ELSEVIER

Available online at www.sciencedirect.com

ScienceDirect

Procedia Technology 25 (2016) 122 – 129

Procedia Technology

Global Colloquium in Recent Advancement and Effectual Researches in Engineering, Science and Technology (RAEREST 2016)

Experimental and Simulation studies on Nitrogen Dynamics in Unsaturated and Saturated Soil using HYDRUS-2D

C.Mekala[a], Indumathi M Nambi[*]

*[a] *Environmental and Water Resource Engineering, Civil Engineering, IIT Madras, Tamilnadu 600036, India*

Abstract

Effective irrigation practices have become an optimal means of providing water and nutrients to crops as well as preventing the vulnerability of ground water contamination. This could be achieved by understanding the fate and transport processes of nitrogen compounds in the subsurface. However, nitrogen dynamics in the plant rhizosphere is very complex, which depends on many factors such as soil temperature, pH, water content, soil microbes, soil type and plant characteristics and cannot be easily quantified. Using state-of-the-art modelling techniques, an attempt was made to evaluate the reactive transport of ammonium nitrogen under continuous and alternate wetting and drying mode (AWD) of irrigation in soil columns using a HYDRUS 2D model. The model quantifies the soil sorption, microbial transformations such as nitrification and denitrification, leaching, and final release to aquifer for ammonium and nitrate input fluxes. This quantification helped in designing an optimal fertigation and irrigation schedule. Soil column study was done with variable saturation and in a combined unsaturated (45 cm) and saturated (5 cm) representing vadose and aquifer. Drip irrigation with wastewater containing 100 mg/L of ammonium and 500 mg/L of organic carbon (acetate) was applied based on the recommended total quantity of nutrients in continuous and pulse modes to the column. The soil parameters, initial and boundary conditions used in the model were obtained through experimental studies. The HYDRUS-2D model was developed, calibrated and validated with experimental results. The model performed could predict well the experimental data. Under continuous irrigation, nitrification (0.23/d) was the predominant process whereas both nitrification and denitrification occurs simultaneously in AWD with the overall nitrate removal efficiency of 60%. Consequently, the scenario prediction using this model for optimal fertigation schedule was done for groundnut crop. Further this model could be extended for various scenario predictions for designing optimal irrigation-fertigation schedules for sustainable agricultural practices.

Keywords: Fertigation; HYDRUS2D; Nitrogen dynamics; Irrigation

---

* Corresponding author. Tel.: +914422574289;
E-mail address: indunambi@iitm.ac.in

doi:10.1016/j.protcy.2016.08.089

1. Introduction

Nomenclature	
h	pressure head
K	hydraulic conductivity
θ_w, θs, θr	Volumetric water content, saturated and residual water conten
q	Darcy flux
D	Dispersion coefficient
S_e	Saturation
Q_{nm}	Plant uptake
Φ_1, Φ_2	First order nitrification and denitrification constant
α,β,η	Fitting parameters
ρ_b	Bulk density
τ	Tortuosity
z	Vertical coordinate

Over the decades, the intensive use of agriculture practices consumes tons of agrochemicals to increase crop productivity. This probably leads to diffusion and leaching of excess chemicals creating various environmental pollution, the significant being groundwater contamination. [1]. Excessive nitrogen containing wastewater irrigation, over fertigation and build up of soil residuals leads to severe nitrate contamination. Numerous ways as numerical modelling and experimental studies are present to estimate irrigation losses, leaching potential by different irrigation methods (drip, subtape, furrow, and sprinkler), crop and soil types. [2,3]. Efficient irrigation with proper fertilizer application to deliver water and nutrients to plants involves a scientific planning based on crop needs, soil conditions, and hydro geological conditions.Hence a holistic approach for water dynamics and scientific understanding of nitrogen compounds in soil and groundwater is essential for design operation and planning of scheduling of irrigation and fertigation[4].

