A NITRIFICATION PREDICTIVE MODEL FOR RECLAIMED WATER DISTRIBUTION NETWORKS: NITRINET

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ABSTRACT

In this work, a new model (NITRINET) to simulate nitrification processes in pressurised irrigation distribution networks fed with reclaimed water (RW) is developed and applied to the Tintín Irrigation District (TID) distribution network as case study (Montilla, southern Spain). Due to water scarcity and climate change scenarios, irrigation with RW has gained interest worldwide, especially in arid and semi-arid regions, like the Mediterranean Basin. The importance of the developed model relies on the fact that the chemical composition of RW varies spatially along the distribution network. The water quality analyses carried out in TID during two irrigation seasons (2019, 2023) have shown that nitrate concentrations increase along the network in contrast to the reduction observed in the ammoniacal forms. This confirms that nitrification processes occur inside the pipes. Therefore, the concentration of nutrients in RW does not remain constant, as it varies from farm to farm. Thus, NITRINET combines the hydraulic simulation of the distribution network and the modelling of nitrification processes to predict the concentration of ammoniacal nitrogen (NH_4^+-N) and nitric nitrogen (NO_3^--N) in RW arriving at farms, so that it can be used as a Decision Support System to optimise fertigation at irrigation district level.

TID covers 150 hectares, where olive and grapevine are the dominant crops. Located in the south of Spain, Montilla has a typical Mediterranean, semi-arid climate, with an average annual rainfall of 590 mm. Rainfall is concentrated in winter and spring, being insignificant in summer. This highlights the need for irrigation in these critical months, when rainfall is negligible and reference evapotranspiration (ET_0) reaches its maximum (with values greater than 8 mm·day^{-1}). All TID farms share the same irrigation system: subsurface drip irrigation, with 2.2 L·h^{-1} pressure-compensating drippers. Since there is no contact at all between RW and the edible part of both woody crops (grapes and olives), according to European Regulation 2020/741 on minimum requirements for water reuse (European Parliament, 2020), RW quality requirements in TID are those of class C, the most lenient category for food crops. Water used for irrigation in TID comes from Montilla wastewater treatment plant (WWTP), where a secondary treatment is performed (extended aeration with activated sludge). Treated wastewater is sent to a settling reservoir (9,100 m^3 of capacity) in TID, which is communicated with a bigger storage reservoir (222,000 m^3 of capacity), where an additional physico-chemical treatment is performed for algicidal and bactericidal purposes, by combining two ultrasonic devices and the addition of potassium permanganate ($KMnO_4$). RW allocation in TID is 1,500 m^3/ha per irrigation season.

Alcaide Zaragoza et al. (2022) and Gómez-Lucena et al. (2024) evidenced that RW quality varies spatially in TID distribution network, as nitrification reactions take place inside the pipes. The main consequence of this phenomenon is an unequal distribution of nutrients among farms, since the greater the distance between the farm and the pumping station, the lower the concentration of NH_4^+-N and the higher the concentration of NO_3^--N in RW reaching the plot. Nitrification is a biochemical process which involves two linked reactions: the oxidation of ammonium (NH_4^+) to nitrite (NO_2^-), and the subsequent oxidation of NO_2^- to nitrate (NO_3^-) (Alexander, 1965). This process is carried out by the nitrifying bacteria, which are sensitive to environmental factors, such as pH, temperature, light intensity, and dissolved oxygen concentration, to name but a few (Groeneweg et al., 1994; Grunditz and Dalhammar, 2001; Ward, 2008). Nitrification processes in RW directly affect plant nutrition, as NH_4^+-N and NO_3^--N are the primary nitrogen forms absorbed by plants through roots, since both ions are readily assimilable (Li et al., 2013).

The environmental conditions in TID distribution network are optimal for nitrification reactions to take place (Alcaide Zaragoza et al., 2022), as there is a complete absence of light, pH is slightly alkaline, nutrient concentration in RW is usually high, and nitrifying bacteria can be present in wastewater (Brion & Billen, 2000). As regards the hydraulic characteristics, TID distribution network comprises over 50 km of underground pipes. The most distant farms are situated 8 km of pipeline downstream from the pumping station, which implies that, in these distant farms, water travel times exceed 2 hours. High retention times along with low flow velocity in terminal pipes (where the ratio surface to volume is higher) favour nitrification. Moreover, if pipes' inner surfaces are considered, RW contacts over 3,900 m^2 of pipe wall on its way from the pumping station to the farthest farms. This variable must be considered, as it determines the amount of bacterial biofilm (including nitrifying bacteria) that can attach and accumulate on inner walls of the pipes (Gieseke et al., 2006; Wang et al., 2020).

