phi_1 = -K_1 \Theta C\,, \tag{5}$$

$$\Phi_2 = K_1 \Theta C - K_2 \Theta Y\,. \tag{6}$$

The rate coefficients K_1 and K_2 are considered as variables dependent upon environmental and other factors such as temperature, pH and aeration (Selim and Iskandar, 1981). In order to incorporate these factors, the coefficients are expressed as

$$K_i = k_i f_i , \tag{7}$$

where k_i is considered constant and represents the maximum value and f_i is an empirical function. For the nitrification rate K_1, the function f_1 is expressed as a function of the pressure head, while the denitrification function f_2 is considered as a function of the degree of water saturation in the soil.

The adsorption of NH_4-N is considered instantaneous and reversible with equilibrium defined by a linear Freundlich type isotherm of the form

$$S = K_D C , \tag{8}$$

where K_D is the distribution coefficient for the reaction.

The plant uptake terms Q_{am} and Q_{ni} are described by a macroscopic model, in which the Michaelis–Menten approach is used to determine the rate of N uptake as a function of root density and concentration of ammonium and nitrate in the soil solution

$$Q_{am} = I_{\max} R(z, t)\, C / [K_m + C + Y] , \tag{9}$$

$$Q_{ni} = I_{\max} R(z, t)\, Y / [K_m + C + Y] , \tag{10}$$

where $I_{\max}$ is the maximum rate of N uptake per unit root length and K_m is the Michaelis constant which represents the concentration of N at $0.5 I_{\max}$.

Initial and boundary conditions for Equations (1), (3) and (4) are

$$h = h_i(z), \quad C = C_i(z) \quad \text{and} \quad Y = Y_i(z) \quad \text{at} \quad z \geqslant 0 \text{ for } t = 0 , \tag{11a}$$

$$q_0 = -K\frac{\partial h}{\partial z} + K \quad \text{or} \quad q_0 = 0 \quad \text{in } z = 0 , \tag{11b}$$

$$J_{in} = q_0 C_0 - \Theta D\frac{\partial C}{\partial z} \quad \text{or} \quad J_{in} = 0 \quad \text{in } z = 0 , \tag{11c}$$

$$\partial C/\partial z = 0 \quad \text{and} \quad \partial Y/\partial z = 0 \quad \text{in} \quad z = d , \tag{11d}$$

where C_0 is the applied concentration of NH_4-N, h_i, C_i, Y_i are the initial distributions of the pressure head and NH_4-N and NO_3-N concentrations, respectively.

3. Numerical Solutions by the Finite Element Method

In the finite element approach, the dependent variable y (= h, C, Y) is approximated by a finite series of the form

$$y(z, t) \approx \hat{y}(z, t) = \sum_{j=1}^{n} \Phi_j(z) y_j(t) \tag{12}$$

where Φ_j are the shape functions, y_j are the nodal values of dependent variables at time t, and n is the number of nodes in the solution domain.

The Galerkin approach requires that the residual $L(\hat{y})$, obtained by substituting

Equation (12) into (1) or (3) or (4), be orthogonal to the selected weighting functions:

$$\int_0^d L(\hat{y})N_i(z)\,\mathrm{d}z = 0 \quad (i = 1,2,3\ldots,n)\,. \tag{13}$$

where N_i are the weighting functions and d the soil depth.

Substitution of the approximation (12), respectively, into Equations (1) or (3) or (4), application of the Galerkin principle (Equation (13)), using Green's theorem to remove the second derivatives and applying integration by parts to the spatial derivatives, leads to:

$$[A_{ij}]\{y_j\} + [\mathrm{B}_{ij}]\left\{\frac{\mathrm{d}y_j}{\mathrm{d}t}\right\} = \{F_i\}\,, \tag{14}$$

where, in the case of water flow

$$[A_{ij}] = \sum_e \int_e K\frac{\mathrm{d}\Phi_j}{\mathrm{d}z}\,\frac{\mathrm{d}N_i}{\mathrm{d}z}\,\mathrm{d}z\,, \tag{15a}$$

$$[B_{ij}] = \sum_e \int_e C_h\Phi_j N_i\,\mathrm{d}z\,, \tag{15b}$$

$$\{F_i\} = q_0 - q_d + \sum_e \int_e K\frac{\mathrm{d}N_i}{\mathrm{d}z}\,\mathrm{d}z + \sum_e \int_e SwN_i\,\mathrm{d}z\,. \tag{15c}$$