Most widely adopted technology was alternate wetting and drying irrigation rather than continuous flooded irrigation because it not only reduces water and fertilizer load to soil and plants but prevents excess leaching and groundwater contamination [5]. Quantifying water and nitrogen losses in plant root zone is complexes due to uncertainties in estimating the actual water content and solute movement even under controlled environment such as lysimeter studies and column experiments [6]. In addition, field experiments will provide a realistic data but there would not be any control in the experimentation, also it is laborious, time consuming and tracking of water drainage flux and solute concentrations will be uncertain. Hence, computer simulations became a valuable tool for understanding the complex nitrogen dynamics and their interaction with soil, crops and the role of water content, soil microbes and soil conditions affecting their transport. Also, assessment of management options for better cropping and safeguarding the environment based on scenario analysis through models will make the work easier [7,8,9].

Several models were present in literature simulate flow and transport processes, nutrient uptake and biological transformations of nutrients in the soil [10] numerical models showing the effect of temperature and dissolved oxygen, water and N dynamics in paddy fields [11], SWMS [12], HYDRUS [13,14,15] HYDRUS 2D/3D [6] has been used extensively for evaluating the effects of soil hydraulic properties, soil layering, dripper discharge rates, irrigation frequency and quality, timing of nutrient applications on wetting patterns and solute distribution [e.g.,16,17,18,] because it has the capability to analyze water flow and nutrient transport in multiple spatial dimensions [19]. Most of models obtain their input data from field studies which were not representative due to uncertainties in sampling, climatic conditions, environment etc. Hence, this study was taken up to develop a model which was calibrated and validated by experimental results which helps in better understanding and predictions. The objective the present study was to develop a model for the transport of nitrogen compounds and simulate water fluxes in an unsaturated and unconfined aquifer system under continuous and alternate wetting and drying irrigation for the scientific understanding and investigate the critical factors.

Table 1. Soil hydraulic properties

Soil Parameter	Values
Porosity	0.37
Bulk density	1564.03 kg/m^3
Hydraulic conductivity	7.75x10^-3 cm/s
Vangenuchten parameters	Θ_r - 0.055, Θ_r -0.37, α - 0.124 , n- 1.8

2. Materials and Methods

2.1 Experimental Set up

The study was conducted in a soil column of 70 cm height and 5 cm internal diameter. The column was packed for a depth of 50 cm with sandy loam soil taken from wastewater irrigated plots of IIT Madras, Tamilnadu. The soil characteristics were shown in Table1. The soil column was irrigated from the small inlet tank with 10-12 needles arrangement to evenly distribute the feed solution on soil surface. Two sets of column studies were done. One with variable saturation denoted as C1 and another with a combined unsaturated and saturated system denoted as C2. The wastewater was feed at a rate of 7 cm/d for C1 and 22 cm/d for C2 studies using syringe pump. There were three sampling ports located at 10 cm, 20 cm and 40 cm soil depth. The bottom has one more port which was connected to a hanging U tube column. This arrangement was done only in C2 column to maintain saturated conditions for 5 cm soil depth at the bottom. Lechate samples were collected in a conical flask connected to a vacuum pump. There were additional two ports for inserting soil moisture probes (Soil sensor, USA) one at top (15 cm) and another at bottom (30 cm) for soil water content measurement during the studies.

2.2 Wastewater irrigation and Analysis

Before irrigating the soil column, the soil was mixed with nitrifying and denitrifying bacterial culture developed from soil [20]. The initial biomass was calculated based on plate count method. Initially the soil column was fully saturated and the excess soil water was removed by draining. In C2 experiment, a 5 cm saturated soil depth was maintained by hanging water column at the bottom of column. Wastewater containing 100 mg/L of ammonium and 500 mg/L of acetate was applied at a constantly for C1 column studies for 20 days and by split irrigation for C2 column studies for 10 days. Spatial and temporal lechate samples were collected and analyzed for ammonium, nitrate and acetate. The soil water content measurements were also made while sampling. The ammonium were analyzed by ion chromatography (IC3500 model, Thermofisher USA) using CS16 column, with 40 mM Methane sulfonic acid as eluent and nitrate, acetate by AS18 column with 35 mM Sodium hydroxide as eluent at 1ml/min.

