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# A process-oriented hydro-biogeochemical model enabling simulation of gaseous carbon and nitrogen emissions and hydrologic nitrogen losses from a subtropical catchment

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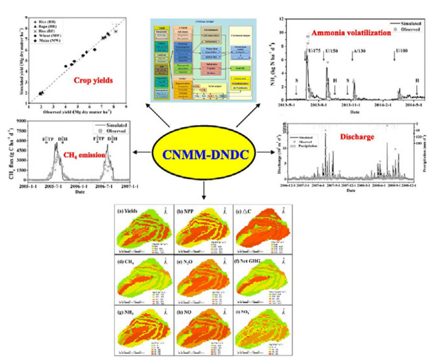
## HIGHLIGHTS

- A catchment model was built by coupling biogeochemical and hydrological models.
- The model was calibrated and validated for a subtropical catchment.
- The model showed encouraging performance for the initial test.
- The model showed scientific predictions at the subtropical catchment.
- The model can provide strategies for establishing sustainable ecosystems.

## GRAPHICAL ABSTRACT

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## ABSTRACT

Quantification of nitrogen losses and net greenhouse gas (GHG) emissions from catchments is essential for evaluating the sustainability of ecosystems. However, the hydrologic processes without lateral flows hinder the application of biogeochemical models to this challenging task. To solve this issue, we developed a coupled hydrological and biogeochemical model, Catchment Nutrients Management Model - DeNitrification-DeComposition Model (CNMM-DNDC), to include both vertical and lateral mass flows. By incorporating the core biogeochemical processes (including decomposition, nitrification, denitrification and fermentation) of the DNDC into the spatially distributed hydrologic framework of the CNMM, the simulation of lateral water flows and their influences on nitrogen transportation can be realized. The CNMM-DNDC was then calibrated and validated in a small subtropical catchment belonged to Yanting station with comprehensive field observations. Except for the calibration of water flows (surface runoff and leaching water) in 2005, stream discharges of water and nitrate in 2007, the model validations of soil temperature, soil moisture, crop yield, water flows in 2006 and associated nitrate loss, fluxes of methane, ammonia, nitric oxide and nitrous oxide, and stream discharges of water and nitrate in 2008 were statistically in good agreement with the observations. Meanwhile, our initial simulation of the

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catchment showed scientific predictions. For instance, it revealed the following: (i) dominant ammonia volatilization among the losses of nitrogenous gases (accounting for 11–21% of the applied annual fertilizer nitrogen in croplands); (ii) hotspots of nitrate leaching near the main stream; and (iii) a net GHG sink function of the catchment. These results implicate the model's promising capability of predicting ecosystem productivity, hydrologic nitrogen loads, losses of gaseous nitrogen and emissions of GHGs, which could be used to provide strategies for establishing sustainable catchments. In addition, the model's capability would be further proved by applying in other catchments with different backgrounds.



## 1. Introduction

Nitrogen is an essential component of ecosystems and a key control of ecological conditions and functions (e.g., Bouwman et al., 2013; Breuer et al., 2008). Intensive modern agriculture with high application rate of nitrogenous fertilizers results in excessive nitrogen remaining in the soil and extraordinary changes in the nitrogen cycle. These changes induce a series of environmental problems at the catchment, regional and even global scales (e.g., Deng et al., 2011a; Galloway et al., 2004; Tilman et al., 2001). Excessive nitrogen can be lost via emissions of nitrous oxide ($N_2O$), nitric oxide (NO) and ammonia ($NH_3$), as well as nitrate ($NO_3^-$) leaching and ammonium ($NH_4^+$) and $NO_3^-$ transport with surface runoff. The various nitrogen losses substantially contribute to concomitant global warming ($N_2O$), air pollution (NO and $NH_3$) and surface/groundwater contamination ($NH_4^+$ and $NO_3^-$) (e.g., Alvarez-Cobelas et al., 2008; Congreves et al., 2016; Fowler et al., 2013). Therefore, understanding of the nitrogen cycle has shifted from a focus on promoting food production to one aimed at realizing the sustainability of ecosystems. Thus, the future sustained ecosystems can not only keep food production in a highly efficient manner but also generate the lowest possible environmental hazards (e.g., Galloway et al., 2008; Tilman et al., 2001).

Reducing net greenhouse gas (GHG) emissions or realizing GHG neutrality is regarded as one of the essential indicators of ecosystem sustainability to adapt to climate change (e.g., Galloway et al., 2008). Net GHG emissions is defined as the sum of the net carbon dioxide ($CO_2$), methane ($CH_4$) and $N_2O$ emissions and is expressed as the amount of $CO_2$ equivalents on a given time horizon, e.g., 20 or 100 years (e.g., IPCC, 2006). Greenhouse gas neutrality refers to the status when the net emission (source) is fully offset by the net removal/uptake (sink). Due to the tight couplings between the transformation processes of carbon and nitrogen in terrestrial ecosystems, any change in nitrogen transportation and/or transformation may alter the production, consumption, and/or transportation processes of not only $N_2O$ but also $CO_2$ and $CH_4$, and thus may alter the net GHG balance. Therefore, interactions between the nitrogen cycle and the net GHG balance at the ecosystem, catchment, regional or even global scale is attracting increasing concern (e.g., Cui et al., 2014).