In the case of equation of NH_4–N transport

$$[A_{ij}] = \sum_e \left\{\int_e \Theta D\frac{\mathrm{d}\Phi_j}{\mathrm{d}z}\,\frac{\mathrm{d}N_i}{\mathrm{d}z}\,\mathrm{d}z + \int_e q\frac{\mathrm{d}\Phi_j}{\mathrm{d}z}\,N_i\,\mathrm{d}z + \int_e \frac{\mathrm{d}q}{\mathrm{d}z}\Phi_j N_i\,\mathrm{d}z + \right.$$

$$\left. + \int_e K_1\Theta\,\Phi_j N_i\,\mathrm{d}z + \int_e R\frac{\mathrm{d}\Theta}{\mathrm{d}t}\,\Phi_j N_i\,\mathrm{d}z\right\}\,, \tag{16a}$$

$$[B_{ij}] = \sum_e \int_e R\Theta\Phi_j N_i\,\mathrm{d}z\,, \tag{16b}$$

$$\{F_i\} = q_d C_d - J_{Cd} - q_0 C_0 + J_{C_0} - \sum_e \int_e Q_{am} N_i\,\mathrm{d}z\,, \tag{16c}$$

and R is the retardation factor (= $1 + \rho K_D/\Theta$) and, in the case of the equation of NO_3–N transport,

$$[A_{ij}] = \sum_e \left\{\int_e \Theta D\frac{\mathrm{d}\Phi_j}{\mathrm{d}z}\,\frac{\mathrm{d}N_i}{\mathrm{d}z}\,\mathrm{d}z + \int_e q\frac{\mathrm{d}\Phi_j}{\mathrm{d}z}\,N_i\,\mathrm{d}z + \int_e \frac{\mathrm{d}q}{\mathrm{d}z}\Phi_j N_i\,\mathrm{d}z + \right.$$

$$\left. + \int_e K_2\Theta\,\Phi_j N_i\,\mathrm{d}z + \int_e \frac{\mathrm{d}\Theta}{\mathrm{d}t}\,\Phi_j N_i\,\mathrm{d}z\right\}\,, \tag{17a}$$

$$[B_{ij}] = \sum_e \int_e \Theta\Phi_j N_i \, dz \, , \tag{17b}$$

$$\{F_i\} = q_d Y_d - J_{Yd} - q_0 Y_0 + J_{Y_0} + \sum_e \left\{ \int_e K_1 \Theta C \Phi_j N_i \, dz - \int_e Q_{ni} N_i \, dz \right\} . \tag{17c}$$

To evaluate the integrals in coefficient matrices (Equations (15), (16) and (17)) the nonlinear coefficients Θ, D, C_h, K, K_1, K_2, R, and q are approached in terms of the shape functions and the values of coefficients at the nodes, by equations similar to Equation (12) (Antonopoulos and Papazafiriou, 1990).

The time derivatives in Equation (14) are approximated by a simple finite-difference scheme, using the following approximation

$$\{dy/dt\}^{t+\Delta t/2} = \{y^{t+\Delta t} - y^t\}/\Delta t \tag{18}$$

and the dependent variables as

$$\{y\}^{t+\Delta t/2} = \omega\{y\}^{t+\Delta t} + (1-\omega)\{y\}^t \, , \tag{19}$$

where Δt is the time step and ω is a temporal weighting factor ($0 \leqslant \omega \leqslant 1$). When $\omega = 0.5$, a Crank–Nicolson scheme is obtained. By defining the matrix Equation (14) at the half-time level ($t + \Delta t/2$) and using Equations (18) and (19), the following set of equations is obtained:

$$[P_{ij}]^{t+\Delta t/2} \{y_j\}^{t+\Delta t} = [Q_{ij}]^{t+\Delta t/2} \{y_j\}^t + \{F_i\}^{t+\Delta t/2} \, , \tag{20}$$

where

$$[P_{ij}] = \omega[A_{ij}] + \frac{1}{\Delta t}[B_{ij}] \, , \tag{21a}$$

$$[Q_{ij}] = (\omega-1)[A_{ij}] + \frac{1}{\Delta t}[B_{ij}] \, . \tag{21a}$$

The results of these substitutions are three systems of linear algebraic equations which have tridiagonal matrices of unknowns. The system describing the flow of water is solved first. The obtained values of pressure head $h(z, t)$ are used to compute $\Theta(z, t)$, $q(z, t)$ and $D(z, t)$, which appear in the systems describing the mass transport of NH_4–N and NO_3–N. Then the system of NH_4–N transport is solved for the desired $C(z, t)$ and finally the system of NO_3–N transport.

4. Results and Discussion

The mathematical model is applied to simulate water, NH_4–N and NO_3–N during nitrogen wastewater application in homogeneous and multilayered soils.