2.3 Coupled water and solute transport simulations by HYDRUS2D

The mathematical model for predicting water flow and the transport of nitrogen species in unsaturated sub-surface system is described in this section to simulate the nitrogen species transport with varying irrigation and moisture conditions. Vertical movement of water in soil under one-dimensional unsaturated condition can be described by Richard's model as expressed in Eqn. (1) [21]

$$C(h)\frac{\partial h}{\partial t} = \frac{\partial}{\partial z}K\left(\frac{\partial h}{\partial z}\right) - \frac{\partial K}{\partial z} \tag{1}$$

where $C(h) = \frac{\partial \theta}{\partial h}$ is specific moisture capacity (1/L); h is the pressure head (L); K is the unsaturated hydraulic conductivity (L/T); t is the time (T); z is the vertical coordinate (L) positive downward.

To solve the Richard's equation the following constitutive relationships are required. Such relations were proposed by Van Genuchten (1980) as given in Eqns. (2) – (4):

$$S_e = \frac{\theta_w - \theta_r}{\theta_s - \theta_r} \tag{2}$$

$$\theta_w = \theta_r + \left[\frac{\theta_s - \theta_r}{1+(\alpha|h|)^{\beta}}\right]^{\eta} \tag{3}$$

$$K(h) = K_s S_e^{1/2}\left[1-\left(1-S_e^{1/\eta}\right)^{\eta}\right]^2 \tag{4}$$

where: θ_w is the water content (L^3/L^3); S_e is the effective saturation; θ_s is the saturated water content; θ_r is the residual water content; K_s is the saturated hydraulic conductivity(L/T); α, β and η are fitting parameters.
The chemical and biological reactions of nitrogen transformation in the soil when wastewater is applied are nitrification, denitrification, uptake of ammonium and nitrate by plants, and adsorption of ammonium on the soil cation exchange sites [22]. To simplify the model formulation, this section considered only ammonium nitrogen and nitrate nitrogen as the main nitrogen species along with adsorption process and nitrification along with denitrification are the key reactions in the nitrogen cycle.

The one-dimensional vertical mass transport and transformations of ammonium nitrogen and nitrate nitrogen under transient flow and variably saturated soil conditions are described in the Eqns. (5) and (6):

$$\theta_w \frac{\partial NH_4-N}{\partial t} + \rho_b \frac{\partial S}{\partial t} = \frac{\partial}{\partial z}\left(\theta_w D \frac{\partial NH_4-N}{\partial z}\right) - q\frac{\partial NH_4-N}{\partial z} + Q_{am} - \phi_1 \tag{5}$$

$$\theta_w \frac{\partial NO_3-N}{\partial t} + \rho_b \frac{\partial S}{\partial t} = \frac{\partial}{\partial z}\left(\theta_w D \frac{\partial NO_3-N}{\partial z}\right) - q\frac{\partial NO_3-N}{\partial z} + Q_{ni} - \phi_2 \tag{6}$$

where NH_4-N is the concentration of ammonium nitrogen; NO_3-N is the concentration of nitrate nitrogen; $D=D_m*\tau+q*\alpha_L$, D is the dispersion coefficient; D_m is the molecular diffusion coefficient; τ is the tortuosity; q is the Darcy velocity; α_L is the longitudinal dispersivity; ρ_b is the bulk density of soil; S ($S = K_d*N_{(NH4/NO3)}$) is the amount of NH_4 or NO_3 in the adsorbed phase per unit mass of soil; K_d is the linear partitioning coefficient of ammonium nitrogen, Φ_1 is the rate of NH_4-N transformation per unit soil volume; Φ_2 is the rate of NO_3-N transformation per unit soil volume; Q_{am} is the rate of plant uptake of NH_4-N per unit soil volume and Q_{ni} is the rate of plant uptake of NO_3-N per unit soil volume. The plant uptake process is not considered in this study.
The transformation terms Φ_1 and Φ_2 describe the nitrification of NH_4-N and denitrification of NO_3-N which are approximated by first-order kinetic type reactions which are given in Eqns. (7) and (8) [21]:

