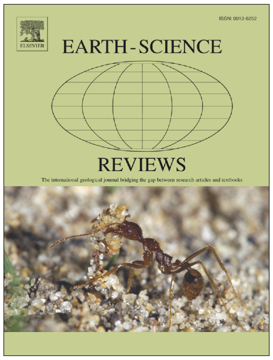

Coupling soil water processes and nitrogen cycle across spatial scales: Potentials, bottlenecks and solutions

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the rainfall event scale, the dry antecedent SWC condition may increase the soil N mineralization and nitrification, which may in turn create a more abundant source of N for leaching (Goldberg and Gebauer, 2009; Castellano et al., 2013; Ouyang et al., 2017). Second, at the yearly scale, dry conditions may limit plant N uptake and result in more legacy N from previous N input (manure, fertilizer etc.) (Loecke et al. 2017; Iqbal et al., 2018). Third, under dry or wet initial conditions, the major component of water source (e.g., lateral flow, shallow ground water flow and matrix flow) in the hydrograph can be different, which could result in different N concentrations in leachate and in the stream (van Verseveld et al., 2008). However, the governing mechanisms for this phenomenon can be vary with respect to different temporal and spatial scales, climate conditions, and geological and pedological backgrounds.

3.3 Models lack robust hydrological or biogeochemical mechanisms

When simulating the soil N cycle in most models at field, watershed and regional scales (e.g., using DNDC, DayCent, SWAT and CLM), soil water processes are usually simplified as parameters easily to be measured or predicted by empirical functions. This includes three main steps. First, soil texture, bulk density and organic matter are used to derive soil hydraulic properties (saturated hydraulic conductivity, SWCs at saturation, field capacity and wilting point) from pedotransfer functions (PTFs). Second, these soil hydraulic properties, as well as other meteorology, vegetation and soil parameters, are used in models to simulate the SWC, water filled pore space, oxygen content and thus oxidization-reduction potential. Third, the oxidization-reduction potential is then used to calculate the nitrification and denitrification rates based on formulas like the Michaelis-Menten equation.

Uncertainty surrounding soil hydraulic parameters has been recognized as one of the major obstacles for achieving optimal simulations (Chirico et al., 2010; Baroni et al., 2017). Direct measurements of soil hydraulic parameters are costly and time-consuming in the laboratory and field, thus restricting the availability of high spatial resolution data for model simulations (Chirico et al., 2010). Indirect methods, especially the PTFs, have been developed to estimate the SHPs from easily measurable soil physical and chemical properties (Saxton et al., 1986). However, previous studies have demonstrated that applying existing PTFs always introduced substantial uncertainty as they were used outside the datasets used to develop them (Chirico et al., 2010; Liao et al., 2014). To improve simulation, accuracies and spatial heterogeneities of soil hydraulic parameters should be considered in modelling (Sciuto and Diekkrüger, 2010). In addition, factors like subsurface flow, soil matric potential, and soil drying-wetting processes should also be properly mathematically formulated and incorporated in model simulations (Lin et al., 2015).

4. Possible solutions

4.1 Hydrogeophysical tools to study the coupled soil water-N cycle

Non-invasive hydrogeophysical tools have been applied to investigate soil water processes from plot to catchment scales (Fig. 4). Although the success of using these tools to detect soil water processes are restricted by various factors like wetness, salinity, soil texture, etc (Doolittle, et al., 2007; Doolittle and Brevik, 2014). For example, Zhou et al. (2001) used ERT to detect the three-dimensional spatio-temporal variations of SWC at the field scale, while Greer et al. (2017) used the same tool to visualize wetting fronts of subsurface flow in coal mine valley fill. Robinson et al. (2012) and Zhu et al. (2010) relied on repeated EMI surveyes to derive the subsurface soil water redistribution and flow paths at the farm scale. Guo et al. (2014) used time-lapse GPR survey to reveal the subsurface lateral preferential flow network at the hillslope scale.