The following applications of the mathematical model presented here are based on the experimental data of Selim and Iskandar (1981). In all the cases studied, nitrogen content wastewater was applied to a homogeneous and a three layered sandy loam soils, under different concentration of NH_4–N in the applied wastewater, duration of application, rate of application and wastewater application cycle.

The physical and chemical properties of these soils are given by Selim and Iskandar (1981). The Θ, h and K relationships for the soil are

$$\Theta(h) = \Theta_s/[1 + (-h/\alpha)^b] , \tag{21a}$$

$$K(\Theta) = \eta \exp (\lambda\Theta) . \tag{21b}$$

The values of constants in Equations (21a, b) for each layer of layered soil, respectively, are 0.44, 0.42, and 0.34 cm^3/cm^3 for the Θ_s, 100, 40, and 30 for the α, 1, 1 and 1 for the b, 9.6×10^{-4}, 2.2×10^{-4} and 2.1×10^{-4} for the η and 27.63, 30.7 and 38.87 for the λ. The bulk density values are: 1.41, 1.59 and 1.55 g/cm^3, respectively.

The parameters of kinetic reactions of nitrogen transformations were considered similar for all applications and the values were: $K_D = 0.25$ cm^3/g, $K_m = 1.0$ ppm, $I_{max} = 0.001$ μg N/h cm, $k_1 = 0.1$ and $k_2 = 0.01$ h^{-1}. The rate coefficients for nitrification and denitrification are considered as functions of pressure head ($K_1 = f(h)k_1$) and degree of water saturation ($K_2 = f(\Theta/\Theta_s)k_2$), respectively.

A two-year-old mixture of reed canary-grass and tall fescue was grown on the soil, which had a constant evapotranspiration rate of 0.25 cm/day, for a short period of one month and the root distribution function is

$$R(z, t) = 226 \exp(-0.1z) . \tag{22}$$

Table I shows the values of the variables that change at each application.

In the first application, the accuracy of the model was assessed by comparison of the results with the finite difference solution of Selim and Iskandar (1981) model. The values of parameter of wastewater application used, were those of case 1 in Table I.

Figure 2 shows the distribution of water content, NH_4–N and NO_3–N respectively, for the first week following the application of 5 cm of wastewater. Water content and NH_4–N distributions predicted by the finite element model are almost identical to those of the finite difference model. The results of NO_3–N distributions, however, are not in close agreement with those of the finite difference model. The NO_3–N

Table I.

Case	Applications				
	Rate q (cm/h)	Duration ta (h)	Depth d (cm)	Concentration C_{am} ($\mu g/cm^3$)	Schedule Ta (days)
1	0.5	10	5	25	7
2	0.5	10	5	50	7
3	0.5	15	7.5	25	7
4	0.5	10	5	25	10
5	1.0	10	10	25	7

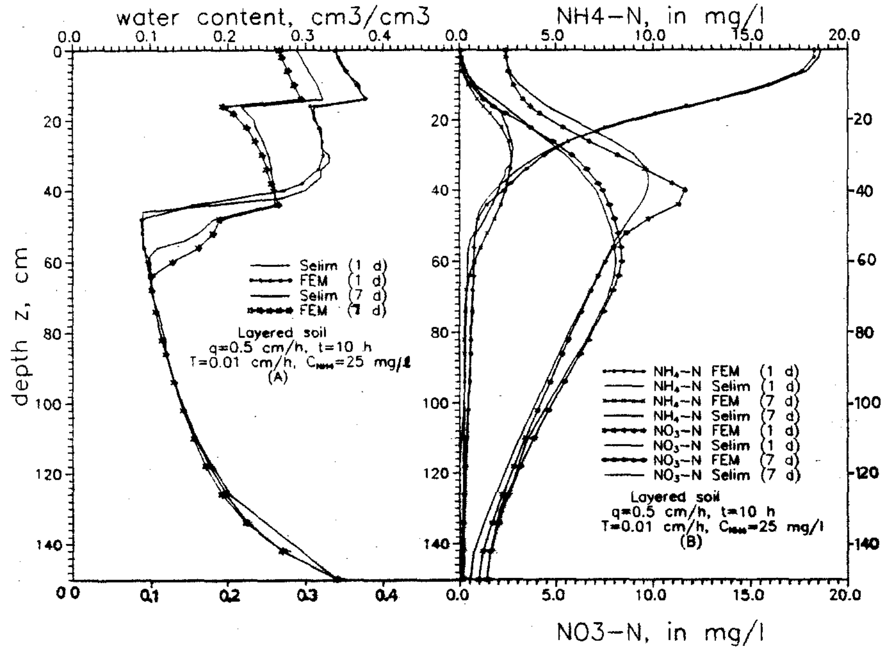

Fig. 2. Comparison results between finite difference and finite element models, (A) water content, (B) NH_4-N and (C) NO_3-N in the layered soil for the first week following wastewater application.