During 2019 and 2023 irrigation seasons, water quality analyses were performed regularly in the following sampling points of TID: settling reservoir, storage reservoir, filtration treatment inlet (FTI), filtration treatment outlet (FTO), and 8 plots distributed across the distribution network, with the aim of studying the spatial variability of water quality during an irrigation episode. Among others, the following parameters were measured: Total N, NH_4^+-N and NO_3^--N, pH, temperature, and dissolved oxygen. The last three variables were measured in situ with a multiparameter meter, whereas the first three were measured in the laboratory of the Environment and Water Agency of Andalusia (AMAYA) (Seville, Spain). Therefore, water samples were collected and immediately refrigerated until analysis. Using EPANET (Rossman et al., 2020), water travel time, total pipe length, total pipe internal surface, and mean velocity were calculated for each selected plot.

Comparing water quality in FTO with the 8 selected plots, changes in NH_4^+-N and NO_3^--N concentrations (ΔNH_4^+-N and ΔNO_3^--N) were determined, as well as pH variation (ΔpH). A Spearman's correlation test was conducted to determine the relationship among ΔNH_4^+-N, ΔNO_3^--N, ΔpH, water temperature, and the previously determined hydraulic variables (water travel time, total pipe length, total pipe internal surface, and mean velocity). In light of the Spearman's test results, water pH, temperature, substrate availability (NH_4^+-N concentration), and water travel time were selected as the main explanatory variables for the developed model. This way, NITRINET performs simultaneously the hydraulic simulation of the network (to calculate the water travel time of each farm) and the simulation of nitrification reaction over time (based on water pH, temperature, and substrate availability). Combining both simulations, the model predicts nutrient concentrations in RW at farm level (see Figure 1).

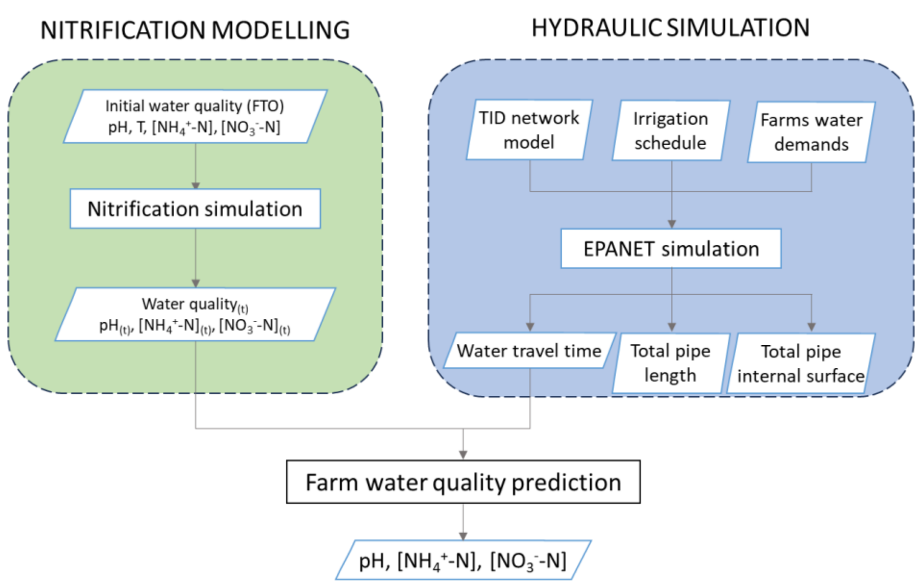

Figure 1. NITRINET model workflow.

To simulate nitrification, three differential equations have been developed. These equations model nitrification over time (t) as function of temperature (θ_T), pH (θ_{pH}), and substrate availability (θ_{NH_4}).

$$\frac{dNH_4}{dt} = -k_a \cdot \theta_{pH} \cdot \theta_T \cdot \theta_{NH_4} \cdot NH_4 \quad (1)$$

$$\frac{dNO_3}{dt} = -\frac{dNH_4}{dt} = k_a \cdot \theta_{pH} \cdot \theta_T \cdot \theta_{NH_4} \cdot NH_4 \quad (2)$$

$$\frac{dpH}{dt} = c \cdot \frac{dNH_4}{dt} \quad (3)$$

θ parameters simulate the influence of environmental variables on nitrification. They are dimensionless and take values between 0 and 1. Values close to 0 indicate unfavourable conditions and low nitrification rates, whereas values close to 1 indicate that conditions are favourable, and the reaction is not being inhibited. To determine the values taken by these parameters, literature has been reviewed (Pambrun et al., 2006) and adapted (Grunditz and Dalhammar, 2001). k_a and c are empirical parameters, which have been estimated using real data from TID water quality analyses and Markov Chain Montecarlo (MCMC) algorithms.