$$\phi_1 = -K_1\theta_w(NH_4 - N) \tag{7}$$

$$\phi_2 = K_1\theta_w(NH_4 - N) - K_2\theta(NO_3 - N) \tag{8}$$

where K_1 and K_2 are the nitrification and denitrification rates.

2.3.1 Initial and Boundary conditions

The schematic diagram of soil domain with initial and boundary conditions was shown in Fig.1. Initial soil water content of the top layer was 0.201.The upper boundary condition constant flux boundary for C1 column and time variable boundary condition with constant flux for C2 study. The bottom boundary was free drainage for C1 and constant pressure head boundary condition, reflecting the position of the groundwater table [11] for C2 study. Duration of wastewater irrigation was 8 h per day at an interval of 24 h. This condition simulates the wetting and drying cycle of AWD irrigation. For continuous irrigation study (C1), the wastewater containing ammonium and acetate were fed continuously for 24 h. The solute was set to third type condition.

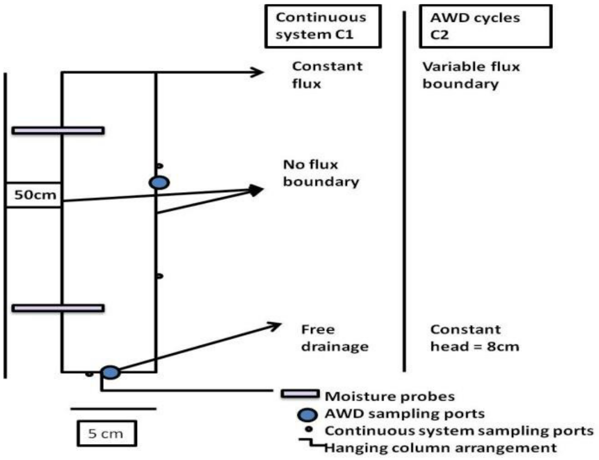

Fig.1. Soil column with boundary conditions and operation cycle

3. Results and Discussion

3.1 Moisture variations

Water contents were measured on daily basis at 15 cm and 30 cm soil depth and were simulated by HYDRUS 2D as shown in Fig.2. The measured water content at top depth showed fluctuations upto 8 days and bottom depth remained similar to simulations after 4 days. However, both followed a similar profile. The average water content was 0.2cm^{3}cm^{-3} which was favourable for root zone of crops. However, the simulated water contents were lower than the measured during the initial phase but matched well at both depths during the later phase. These higher variations were due to soil evaporation, preferential flow, assumption of flux boundary which may be different from transient conditions. Similar trend was observed by [20] for assessing the salinity and nitrate for citrus plantations and other studies [21,16,22]. In case of alternative wetting and drying cycles of irrigation for C2 column with a combined saturated and unsaturated system, the model was able to simulate the water saturations profile moderately (the data not shown here).