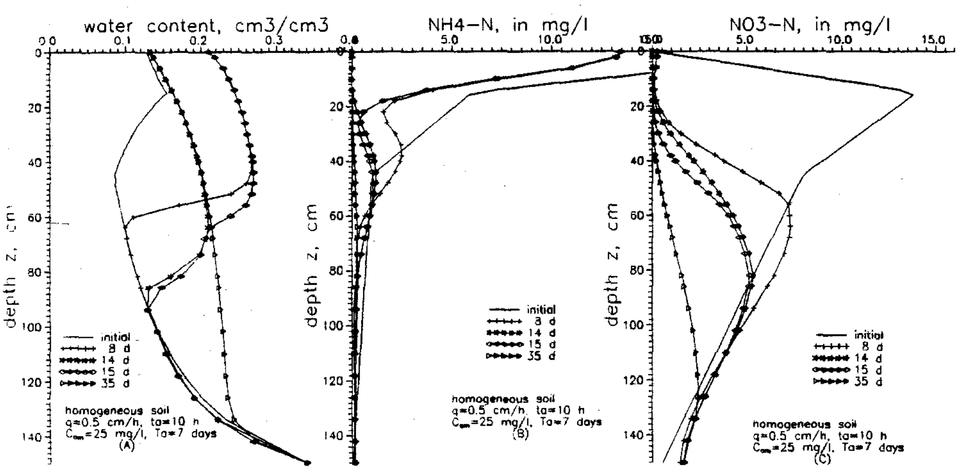

Fig. 3. Distribution of (A) water content, (B) NH_4-N and (C) NO_3-N in the homogeneous soil following weekly wastewater applications.

distribution on the first day presents a peak identical to that of the initial distribution, while the distribution of finite difference is more dispersed.

Figure 3 shows the distributions of water content, NH_4-N and NO_3-N in the homogeneous soil and Figure 4 in the layered soil for the values of wastewater application of case 1 (Table I), before and after the weekly wastewater applications.

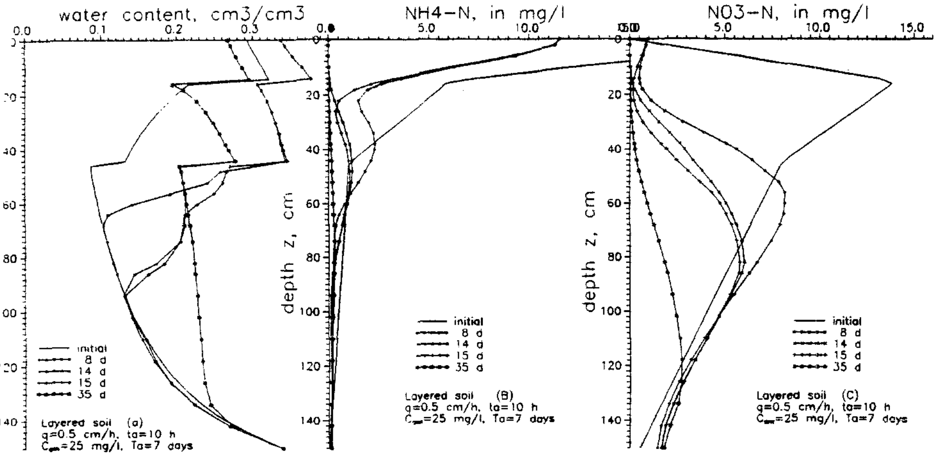

Fig. 4. Distribution of (A) water content, (B) NH_4-N and (C) NO_3-N in the layered soil following weekly wastewater applications.

This case of application is considered the base case for comparison to the other cases of wastewater application. The results show different distributions of water, NH_4-N and NO_3-N in the two soils. The distributions of water content and NH_4-N in the upper layers were the same after and before each irrigation, while the NO_3-N distribution has shown a deeper movement of profiles and a decrease in the maximum concentration.

Figure 5 shows the total mass of water content, NH_4-N in soil solution and solid phase, and NO_3-N in soil solution during the simulation period of the first case of application. This figure shows that the total water content in the soil profile increased after wastewater application and decreased during redistribution and evapotranspiration. The mean total mass of water content and NH_4-N in the soil solution is approximately the same between successive wastewater applications but the total mass of NO_3-N is continuously decreasing.

