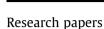
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## Numerical simulation and experimental study on farmland nitrogen loss ( to surface runoff in a raindrop driven process



HYDROLOGY

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#### ABSTRACT

It has been widely recognized that surface runoff from agricultural field is an important non-point pollution source, which however, the chemical transfer amount in the process is very difficult to be quantified in field since some variables and natural factors are hard to control, such as rainfall intensity, temperature, wind speeds and soil spatial heterogeneity, which may significantly affect the field experimental results. Therefore, a physically based nitrogen transport model was developed and tested with the so called semi-field experiments (i.e., artificial rainfall was used instead of natural rainfall, but other conditions were natural) in this paper. Our model integrated the raindrop driven process and diffusion effect with the simplified nitrogen chain reactions. In this model, chemicals in the soil surface layer, or the 'exchange layer', were transformed into the surface runoff layer due to raindrop impact. The raindrops also have a significant role on the diffusion process between the exchange layer and the underlying soil. The established mathematical model was solved numerically through the modified Hydrus-1d source code, and the model simulations agreed well with the experimental data. The modeling results indicate that the depth of the exchange layer and raindrop induced water transfer rate are two important parameters for the simulation results. Variation of the water transfer rate, e<sub>n</sub> can strongly influence the peak values of the NO<sub>3</sub><sup>-</sup>N and NH<sub>4</sub><sup>+</sup>N concentration breakthrough curves. The concentration of NO<sub>3</sub><sup>-</sup>N is more sensitive to the exchange layer depth,  $d_e$ , than NH<sup>+</sup><sub>4</sub>-N. In general, the developed model well describes the nitrogen loss into surface runoff in a raindrop driven process. Since the raindrop splash erosion process may aggravate the loss of chemical fertilizer, choosing an appropriate fertilization time and application method is very important to prevent the pollution.

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#### 1. Introduction

Non-point source pollution (NPSP) has become a very important environment pollution problem in China, largely because of the agricultural non-point source pollution (ANPSP). The pollution has posed a threat to the surface water and groundwater resources in China. There are a number of pathways through which agricultural chemicals could reach waterways. The solute transfer from soil to runoff has been recognized as a major ANPSP source. Therefore, a sound, accurate and physical based model for soil chemical transfer into runoff is required for quantitatively predicting NPSP, and reducing the ANPSP.

Traditionally, there are two methods to describe chemical transfer into runoff, the lumped, mixing-layer approach and the diffusion

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http://dx.doi.org/10.1016/j.jhydrol.2017.01.035 0022-1694/© 2017 Published by Elsevier B.V. approach. The diffusion approach is based on the assumption that there exists a stagnant film of water at the soil-runoff interface. from which solute transfer to runoff takes place by molecular diffusion (Wallach, 1991; Wallach and van Genuchten, 1990; Wallach et al., 1988). The diffusion-based models could be reasonably fitted with the experimental data, but the impact of raindrops to the whole process was not considered and the diffusion coefficient is not well defined physically (Ahuja, 1990). For the mixing-layer approach, a thin surface layer on soil is defined as the mixing zone, in which rainfall or irrigation water and the soil solution could be instantaneously mixed (Zhang et al., 1997). The soil solution is considered as the only source of solute transfer to runoff. This approach has been widely accepted and many related models have been developed (Ahuja et al., 1981; Ahuja and Lehman, 1983; Steenhuis, 2001; Steenhuis and Walter, 1980; Steenhuis et al., 1994; Zhang et al., 1997, 1999; Gao et al., 2004, 2005; Tong et al., 2009).

Based on the mixing-layer theory and Rose soil erosion model (Rose, 1985; Rose et al., 1994, 1998; Hairsine and Rose, 1991), Gao et al. (2004, 2005) proposed a physically based model that couples

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raindrop-driven transport of solutes from the mixing layer or 'exchange layer' into surface runoff with diffusion-driven transport from deeper soil layers into the mixing layer. In this model, all parameters were measured or based on previously published results, simulations could fit to the experimental data very well. Walker et al. (2007) used a simple laboratory experiment to explore the impact of the infiltration process on the raindrop-impact induced soil erosion, and they found that infiltration profoundly reduced soil erosion from raindrop-impact. Walter et al. (2007) used previously published experimental data (Ahuja et al., 1983) to test Gao's model (Gao et al., 2004, 2005) under both infiltration and non-infiltration conditions. In their study, it was assumed that the chemical concentrations in the runoff layer, prior to the generation of rainfall (that means the runoff layer hasn't been produced), were not zero. Considering the increase process of ponded water before the surface runoff occurrence. Bao et al. (2009) used two different kinds of soils to explore the raindrop-driven solute transport from soil to surface runoff and further tested Gao et al.'s (2004, 2005) model. However, their simulation results did not fit the observed data well at the early runoff time. Although the models developed above effectively incorporated both rain-drop induced mixing and diffusion processes into the surface runoff model and has been tested through many laboratory experiments, they have not been applied to field sites. Moreover, these studies focus on nonreactive chemicals like Chloride (Cl<sup>-</sup>) and Bromide (Br<sup>-</sup>) to investigate mechanism of soil chemical transfer into runoff. However, many reactive chemicals such as nitrogen and pesticides have been found to transport into runoff under raindrop erosion condition.