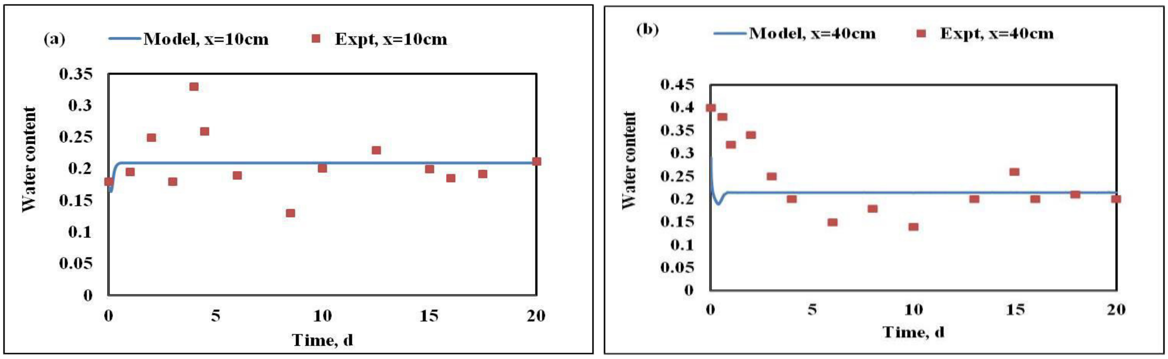

Fig.2 Experimental and predicted water content variation for unsaturated soil column C1at (a) x= 10cm soil depth, (b) x=40 cm soil depth

3.2 Nitrogen distribution dynamics

Comparison between daily measured and simulated concentrations of ammonium and nitrate were shown in Fig.3 (a) and (b) at 15 cm, 30 cm and 50 cm soil depths. For ammonium, the model was over predicting at 15 cm soil depth where as the other two depths were well matching except for some variation due to dispersion was observed at 50 cm depth for experimental values.

In case of nitrate breakthrough curve, the model showed a good correspondence with experiments with only slight variations observed at 15 cm soil depth. The model was under estimating the nitrate concentrations at x= 15 cm and 30 cm. A similar match of nitrate distributions has been reported in other studies as well [20, 22, 21]. The reason behind such variations may be variations in heterogeneity of soil packing, anisotropy, nature of sampling method which gives as representative of an area, preferential flow due to soil properties, variation in water content, which in turn affecting the dispersion. The model considers the only the nitrification, denitrification, sorption reactions in soil, whereas mineralization, immobilization through carbon–nitrogen complex formation and microbial interaction, inhibition due to oxygen, substrate and other byproducts formation were not taken into account. This could be done by using advance modeling by Wetland modules (CW2D and CWM modules) of HYDRUS 2D software. There were other several factors as reported by [22] influencing the correspondence between measurements and simulations of water contents and solute concentrations in the soil.

Coming to the depth wise profile as shown in Fig.3(d), the ammonium concentration reached a maximum concentration of 78 mg/L at top and least (51 mg/L) at bottom depth. This shows that, there was gradation along depth wise occurring due to sorption and nitrification occurring along the length of the column. The reduction in concentration was mainly due to nitrification reaction which needs a continuous supply of oxygen. This was provided by top atmospheric boundary. The estimated nitrification coefficient was 0.23/d [22] based on model simulations. Since there was a continuous irrigation, the ammonium leaching was around 50 mg/L after 4 days. This amount will get reduced if alternate or split irrigation is practiced. The overall removal rate by nitrification and sorption was 50%. Nitrate formation and leaching occurred around 3 days. The nitrate formed migrates to bottom of column where anoxic conditions were prevails favoring denitrification accounting to 0.023/d.