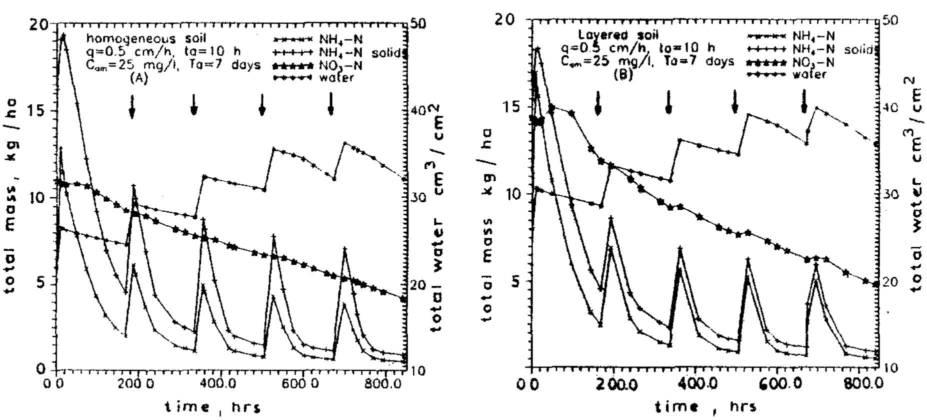

Fig. 5. Total water content, NH_4-N in soil solution and solid phase and NO_3-N in the soil solution with time in (A) the homogeneous and (B) the layered soils for the 1st application case.

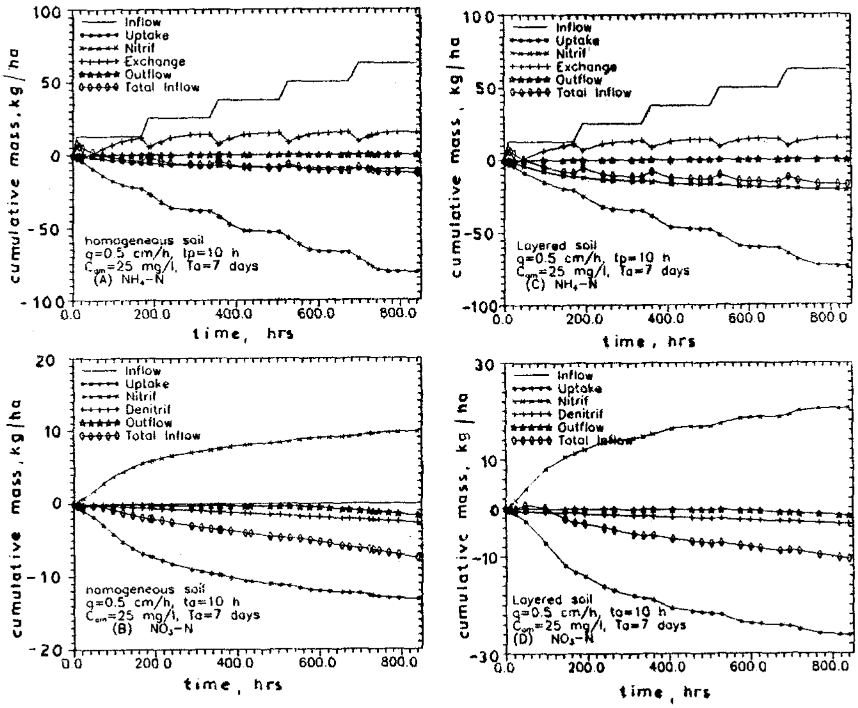

Fig. 6. Cumulative mass of inflow, uptake, nitrification, denitrification, exchanged, outflow and inflow balance for NH_4-N and NO_3-N with time during 5 weeks in the homogeneous (A and B) and the layered (C and D) soils.

Figure 6 shows the cumulative mass of NH_4-N inflow, NH_4-N and NO_3-N uptake, NH_4-N nitrification, NO_3-N denitrification, NH_4-N and NO_3-N outflow and the total mass inflow of NH_4-N and NO_3-N in the two soils, respectively. Simulated results show that NH_4-N uptake was much greater than that of NO_3-N on all times. This is due to the low concentration of NO_3-N in the top portion of soil profile as shown in Figures 3c and 4c, because of their leaching. The cumulative mass of NO_3-N denitrification was much more lower than that of NH_4-N nitrification. The NH_4-N and NO_3-N uptake and denitrification were the main processes of N removal from the soil system. The leachate cumulative mass of NH_4-N and NO_3-N was non-significant for the simulative period. From the fluctuation of cumulative inflow mass, it is shown that in the two soils a mass deficit is created after the second irrigation, it seldom remains constant for the NH_4-N and it increases slowly for the NO_3-N.

