Process-based model for treatment of nitrogen fractions in biofilters

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Highlights

- A process-based model to ammonia and nitrate fractions is presented.
- Water flow module present average NSE of 0.82 for seven monitored events.
- Nitrogen quality model present good pollutant mass balance for one monitored event.

Introduction

Extreme hydrological events, such as droughts and floods, are one of the main causes of disasters worldwide, and it tends to be aggravated by climate and land use changes (Carter et al., 2015). Consequently, risks to the population increases, once flood events in urban centres become more frequent and the parallel between higher demand and resources scarcity contributes to increase water, energy and food insecurity. In this context, the approach Nexus – water, energy, food emerges, integrating these three resources to turn the society more resilient and increase sustainable communities, aiming to the UN Sustainable Development Goals (SDG) (Hoff, 2011). Low Impact Development (LID) practices can be used as a tool to achieve more resilient cities and communities, if integrating purposes of runoff retention, water quality improvement and stormwater harvesting, for others then just water reuse (Fletcher et al., 2015, Macedo et al., 2017).

There are still limitations on LID real, practical and low-cost employability facing climate change, mitigation, adaptation and re-use for water-energy-food security risks. Considering the design and operation, the key-factors influencing in the water quality improvement, stormwater harvesting, and runoff retention still need to be explored better. After identified these factors, they should be equated to allow multi-objective optimization for water reuse and flood control. Moreover, these gaps intensify especially in cities with a subtropical climate, since the most of studies are conducted in temperate areas, where geoclimatic, sanitary and social conditions are very different from those in subtropical climate. Thus, adapting LID systems for tropical and subtropical regions is still a shortcoming.

One of the ways to explore different future design and operation scenarios, allowing to identify its key factors, is from the modelling of the systems. Several models have already been developed to simulate the hydraulic-hydrological behaviour in different LID systems. However, there are still few models for nutrients, especially for total nitrogen or its fractions. Therefore, in this study we aim to present an initial approach to a process-based model to simulate the ammonia and nitrate fractions in a biofilter system, with the processes of nitrification, denitrification, adsorption and plant uptake.

Methodology

Based on previous studies by Shen et al. (2018), Randelovic et al. (2016) and Akan (2016), the model developed employs the "three-bucket" approach, in which each bucket represents the main zones found in a biofilter: ponding zone, unsaturated zone and submerged zone. In addition, there is a separation into two modules: water flow module and nitrogen quality module.

Water flow module

The water flow module aims to describe the hydraulic-hydrological behaviour of a biofilter system. The main simulated processes consist of infiltration from the ponding zone to the unsaturated zone, infiltration from the unsaturated zone to the submerged zone, outflow from an underdrain, overflow from an weir, evapotranspiration and capillary rise. For the underdrain and weir, the equations for the orifice and the equation for the triangular weir were used respectively, together with a mass balance of the respective zone of influence. For the infiltration processes, the Green-Ampt equation with suction head values for each zone was used. The evapotranspiration and capillary rise equations proposed in the study of Shen et al. (2018) were adopted. The calculation of the water level in the ponding zone was obtained by the interactive method of the adapted PULS (Ferreira et al., 2019). Further details of each of the equations can be obtained in the studies cited.

This module was calibrated using genetic algorithms from the maximization of the NSE, considering the values of outflow through the underdrain and the height of the water level in the ponding zone for three events monitored in a biofilter box in the laboratory. Subsequently, results were validated for four more events.

Nutrient quality module

For the quality module, each of the buckets is simulated considering the predominant processes in each of the zones. For the ponding zone, it is considered that there is a complete mixing occurring, with denitrification reactions predominating (for high flooding periods). The mass balance in this zone follows equation 1. For the unsaturated zone and submerged zone, the mass balance is made for different layers within each zone, using the solute transport equation in soils, adding a source sink and plant uptake terms (equation 2). The process of interaction between soil – liquid phase of the pollutant is considered only for ammonia, since nitrate is highly soluble. This process is simulated through a linear adsorption equation (equation 3), but considering a desorption factor separately, considering that these processes predominates in different times in the biofilter media (Shen et al., 2018). For the ponding zone and unsaturated zone, the source sink term is calculated according to equation 4 and for the submerged zone, according to equation 3. For plant uptake, the model uses the Michalis-Menten equation (equation 6 and 7). The advection term in equation 1 is calculated by upwind or central differences, depending on the value of Peclet number, while the dispersion term is approximated by central differences (Randelovic et al., 2016).

The nutrient quality module is still being adapted and has not yet been calibrated. An initial assessment was made for an event, with the calibrated data from the water flow module.

$$\frac{\partial (C_{1,i+1}\, h_i\, A_b)}{\partial t} = C_{In_i} . Q_{In_i} - C_{1,i} . \left(Q_{Inf,p_i} + Q_{over_i} \right) + \sum R_{x_{1,i}} \qquad \text{(Eq. 1)}$$

$$\frac{\partial \theta C_{l,i+1}}{\partial t} + \rho \frac{\partial C_{s,i+1}}{\partial t} = \frac{\partial}{\partial z}\left(D_e \theta \frac{\partial C_{l,i}}{\partial z} \right) - \frac{\partial\, q_{l,i}\, C_{l,i}}{\partial z} + \sum R_{x_{l,i}} + \emptyset J_{x_{l,i}} \qquad \text{(Eq. 2)}$$

$$\rho \frac{\partial C_{s,i+1}}{\partial t} = \theta . k_{ads} . C_{l,i} - \rho . k_{des} . C_{s,i} \qquad \text{(Eq. 3)}$$

