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Development and application of a fully integrated model for unsaturated-saturated nitrogen reactive transport

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ABSTRACT

This paper presents a fully integrated model to simulate coupled unsaturated-saturated flow and reactive transport of ammonium and nitrate, the two major nitrogen species. Based on our previous work of developing a coupled model of unsaturated-saturated flow and solute transport of a single species, the key contribution of this study is to develop a new mathematical model and the new computer code for a comprehensive list of biogeochemical reactions, which are necessary for simulating nitrogen reactive transport. The computer code is verified by comparing its simulated results with those obtained using another model for a synthetic case. Model calibration and validation are conducted for two real-world cases to simulate nitrogen reactive transport. The two cases are at the experimental plot scale with the sewage water irrigation and at the field scale with the septic tank effluent infiltration, respectively. Quantitative evaluation of the numerical modeling results indicates that the new model and computer code can accurately simulate field observations of moisture content, water table elevation, and nitrogen concentration. For example, the root mean square error for simulating moisture content can be as small as 0.01. The code is computationally efficient to capture spatial and temporal trends of nitrogen concentrations at the field scale with a large number of computational nodes and time steps. The fully integrated model is a promising tool for large-scale modeling of water flow and nitrogen transformation and transport under complex conditions in agricultural and urban environments.

1. Introduction

As nitrogen is an essential nutrient for crop growth, applying nitrogen fertilizer is necessary to replenish soil nitrogen deficiency and to increase crop yield. However, excessive use of nitrogen fertilizer has caused high nitrogen concentration in crop soils and groundwater aquifers (Brady and Weil, 2008; Gastal and Lemaire, 2002). Nitrogen pollution in crop soils and/or groundwater has a number of adverse impacts on human health and environmental quality (Jalali et al., 2008; Muyen et al., 2011; Valipour, 2014a). For example, high nitrate concentration in drinking water is carcinogenic, and may also cause blue baby syndrome (Wolfe and Patz, 2002). Environmental regulations have been established for monitoring nitrate concentration in drinking water for human consumption (USEPA, 2012). In order to improve nitrogen management in agricultural areas and to minimize nitrogen pollution risks, it is important to estimate nitrogen contributions from various contamination sources to the subsurface and surface environments. This entails quantitative simulation of transformation and transport of nitrogen in soil zones and groundwater aquifers.

A large amount of efforts have been spent to characterize and simulate physical, chemical, and biological processes that control nitrogen transformation and transport among different nitrogen pools in soil zones and groundwater aquifers. The processes and their interactions are complicated, including mineralization, immobilization, nitrification, denitrification, and volatilization (Xu et al., 2012; Canion et al., 2014). In addition, these processes are heavily influenced by human activities, soil water dynamics, groundwater recharges, and soil vegetation systems (Huang and Huang, 2009). To comprehensively investigate the processes from a system perspective, modeling approaches have been widely used to provide quantitative estimates of soil water flow and nitrogen reactive transport especially at field scales (Wriedt and Rode, 2006). During the past several decades, a number of nitrogen reactive transport models have been developed, such as DAISY (Hansen et al., 1991), ANIMO (Groenendijk and Kroes, 1999), RISK-

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N (Oyarzun et al., 2007) and ArcNLET (Rios et al., 2013; Wang et al., 2013; Zhu et al., 2016). These models have different levels of complexity for simulating nitrogen reactive transport in both unsaturated and saturated zones. While the models usually include a module for simulating complex soil nitrogen transformation, they are inadequate to simulate three-dimensional (3-D) groundwater flow and nitrogen transformation in groundwater aquifers, which limits their applications to complex regional domains with both soil and groundwater flow. Therefore, a fully 3-D unsaturated-saturated model is necessary for nitrogen reactive transport modeling (Wang et al., 2003). However, the computational cost of such a model may not be practically affordable due to high non-linearity of unsaturated flow.

In order to reduce the computational burden, coupled unsaturated-saturated models have been developed by explicitly or implicitly linking an unsaturated soil nitrogen model with a saturated groundwater nitrogen model (Stenemo et al., 2005; Ajdary et al., 2007; Rahil and Antonopoulos, 2007; Bonton et al., 2012). In the explicit coupling method, unsaturated water flow and nitrogen transformation processes are simulated using soil-water and nitrogen models, such as EPIC (Williams, 1995), Agriflux (Banton and Larocque, 1997) and mRISK-N (Wriedt and Rode, 2006); groundwater flow and nitrogen transport processes are simulated using groundwater models, such as RT3D (Clement, 1997), MT3DMS (Zheng and Wang, 1999), and HydroGeoSphere (Therrien et al., 2006). The soil and groundwater models are executed separately, and water and nitrogen fluxes computed by the soil nitrogen models are used as the upper boundary condition of the groundwater nitrogen models. The explicit coupling methods usually require a fixed water table, which may limit feedbacks between the linked models (Wriedt and Rode, 2006). In practice, the explicit coupling methods are unsuitable under dynamic water flow conditions, since soil water and groundwater hydraulic conditions change substantially due to climate conditions and human activities. Therefore, the implicit coupling methods are necessary to simultaneously simulate flow and nitrogen reactive transport in soil and groundwater systems. Following Gärdenäs et al. (2005), implicitly coupled models are referred to as integrated models hereinafter. However, it happens often that the nitrogen reactions in either soil or groundwater system are oversimplified in existing integrated models, which hampers the model compatibility and adaptability to general hydrological and nitrogen transport conditions (Lee et al., 2006; Bonton et al., 2012). This problem can be resolved by developing an integrated model that adequately simulates nitrogen reactive transport processes in both soil zones and groundwater aquifers.