The effects of double concentration in applied wastewater (case 2), greater duration of application (case 3), different schedule of wastewater application (case 4) and wastewater application rate (case 5) on nitrification, denitrification, uptake, recharge and leaching to groundwater, are shown in Figures 7 to 10 for the homogeneous and the layered soils.

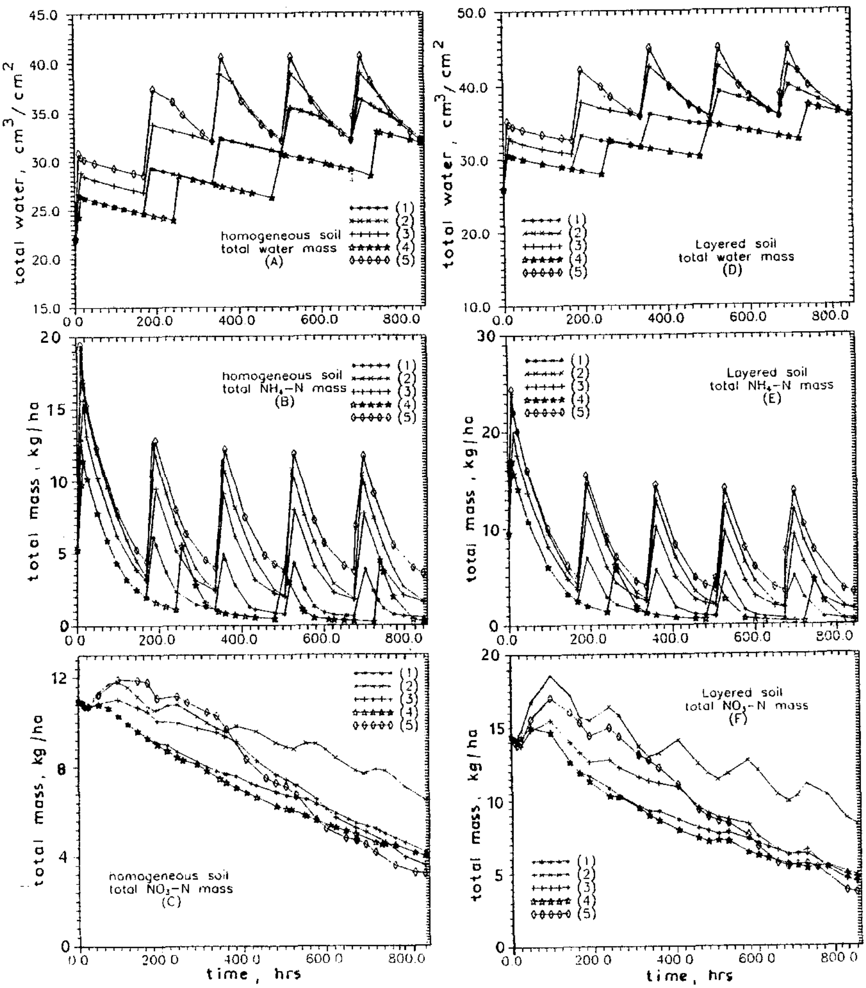

Fig. 7. Comparison of total water, NH_4-N and NO_3-N mass in soil solution during 5 weeks period for the five cases of applications.

Increasing NH_4-N applied mass (case 2) has the effect of increasing NH_4-N in the soil profile and consequently the NO_3-N mass as result of ammonia nitrification. In case 5, however, when the applied mass of NH_4-N is the same to that of case 2, the mass of NO_3-N in the soil decreases rapidly due to greater leaching of NH_4-N and NO_3-N (Figures 7C and F). In all application cases there is a trend of the mean mass of water in soil to increase between applications, of the NH_4-N in the soil solution to become constant and of the mean total mass of NO_3-N to decrease. The last decreases rapidly in the third and fifth cases, when the leaching rates are greater.