China is now the largest user of synthetic nitrogen fertilizer in the world (Sun et al., 2012), and the nitrogen fertilizer is an important approach to improve grain production in China. However, as the main cause for ANPSP, more attention should be paid on excessive or improper use of the nitrogen fertilizer. Minimizing nitrogen loss from an agricultural land is one approach to prevent surface water eutrophication and groundwater pollution. Large amount of studies have been conducted to investigate the transport process of nitrogen transfer from soil surface to overland flow. Higashino and Stefan (2014) developed a model to simulate NO<sub>3</sub>-N release process in a rice paddy field during the monsoon season. Their study results indicate that raindrop-induced pumping is an important mechanism that enhances NO<sub>3</sub><sup>-</sup>-N loss in runoff from rice paddy field. Based on their laboratory experimental results, An et al. (2013) found that water saturation and seepage conditions would affect soil loss and nutrient transport (NO<sub>3</sub><sup>-</sup>-N, NH<sub>4</sub><sup>+</sup>-N and PO<sub> $\overline{4}$ </sub>P) more than free drainage condition did, and raindrop impact could significantly promote nutrient loss by eroding sediments. Kwong et al. (2002) investigated the transport of N and P through surface runoff in the humid tropical countries, and their study results showed that application of nutrients during the dry season, as practiced in sugarcane cultivation, would reduce the off-site transport of N and P by runoff. Elrashidi et al. (2011) proposed a user-friendly technique to estimate nitrate-N loss by runoff and leaching for agricultural land, and the technique can be applied to a small agricultural watershed with several given climate and soil information data, such as the precipitation, soil series, land covers, acreage and hydrologic soil group. Williame and Michaeld (2011) established a paired-watershed field site to evaluate surface runoff loss of N, P and suspended sediment (SS) from different management systems for silage corn production, and ultimately developed a cropping system that could slow down the deterioration of water quality. In summary, some of the above studies tended to use laboratory results to explore the mechanism of nitrogen transport to the runoff, while others focused on investigating the loss of nitrogen in a watershed scale. However, it is still very limited for using modeling method to study nitrogen release from soil to surface runoff under raindrop-driven process in a field scale.

The objective of this study is to modify the model proposed by Gao et al. (2004, 2005) for raindrop impact on chemical release process and establish a model to predict nitrogen transfer from the initially unsaturated soil into the surface runoff under rainfall conditions. By modifying Hydrus-1D source code (Šimůnek et al., 2013), solved by the finite element method and the finite difference method, we obtain the numerical solution to the mathematical model. The developed model was tested with a series of experiments that are conducted in a bare soil plot.

### 2. Model description

#### 2.1. Soil water flow model

The governing equation for the water flow in the Hydrus-1D within the study domain [0, L] is given by the Richards' equation (Šimůnek et al., 2013):

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[ k \left( \frac{\partial h}{\partial z} + \cos \alpha \right) \right] - S \quad z \in [0, L], \tag{1}$$

where  $\theta$  is the soil water content [L<sup>3</sup> L<sup>-3</sup>]; *t* is time [T]; *h* is the pressure head [L]; *S* is the source/sink items [T<sup>-1</sup>]; *k* is the saturated hydraulic conductivity [LT<sup>-1</sup>];  $\alpha$  is the angle between the flow direction and the vertical axis; *z* is the vertical coordinate [L] (positive downward).

The initial hydraulic condition within the study domain [0, L] is,

$$\begin{aligned} h(z,0) &= h_i(z) & t = 0, z \in [0,L] \\ or \ \theta(z,0) &= \theta_i(z) & t = 0, z \in [0,L] \end{aligned}$$

where  $h_i$  [L] and  $\theta_i$  [L<sup>3</sup> L<sup>-3</sup>] are prescribed linear functions of z; t = 0 is the starting simulation time and L is the depth of the study domain.

For the upper boundary, if the rainfall intensity exceeds the soil water infiltration capacity, ponded water occurs, a "surface reservoir" boundary condition can be applied as,

$$-K\left(\frac{\partial h}{\partial z} + \cos\alpha\right) = q_0(t) - \frac{dh}{dt} \quad z = 0,$$
(3)

where  $q_0$  [L T<sup>-1</sup>] is the net infiltration rate, i.e., the difference between precipitation and evaporation.

For the bottom boundary condition, the subsurface drainage is controlled by the height of the water table, which is considered as the constant head boundary condition for simplicity,

$$h(z,t) = L_w \quad z = L, \tag{4}$$

where  $L_w$  is the water table level above the bottom [L].

### 2.2. Nitrogen transport and transformation model

After the surface water started on the soil surface, the soil water system can be divided into three layers vertically: the ponded-runoff layer, the exchange layer, and the soil below the exchange layer (Fig. 1). As shown in Fig. 1, the exchange layer is a thin layer above the soil profile, where raindrops drive the solute movement between runoff layer and surface soil. The solute concentration in the exchange layer can be expressed as  $c_{ei}$  [M L<sup>-3</sup>], where subscript letter *i* equals to 1, 2, 3 and denotes the N species, i.e., urea, NH<sub>4</sub><sup>4</sup>-N and NO<sub>3</sub><sup>-</sup>-N, respectively. The transport processes in the exchange layer are controlled by the interactions between raindrops and the soil surface, the raindrop induced mass transfer coefficient,  $e_r$  [L T<sup>-1</sup>] was calculated as in Gao et al. (2004, 2005),

$$e_r = \frac{ap}{\rho_b} \theta_s \tag{5}$$

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