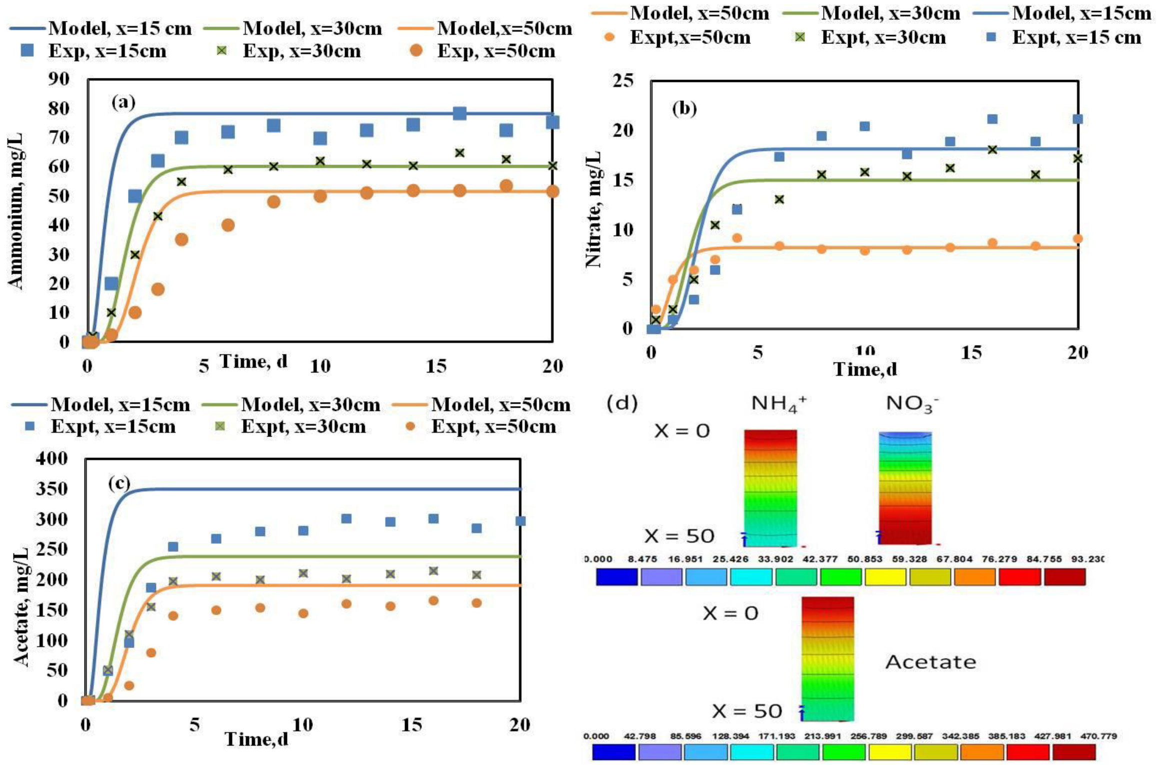

Fig.3 Continuous irrigation in unsaturated soil column C1 (a) Breakthrough curve showing model and experimental values at x=15 and x=45 cm depth for ammonium, nitrate and acetate (b) showing depth wise variations of ammonium, nitrate and acetate concentrations and water saturations

In case of AWD irrigation in an unconfined aquifer system, as shown in Fig 4 (a) and (b) the model moderately simulated the flow through the column but could not estimate the nitrification rates. The model was moderately estimating the ammonium concentrations but under predicting the nitrate ions. Since nitrification and denitrification rate were dependent on moisture content [2122], the model was modified enabling water content dependence parameters to estimate the proper kinetic rates. Based on that, the estimated first order nitrification and denitrification rates were 0.21/d and 0.082/d.

Addressing the depth wise distribution as in Fig 4(c), the ammonium concentration reached 40 mg/L around 2 days and remained constant thereafter. This high potential of nitrogen leaching depends on water flow and bottom boundary conditions.