To establish sustainable ecosystems, it is essential to accurately quantify the nitrogen losses and the net emissions of GHG from terrestrial landscapes or catchments (e.g., Deng et al., 2011a, 2011b; Gao et al., 2014). Therefore, many field experiments have been conducted to investigate nitrogen losses or GHG fluxes at different spatial scales (e.g., Alvarez-Cobelas et al., 2008; Garnier et al., 2014; Pacheco et al., 2015; Zhou et al., 2013, 2015). However, field experiments generally only focus on one portion of nitrogen or GHG-relevant processes. Therefore, field experiments alone are limited to simultaneously quantify all of the nitrogen losses and the net fluxes of different GHGs. Furthermore, the high spatial and/or temporal heterogeneity of nitrogen and carbon processes create an enduring challenge to extrapolate field measurements to a catchment, or longer time periods. Process-based models have been developed to overcome this limitation. Because of the high complexity of nitrogen losses jointly controlled by water flows and multiple transformations of this element in soils, to date, few models include both comprehensive hydrologic and biogeochemical processes. This situation hinders the accurate estimation of total nitrogen losses and GHG fluxes from a catchment. The well-developed distributed hydrological models focus mainly on the simulation of water and nutrient movements that are driven by heterogeneous environmental factors (e.g., Bosch et al., 2011; Ferrant et al., 2011; M. Liu et al., 2014). But the models simplify the simulation of nitrogen transformations in soil, which is usually a significant limitation on the accurate estimation of nitrogen losses by species and related GHG emissions by gas (e.g., Breuer et al., 2008). In contrast, process-oriented biogeochemical models, such as the DeNitrification-DeComposition (DNDC) model (Li et al., 2000, 2006, 2012; Li, 2007), have been well developed in recent decades and are able to comprehensively simulate nitrogen transformation, vertical movements of water and nitrogen in soil and effluxes of carbon and nitrogen gases. These types of models can perform well on flat lands, yet are inapplicable to assessing lands with significant slopes (Deng et al., 2011a). Because they generally ignore the lateral flow and related lateral nutrient movements (e.g., Chen et al., 2008; Li et al., 2006; Li et al., 2014). Several studies have shown that the accuracy of total nitrogen loss simulation from catchments can be improved by incorporating biogeochemical models with more detailed nitrogen transformation/transportation into distributed hydrological models (Breuer et al., 2008; Chen et al., 2008; Ferrant et al., 2011).

In recent years, some efforts have been made to couple hydrological and biogeochemical models. For instance, Pohlert et al. (2007) improved the nitrogen processes in SWAT (Neitsch et al., 2002) based on those of DNDC (Li et al., 2000). However, this model was not widely used as the new version did not perform better than before on the estimation of non-point source pollutions in mesoscale catchments (Bosch et al., 2011). Deng et al. (2011a, 2011b) incorporated two fundamental hydrologic features of surface runoff production and sediment erosion into the DNDC to simulate the nitrogen load of surface water in a small-scale catchment. In their study, only the vertical movement and surface lateral transport of water and nutrients were simulated, assuming that the laterally transported water and nutrients directly flow into the stream. However, the exchanges and/or interactions of water and nitrogen among adjacent simulation units were ignored (Deng et al., 2011a). This limitation may hinder the model's application in other catchments or for virtual experiments to understand these complex interactions. Haas et al. (2013) coupled the biogeochemical model LandscapeDNDC (e.g., Chirinda et al., 2011) with the catchment hydrological model CMF (e.g., Kraft et al., 2011) using a coupler. They tested the coupled model in simulating nitrogen transformation and movement along a virtual hill slope.

The Catchment Nutrients Management Model (CNMM) is a very recently established hydro-biogeochemical model, focusing on the simulation of nitrogen and phosphorous losses at the catchment scale. This model has been validated in a typical subtropical catchment in central China (Li et al., 2017). CNMM is established on basic hydrologic theories and functions for vertical and horizontal hydrologic processes, which are referred to those adopted by the Distributed Hydrology-Soil-Vegetation Model (DHSVM, Wigmosta et al., 1994) and GEOtop (Rigon et al., 2006). But it incorporates relatively simplified biogeochemical processes, which in turn rely on calibration with local data. Nevertheless, CNMM is designed with flexible interfaces that enables convenient coupling with other biogeochemical models (such as DNDC) using modules (Li et al., 2017).