$$R_{x_{l,i}} = \pm R_{nit} = k_{nit}\ [NH_4]_{l,i}\ ,\ R_{nit} = \begin{cases} + ,\, if\ [NO_3] \\ - ,\, if\ [NH_4] \end{cases} \qquad \text{(Eq. 4)}$$

$$R_{x_{l,i}} = - R_{denit} = - k_{denit}\ [NO_3]_{l,i} \qquad \text{(Eq. 5)}$$

$$J_{x_{l,i}} = Fm_{NH4} \frac{\theta C [NH_4]_{l,i}}{Km_{NH4} + \theta C [NH_4]_{l,i}} \qquad \text{(Eq. 6)}$$

$$J_{x_{l,i}} = Fm_{NO3} \frac{\theta C [NO_3]_{l,i}}{Km_{NO3} + \theta C [NO_3]_{l,i}} \qquad \text{(Eq. 7)}$$

Where: C_1 is the concentration in the ponding zone, C_{in} is the concentration of the inflow, Q_{in} is the inflow, Q_{inf} is the infiltration to the unsaturated zone, Q_{over} is the overflow through weir, C_l is the concentration in the different layers of the unsaturated and submerged zone, ρ is the soil bulk density, C_s is the concentration in the soil fraction, D_e is the diffusion coefficient, θ is the water fraction, q is the unitary flow in each layer (also known as water velocity in the soil), Rx is the source sink factor for each layer, Jx is the plant uptake factor for each layer, ø is the fraction of roots in the soil, i is the index of time and l is the index of layer, k_{ads} is the adsorption constant for each pollutant, k_{des} is the desorption constant, k_{nit} is the nitrification constant for first kinetic order reaction, k_{denit} is the denitrification constant, Fm_{NH4} and Fm_{NO3} are the maximum influx of ammonia and nitrate to the roots, Km_{NH4} and Km_{NO3} are the Michaelis constant for plant uptake for ammonia and nitrate.

Results and discussion

The water flow module of the model presented presents a good fit with the real data, for a total of 7 events evaluated, with average NSE in all the events of 0.82 The comparison of the modelled data with the real ones can be seen in Figure 1.

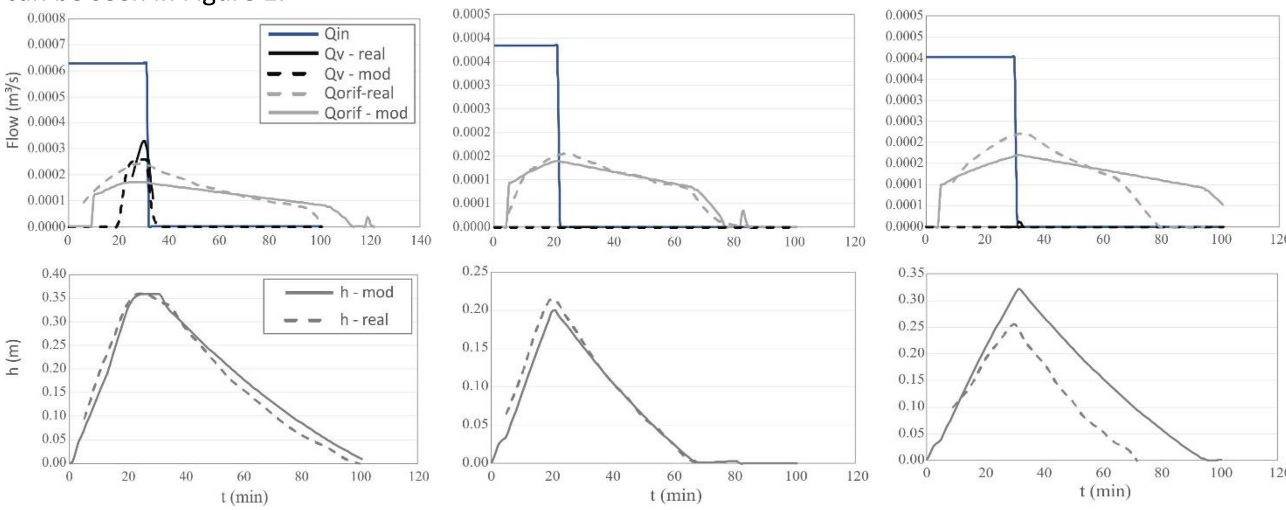

Figure 1. Hydrographs and water level in ponding zone for events 1, 5 and 6. Event 1 is the only one with overflow, event 5 was used for first evaluations of nutrients quality module and event 5 present the worst fit of all events evaluated in the water flow module.

The preliminary results of the nitrogen quality module present a satisfactory general behaviour, with values of removal rates for ammonia and nitrate of 70% and 93%, for an isolated event (event 5). However, the main processes involved in nitrogen removal (nitrification, denitrification and plant uptake) occur mainly inter-event, requiring a longer period for evaluation. Therefore, these initial results rely mainly on the process of adsorption and transport of solutes in the soil.

This abstract presents only the preliminary results of the nitrogen quality module. Final results of the quality module, considering longer series of events (accounting with wet and dry period) and calibration of the parameters will be performed and presented in the full paper and in the conference presentation. Additionally, sensitivity and uncertainty analysis will be explored and discussed, identifying the key-process involved for the nitrogen treatment, in biofilter systems.

Conclusions and future work

The water flow module presents satisfactory NSE results (0.82) when evaluating seven monitored events. For the nitrogen quality module, further investigation is still necessary, considering a longer series of events, so that the influence of nitrification, denitrification and plant uptake can be better evaluated. Later, sensitivity analysis should be conducted to identify the key factors in the biofilter design.

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