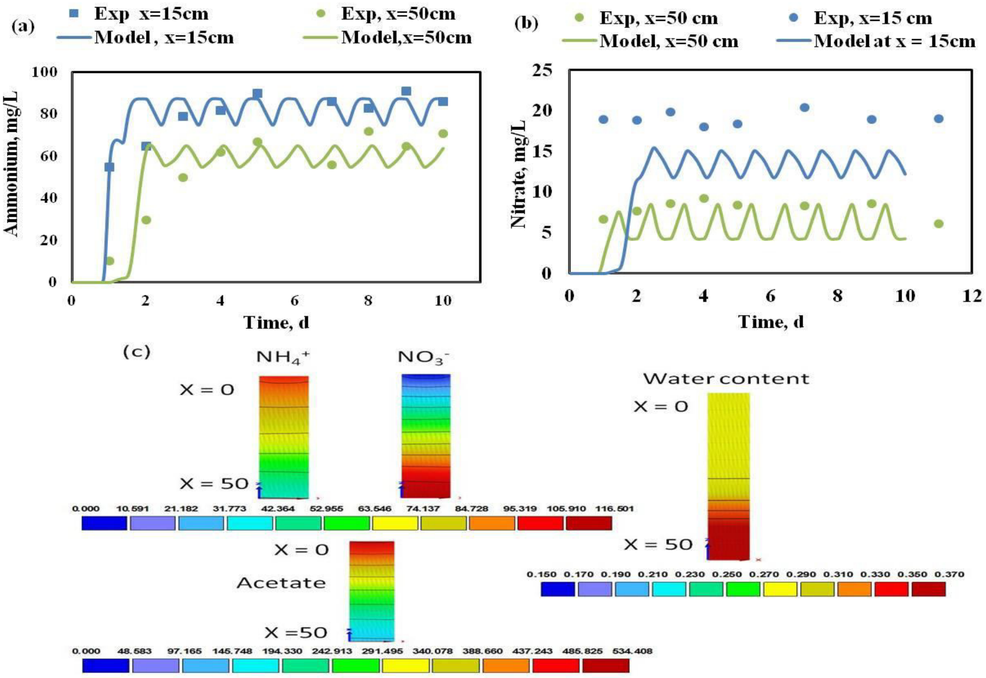

Fig.4 Alternate Wetting and drying irrigation (AWD) showing (a)Breakthrough curve showing model and experimental values at x=15 and x=45 cm depth for ammonium, nitrate and acetate (b). Depth wise variations of ammonium, nitrate and acetate concentrations and water saturations

4. Conclusions

The effects of drip system on unsaturated columns and unconfined aquifer were simulated using a transport model (HYDRUS-2D). The following conclusions were drawn from the present study:

- The HYDRUS-2D model performed reasonably well in predicting soil water content and nitrogen dynamics. The nitrate movement greatly dependent on hydraulic loading and moisture profile. In continuous irrigation with wastewater, nitrogen losses were accounted to be 50% than split method. Also, the soil uptake efficiency decreases with continuous application of wastewater.
- In an unconfined aquifer system, with alternate wetting and drying enhanced the nitrification and denitrification processes in root zone where variable, as oxidation-reduction environment alternated. The analysis of the nitrogen balance shows that on average, about 40 % of total is removed from the soil profile by nitrification, 3% by sorption , 23% (at 50 cm) leaches to groundwater, and about 30.2% is lost due to denitrification. A further improvement of models to be done by considering the plant component, all bio-geo chemical reactions.

References

[1] Candela,L, Wallis K.J, Rosa Maria Mateos. Non-point pollution of groundwater from agricultural activities in Mediterranean Spain: The Balearic Islands case study. Environmental Geology 2008; 54(3):587-595.

[2] García-Garizábal, I, Causapé, J.,Abrahao,R., Nitrate contamination and its relationship with flood irrigation management. Journal of Hydrology 2012;442–443,15–22.

[3] Cavero, J., Barros, R., Sellam, F., Topcu, S., Isidoro, D., Hartani, T., Lounis, A., Ibrikci, H.,Cetin, M., Williams, J.R., Aragüés, R., APEX simulation of best irrigation and N management strategies for off-site N pollution control in three Mediterranean irrigated watersheds. Agricultural Water Management 2012;103, 88–99.

[4] Li, J, Yoder, R.E, Odhiambo, L.O, Zhang, J. Simulation of nitrate distribution under drip irrigation using artificial neural networks. Irrigation Science 2004;23, 29–37.

[5] Tan,X., Shao,D., Liu, H., Yang, F., Xiao, C., Yang, H. Effects of alternate wetting and drying irrigation on percolation and nitrogen leaching in paddy fields. Paddy Water Environ 2013;11 (1–4),381–395.