NITRINET simulates both the oxidation of NH_4^+ to NO_3^- and the associated pH reduction (Figure 2), predicting NH_4^+-N and NO_3^--N concentrations, along with water pH, with mean absolute errors of 1.49 mg·L^{-1}, 1.25 mg·L^{-1}, and 0.32 units, respectively. It should be noted that nitrification is complex to model, since it is influenced by several biological and physicochemical factors. The main purpose of NITRINET is that it can be used as a Decision Support System when planning fertilisation at irrigation district level.

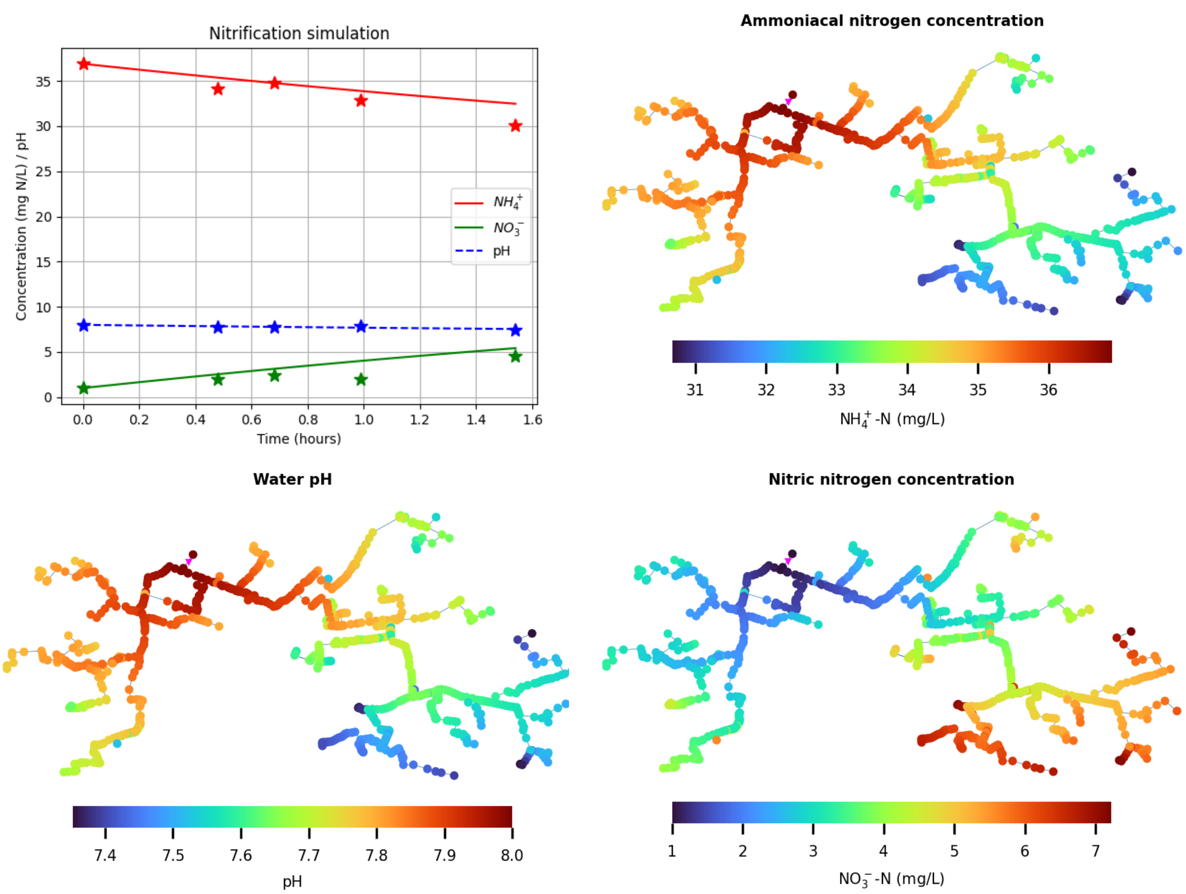

Figure 2. Simulation performed with NITRINET contrasted with real data

The model is of great applicability to the irrigation sector, given that to carry out precision fertigation strategies and optimize the amount of fertilizer applied, it is necessary to determine the concentration of nutrients present in the water arriving at farms. The nutrients that RW already carries must be considered when planning fertilization. This allows for a reduction in the amount of fertilizer applied to the soil, which has a positive impact both on the environment and on farmers' economy.

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