The cumulative NH_4-N uptake increases with the total applied mass of ammonia

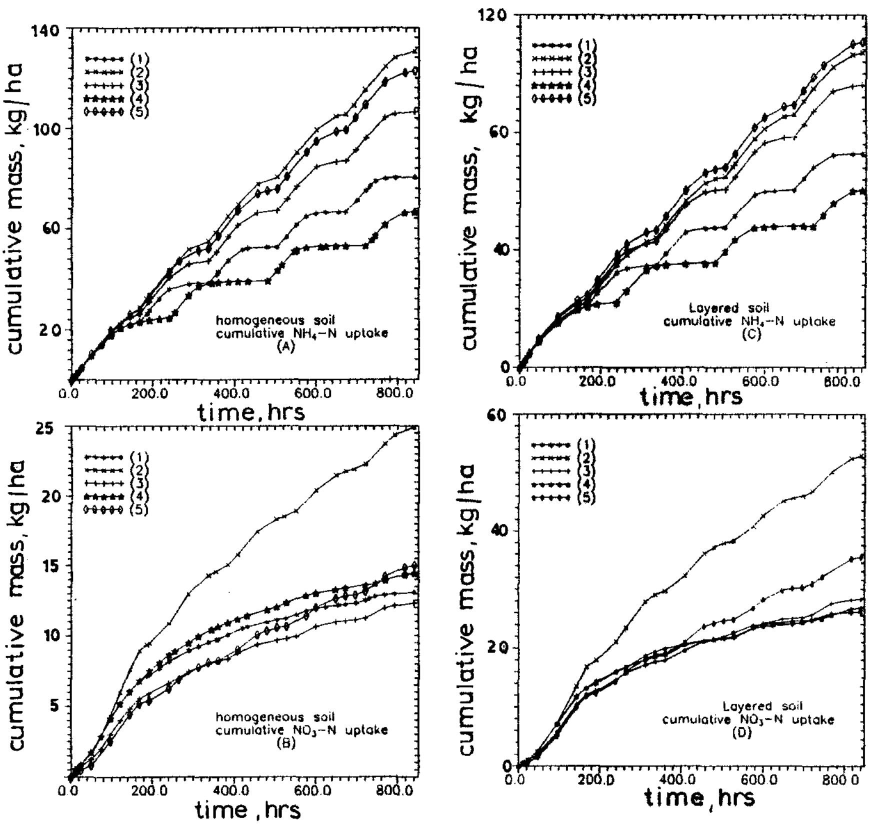

Fig. 8. Cumulative plant N uptake during simulation period for the five cases of applications in the two soils.

nitrogen, as in the cases (2), (5) and (3) (Figure 8). The increased mass of ammonia in the soil has the effect of increasing NH_4-N uptake as shown in case (2). Denitrification is greater when the conditions in the soil are anaerobic, as in the case (5) and somewhat smaller in the case (3) (Figure 9B and D). Figures 7A and 7D show that the total water in the soil retains in higher level after and before each applications of these case.

The mass of water, NH_4-N and NO_3-N, which percolate, play an important role in land treatment systems because of the groundwater pollution.

As shown in Figure 10 the cumulative deep flow of water is significant in the case (5) and after the second irrigation it increases rapidly, at a rate of 1 cm/day. The cumulative drainage water of the 3rd case is lower than the previous case, at a rate of 0.8 cm/day after the third irrigation, while in the 2nd case it is much lower, at a rate of 0.4 cm/day after the fourth irrigation. The leached NH_4-N (Figures 10C and F) is more significant in the 5th case and less significant in the 3rd case and following then in the 2nd and 1st cases. The leached NO_3-N

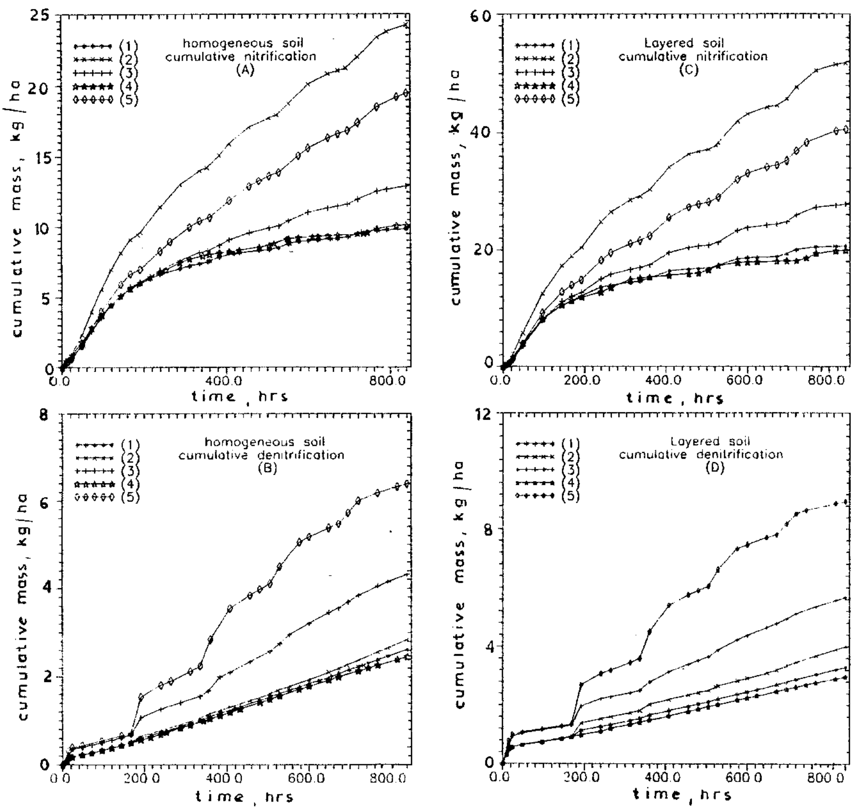

Fig. 9. Cumulative nitrification and denitrification mass during simulation period for the five cases of applications in the two soils.

mass (Figures 10B and E) has the same importance to groundwater pollution as that of NH_4-N. The leached NO_3-N increases rapidly in the 5th and 3rd cases of applications.