[6] Yao,F, Huang, J, Cui, K, Nie, L, Xiang, J, Liu, X, Wu, W, Chen, M, Peng, S. Agro-nomic performance of high-yielding rice variety grown under alternate wetting and drying irrigation. Field Crop Res 2012;126, 16–22.

[7] Van der Laan M, Stirzaker R J, Annandale J G, Bristow K L, du Preez C C.. Monitoring and modeling draining and resident soil water nitrate concentrations to estimate leaching losses. Agricultural Water Management 2010 ;97,1779–1786.

[8] Pang, X.P, Letey, J. Development and evaluation of ENVIRO-GRO, an integrated water, salinity, and nitrogen model. Soil Sci. Soc. Am. J. 1998; 62, 1418–1427.

[9] Li J, Zhang J J, Ren L. Water and nitrogen distribution as affected by fertigation of ammonium nitrate from a point source. *Irrigation Science*, 2, 19–30.

[10] Li, J, Liu, Y. Water and nitrate distributions as affected by layered-textural soil and buried dripline depth under subsurface drip fertigation. Irrig. Sci. 2011;29,469–478.

[11] Antonopoulos, V.Z., Modelling of water and nitrogen balances in the ponded water and soil profile of rice fields in Northern Greece. Agric. Water Manage. 2010;98(2), 321–330.

[12] Tournebize, J., Gregoire, C., Coupe, R.H., Ackerer, P., Modelling nitrate transport under row intercropping system: Vines and grass cover. Journal of Hydrology .2012.440–441, 14–25.

[13] Garg, K.K, Das, B.S, Safeeq, M, Bhadoria, P.B.S. Measurement and modeling of soil water regime in a lowland paddy field showing preferential transport. Agric.Water Manage 2009;96 (12), 1705–1714.

[14] Simunek J, van Genuchten M T, Sejna M. The HYDRUS Software Package for Simulating Two- and Three- Dimensional Movement of Water, Heat, and Multiple Solutes in Variably-Saturated Media. 2011;Technical Manual, ver. 2.0 PC Progress, Prague, Czech Republic.

[15] Hanson, B.R, Simunek, J, Hopmans, J.W. Evaluation of urea–ammonium–nitrate fertigation with drip irrigation using numerical modeling. Agric. Water Manage 2006; 86 (1–2), 102–113.

[16] Ajdary, K, Singh, D.K, Singh, A.K, Khanna, M. Modelling of nitrogen leaching from experimental onion field under drip fertigation. Agric. Water Manag 2007;89,15–28.

[17] Mekala.C and Indumathi M,N. Transport of Ammonium and Nitrate in Saturated Porous Media Incorporating Physiobio transformations and bioclogging , Bioremediation Journal; 20 (2), 117-132

[18] Ramos,T.B, Simunek, J, Gonc¸ alves, M.C, Martins, J.C, Prazeres, A, Pereira, L.S. Two-dimensional modelling of water and nitrogen fate from sweet sorghum irrigated with fresh and blended saline waters. Agric. Water Manage 2012;111, 87–104.

[19] Antonopoulos, V.Z. Water movement and heat transfer simulations in a soil under ryegrass. Biosyst. Eng. 2006; 95(1), 127–138.

[20] Skaggs, T.H, Trout, T.J, Rothfuss, Y. Drip irrigation water distribution pattern: effects of emitter rate, pulsing and antecedent water. Soil Sci. J. Soc. Am 2010;74, 1886–1896.

[21] Hanson, B.R, Simunek, J, Hopmans, J.W. Evaluation of urea–ammonium– nitrate fertigation with drip irrigation using numerical modelling. Agric. Water Manage 2006;86, 02–113.

[22] Hassan, G, Reneau Jr, R.B., Hagedorn, C. Modeling effluent distribution and nitrate transport through an on-site wastewater system. Journal of Environmental Quality 37, 2008; 1937–1948.