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Numerical modelling on transport of nitrogen from wastewater and fertilizer applied on paddy fields

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ABSTRACT

A numerical model is developed to predict the nitrogen species concentration in an unsaturated subsurface system due to vertical leaching from wastewater and urea applied paddy field. The important processes like oxygen mass transfer from air phase to water phase and biological clogging due to microbial growth and their impact on nitrogen transformation are considered in this study. Results suggest that a rising and falling trend is observed for hydraulic conductivity in the presence of biological clogging, in which the rise is due to the influence of increase in water saturation and the fall is due to the increase in microbial saturation. The numerical results show that when the total nitrogen applied is 25 mg/l continuously by wastewater application, the nitrate nitrogen concentration varies between 18 and 23 mg/l at different depths in the absence of biological clogging and between 0 and 24 mg/l in the presence of biological clogging. But in the case of 360 kg N ha^{-1} urea applied during the transplanting time (first day), the nitrate nitrogen concentration varies between 3 and 8 mg/l at different depths in the absence of biological clogging and approximately 0 mg/l throughout the depth of the soil column in the presence of clogging. The nitrate nitrogen concentration is 12 and 6 mg/l at 100 and 200 cm depth, respectively, for the case of three-time split fertilizer application in the presence of biological clogging. In both wastewater and fertilizer application cases, the biological clogging process induces unsaturated hydraulic conductivity reduction which helps to increase the contact time, accelerates nitrogen species transformations and eventually reduces the risk of nitrogen species contamination in groundwater.

1. Introduction

Rice demands significant amount of fertilizer utilization among agricultural crops. Therefore farmers tend to apply considerable amount of nitrogen fertilizer to paddy field. Urea is the most commonly used nitrogen (N) fertilizer (Ghosh and Bhat, 1998; Guo et al., 2004) for rice crop. On the other hand, industrial and municipal wastewater is also extensively used as a source of irrigation water in water-shortage countries (Kim et al., 2008). Wastewater reuse for irrigation can have several advantages including economic benefits, presence of nutrient contents and further it significantly reduces the requirement of fertilizers. Nitrate-nitrogen is one of the main nutrients for plant growth, which is available in irrigated water through fertilizer application or wastewater. Nitrite nitrogen (NO_2-N) is derived from ammonium nitrogen (NH_4-N) followed by nitrate nitrogen (NO_3-N) during nitrification process and the same can be converted to nitrogen gas (N_2) during de-nitrification process. The portion of nitrate nitrogen that is not utilized by the crop can be leached below the root zone into groundwater causing a serious problem as the nitrate concentrations frequently exceed allowable contamination limits (Strebel et al., 1989). Large amount of nitrate nitrogen in drinking water can cause various health problems (Chen et al., 2003) including cancer for human and animals (Chen et al., 2007). Therefore, it is very important to model the fate and transport of nitrogen species from fertilizer and/or wastewater applied paddy field to predict the spatial and temporal distributions of concentrations in the vadose zone.

In general, ammonia-oxidizing bacteria and autotrophic nitrite-oxidizing bacteria are responsible for nitrification process and heterotrophic bacteria are responsible for de-nitrification process. Thus, the presence of bacteria plays a predominant role for nitrogen transformation process in soil water environment. Many studies have experimentally proved that clogging due to bacteria can significantly change saturated as well as unsaturated porous medium properties such as hydraulic conductivity, porosity and

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dispersivity (Frankenberger et al., 1979; Taylor and Jaffe, 1990; Cunningham et al., 1991; Vandevivere and Baveye, 1992; Rockhold et al., 2005; Mostafa and Van Geel, 2012). Similarly conceptual models have also been developed to predict the permeability changes due to biological clogging in saturated as well as unsaturated soil (Taylor and Jaffe, 1990; Clement et al., 1996; Rockhold et al., 2005; Mostafa and Van Geel, 2007; Soleimani et al., 2009). Recently Mostafa and Van Geel (2012) experimentally and numerically have shown that active biomass, extracellular polymeric substances (EPS) and inert biomass fraction are significantly affecting the relative permeability. Therefore, it is extremely important to incorporate the effects of biological clogging and its associated nitrogen transformation in a typical soil–water environment in order to better understand the effective utilization of wastewater and fertilizer.

However, modelling the fate and transport of nitrogen species in flooded paddy fields is quite complicated due to a series of nitrogen transformation processes (Yoshinaga et al., 2004; Evans et al., 2006) and it is further complicated in the paddy soils due to the coupled physical, chemical and biological processes (Nakasone et al., 2004; Liang et al., 2007). Many sophisticated numerical models have been developed earlier for simulating nitrogen species behaviour in an unsaturated porous media (Iskandar and Selim, 1981; Antonopoulos, 1993; Tindall et al., 1995; Lafolie et al., 1997; Berlin et al., 2014) as well as in the saturated porous media (MacQuarric and Sudicky, 2001; Lee et al., 2006). Although several studies have reported the nitrogen species concentration in a paddy soil by experimental and field monitoring (Chen et al., 2007; Li et al., 2008; Zhao et al., 2009), only very few studies have attempted the modelling of nitrogen species concentrations in the paddy soil under saturated/unsaturated conditions (Nakasone et al., 2004; Liang et al., 2007). For example, to mention a few, Ling and El-Kadi (1998) have developed a lumped parameter model for the evaluation of nitrate leaching. Nakasone et al. (2004) have investigated nitrogen transformations studies under different flow conditions in paddy soils. Although, Ling and El-Kadi (1998) and Nakasone et al. (2004) have considered water and fertilizer applications, plant uptake, climate and its associated nitrogen transformation processes in their models, the effect of biological clogging, which significantly reduces the permeability of both wastewater and fertilizer applied paddy fields have not been investigated earlier, at least to the authors knowledge.