The results of 2nd and 5th application cases indicate that when the same amount of NH_4-N is applied in the soil, the leached N mass is greater in the case of higher water application rate. Therefore the impacts of N wastewater application don't depend on total amount applied, but on water application rate and duration.

5. Conclusions

A mathematical model was developed to simulate water movement, mass transport and nitrogen transformations in soils covered by plants during wastewater application on the soils.

The model is one-dimensional and based on the Galerkin finite element method. The model incorporates: the plant uptake of water, the mass transport by dispersion and convection of ammonium and nitrate nitrogen, the nitrification of ammonium

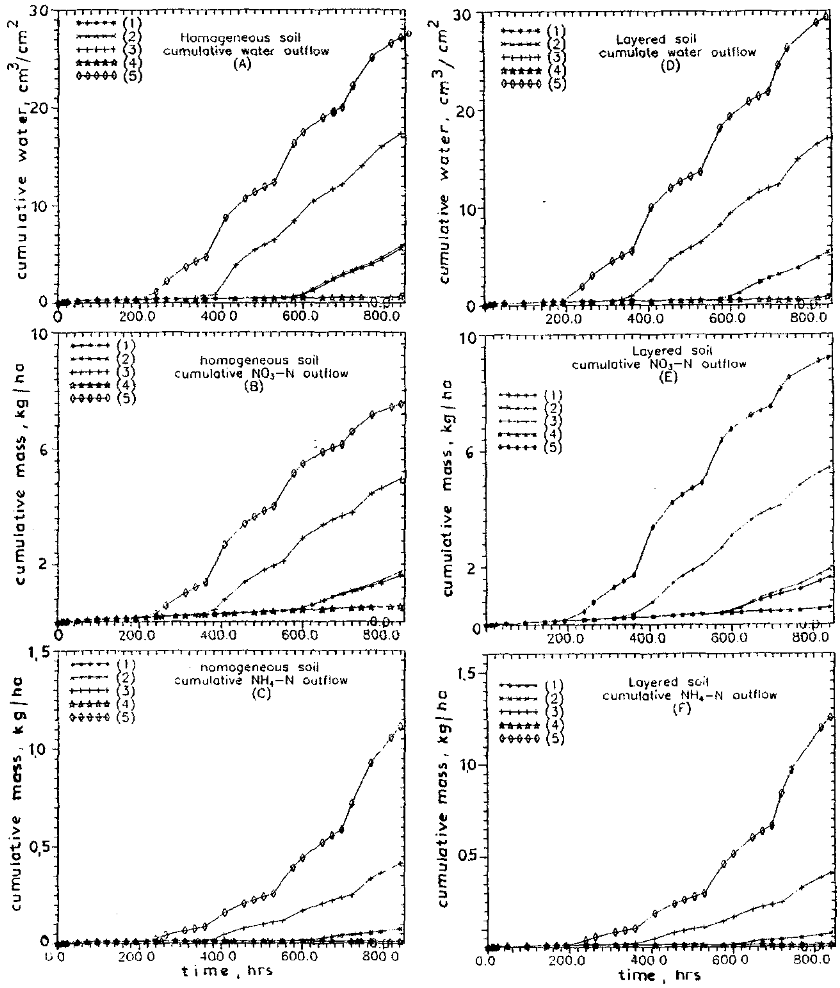

Fig. 10. Cumulative drainage water, leached NH_4-N and NO_3-N mass during simulation period for the five cases of application in the two soils.

to nitrates in one step, the denitrification of nitrates, the ammonium exchange and the uptake of NH_4 and NO_3 ions.

An analysis is carried out on application rate, N concentration, duration and scheduling of application to ascertain their impacts on groundwater recharging and N leaching, on nitrification, denitrification and N uptake by plant roots.

The model can be used to predict the fate of nitrogen in land treatment systems and in the soil when nitrogen is applied by fertilizer, to estimate the nitrogen application load and the uptake by plants, and as research or management model for N behaviour in land treatment.

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