The objective of this study is to develop a fully integrated model of nitrogen reactive transport for simulating nitrogen contaminant transport in soil and groundwater systems. This development is based on the existing integrated model developed in our previous work for simulating unsaturated-saturated flow and solute transport (Zhu et al., 2012, 2013). The previous model only considers transport of a single species, and cannot be used for simulating reactive transport of multiple nitrogen species. The model is extended in this study by including the transport and transformation processes of multiple nitrogen species. In the existing integrated flow and transport model, one-dimensional (1-D) average vertical unsaturated flow and nitrogen reactive transport are simulated in the soil zone, and 3-D groundwater flow and nitrogen reactive transport are simulated in the groundwater system. In this study, the unsaturated and saturated zones are integrated as a whole to couple flow components, solute transport, and nitrogen reactions with their specific characteristics in the unsaturated-saturated zones. The model accuracy and computational efficiency are evaluated in three cases, including a hypothetical 1-D case, a field case with treated sewage water irrigation, and a 3-D case with point nitrogen sources from septic systems. The integrated model is in spirit similar to TOUGHTREACT-N (Gu and Riley, 2010; Finsterle et al., 2012) in that the latter one is also based on an integrated model that simulates coupled processes of advective and diffusive nutrient transport in soil and groundwater. However, our model solves the partial differential equations of groundwater flow and saturated solute transport in a different way, using the finite volume method and a hybrid method of finite element and finite difference. Our numerical methods have the advantages of keeping mass balance and obtaining accurate solution near irregular domain boundaries (Zhu et al., 2012, 2013). Furthermore, our model is more computationally efficient, because the unsaturated domain is divided into a number of sub-areas and the unsaturated flow and transport in each sub-area is simplified to be one dimension. This reduces the number of computational nodes to save computational cost for large-scale nitrogen reactive modeling.

2. Methodology

The model presented in this paper is an extension of our previous model of integrated unsaturated-saturated flow and solute transport (Zhu et al., 2012, 2013) by including a comprehensive list of biogeochemical reactions involved in nitrogen reactive transport. The major nitrogen transformations in the unsaturated and saturated zones considered in the model are shown in Fig. 1. The soil nitrogen includes both organic and inorganic nitrogen. The organic nitrogen is in two major pools: (1) the litter pool composed of crop residuals, dead roots, and microbial biomasses, and (2) the humus pool composed of stabilized decomposition products. The inorganic nitrogen are ammonium and nitrate. All the soil nitrogen transformation processes depicted in Fig. 1 (i.e., mineralization/immobilization, nitrification, denitrification, and volatilization) are simulated in the integrated model. Denitrification in groundwater aquifers is designed in the model as a user option. When the temperature is suitable and sufficient organic carbon exists, the denitrifying bacteria can survive in this anaerobic environment and denitrification occurs (Soares, 2000; Hantush and Mariño, 2001). Otherwise, users do not activate the denitrification function of the model. Nitrification of ammonium is also kept in the model as a user option, and it is activated if nitrification is observed in laboratory and field studies (Smith et al., 2006).

Fig. 2 shows the flowchart of the nitrogen reactive transport modeling. Within each time step, the simulation starts with solving the water flow equations. Subsequently, the transformation processes related to ammonium (i.e., volatilization, mineralization/immobilization, and nitrification) are simulated as source terms of the ammonium transport equations. After obtaining the ammonium concentration, the model starts to simulate the nitrate transformation processes by solving the transport equations. The 1-D and 3-D advection-dispersion equations (ADEs) are used to describe nitrogen transport in soil and groundwater, respectively. The equations are discretized and solved instantaneously by assembling a unified matrix with linking mass fluxes (Zhu et al., 2013). The details of reactive nitrogen transport modeling are given in Sections 3.2 and 3.3.

3. Model development

3.1. Unsaturated-saturated water flow dynamics

The integrated flow model is used as the flow module of the integrated model. This module is described briefly here to make the paper self-contained, and more details are referred to Zhu et al.