The focus of the present paper is to develop a numerical model to simulate the spatial and temporal dynamics of nitrogen species in a paddy soil from wastewater and fertilizer applied paddy fields along with biological clogging effect in a one-dimensional framework. Urea is considered as the fertilizer to be applied, which is the most common form of nitrogen fertilizer used. The numerical model incorporates urea hydrolysis, nitrification and de-nitrification processes in the paddy soil. In essence, the model takes into account the vertical water flow, oxygen mass transfer from air phase to water phase, microbial reactions as well as biological clogging to predict the vertical movement of nitrogen species in the paddy soil. The ultimate goal of the present work is to offer a comprehensive model that can be applied in wastewater and fertilizer applied paddy fields in order to estimate the nitrogen leaching loads to soil water in root zone and groundwater for implementing fertilizer management practices.

2. Mathematical modelling

Vertical movement of water in paddy soil under one-dimensional unsaturated condition can be described by Richard's model as expressed in Eqs. (1)–(3) (Tournebize et al., 2006; Soleimani et al., 2009).

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

$$K = K_r K_{sat} \quad (2)$$

$$\theta_w = \theta_r + \frac{\theta_s - \theta_r}{(1+|\alpha h|^{\beta})^{\eta}} \quad (3)$$

where $C(h) = \partial\theta_w/\partial h$ is the 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, K_{sat} is the saturated hydraulic conductivity and K_r is the relative permeability, θ_w is the water content (L^3/L^3); θ_s is the saturated water content; θ_r is the residual water content; α, β and η are fitting parameters.The diffusion of oxygen from the atmosphere to the soil and mass transfer from air phase to water phase (oxygen dissolution) are important processes in the unsaturated zone (Reible et al., 1989). The air phase oxygen concentration can be simulated using one-dimensional diffusive transport (Simunek and Suarez, 1994) process as expressed in Eq. (4).

$$\theta_g\left[\frac{\partial}{\partial t}(O_{2,g})\right] = \theta_g D_0 \frac{\partial}{\partial z}\left[\tau\frac{\partial O_{2,g}}{\partial z}\right] + \omega\left(O_2 - \frac{1}{H}O_{2,g}\right) \quad (4)$$

The tortuosity factor (τ) is a function of the air-filled porosity θ_a and the total porosity θ_s and is evaluated using the expression provided by Millington (1959) and the same is represented by Eq. (5).

$$\tau = \frac{\theta_a^{7/3}}{\theta_s} \quad (5)$$

The inter-phase mass transfer between gas and water phase is expressed by Henry's equilibrium law (Alfnes et al., 2004) as given in Eq. (6).

$$\theta_w\left[\frac{\partial}{\partial t}(O_2)\right]_{\text{exchange}} = -\omega\left(O_2 - \frac{1}{H}O_{2,g}\right) \quad (6)$$

where O_2 is the concentration in the water phase (ML^{-3}), H is the dimensionless Henry law constant, ω is the first order mass transfer coefficient (T^{-1}), $O_{2,g}$ is the oxygen concentration in the gas phase (ML^{-3}), $\theta_g = \theta_s - \theta_w$ is the volumetric air content, D_0 is the gas diffusion coefficient (L^2/T).

The conceptual understanding of nitrogen fate pathways in the root zone is shown in Fig. 1. The major processes that affect the nitrate leaching below root zone are the vertical water movement, wastewater or fertilizer application on paddy field, nitrogen transformations due to microbial reactions, dissolved organic carbon (DOC) and dissolved oxygen (DO) variation, adsorption in soil and biological clogging.

Nitrification and de-nitrification processes are the main transformation reactions in the nitrogen cycle. In the present work, dissolved organic carbon (DOC) is represented by the simplified chemical formula CH_2O, and assumed to be degraded by heterotrophic microorganisms aerobically.

Reaction equations for nitrogen species and DOC are expressed by Eqs. (7)–(10) (Reddy and Patrick, 1975; Lee et al., 2006).

$$r_1: \quad NH_4{}^+ + \frac{3}{2}O_2(aq) \rightarrow NO_2{}^- + H_2O + 2H^+ \quad (7)$$

$$r_2: \quad NO_2{}^- + \frac{1}{2}O_2(aq) \rightarrow NO_3{}^- \quad (8)$$

$$r_3: \quad CH_2O + \frac{4}{5}NO_3{}^- \rightarrow \frac{2}{5}N_2 + \frac{4}{5}HCO_3{}^- + \frac{1}{5}CO_2(aq) + \frac{1}{5}H_2O \quad (9)$$