Fig. 6. Scheme of coupling the soil water-N cycle across different spatial scales. Geophysical tools are used to detect the soil water processes at small scale; soil hydrology and N cycling models are used to derive critical parameters and functions through small scale study; hydropedological functional units are the basis the small scale monitoring and simulation, as well as the key to upscaling.

Because hydrogeophysical tools can be used to determine the spatio-temporal variation of soil water processes, they have great potential to reveal subsurface N loss paths and hot spots/moments of N biogeochemistry associated with soil water processes (Fig. 4). Some attempts have been made to use hydrogeophysical tools to study the soil N cycle. For example, Kennedy et al. (2018) used GPR to map the thickness of peat and then, coupled with conventional measurements of peat N concentrations, calculated the N stock. McDaniel et al. (2017) built a relationship between measured apparent electrical conductivity and N_2O flux and then used this relationship to map the spatial pattern of N_2O flux. However, most of these studies focused on indirect measurement and mapping of soil N stock and flux based on relationships with soil properties that affected the readings of these hydrogeophysical tools.

In the future, hydrogeophysical tools will be linked to innovations in soil N-sensing techniques (Fig. 4). New electrochemical tools promise to allow *in situ* measurement of N dynamics without disturbance to soil structure as current methods demand (e.g., Ali et al., 2017). The U.S. National Academy of Science identified the development of ‘highly sensitive, field-deployable sensors’ as one of five breakthroughs that are required to meet challenges facing food and agricultural sciences (National Academies of Sciences, Engineering, and Medicine, 2018). However, several difficulties remain in this aspect. First, knowledge gaps between soil water processes and the N cycle have not been addressed and fully resolved. Further analyses are still needed by soil hydrologists, biogeochemists and microbiologists to interpret the outputs of these tools. Second, errors and uncertainties have also been reported when using these tools to detect SWC, subsurface flow and soil N parameters (Doolittle et al. 2007; Zhu and Lin, 2009). New technologies and methods of analysis will be required to meet these challenges. Coupled use of automatic high-resolution and high-accuracy hydrogeophysical tools and electrochemical N sensors will create an enormous amount of data. With further development of machine learning and artificial intelligent techniques, we would expect a bright future for using these tools to visualize the spatial and temporal variations of the soil N cycle.

4.2 Upscaling based on the concept of hydropedological function units

To couple the soil water process with soil N cycle, observations and simulations at small spatial scale should be properly upscaled (Fig. 6). The concept of hydropedological function units can be useful in the upscaling of soil water-N cycling dynamics (Lin, 2011). Soil water-N cycle is jointly and interactively affected by topographic, pedological and hydrological properties (Sogbedji et al., 2000; Stewart et al., 2014; Zhu et al., 2015). The concept of hydropedological function units is used to delineate a large study area into small units and assumes that topographic, pedological and hydrological properties controlling soil water-N cycle are comparatively homogeneous within each unit. Critical soil water and N cycling parameters and mechanisms of these units can be upscaled by constructing the empirical functions between these parameters and ancillary soil, topography and vegetation variables, and then incorporating them into the large scale models and investigations. This upscaling can be based on time stability concepts and block kriging (Crow et al., 2012), and hydrological connections and flows among different units should be addressed at large scales. For example, to upscale the N leaching simulation, Schmidt et al. (2008) delineated so-called "nitrogen response units" and regressed N leaching with percentages of cereals in crop rotations and livestock. In addition, critical functions determined at small scales can also be used to revise or add new modules to the large scale models. For example, to incorporate the small scale observations of subsurface flow at soil-bedrock interface, Fu et al. (2014) revised the SWAT model by adding the corresponding module.

4.3 Coupling soil hydrology and N biogeochemistry models

Coupling soil hydrology models with N biogeochemistry models can be another strategy for integrating soil water-N cycles to improve simulations (Fig. 4). Models are usually developed for certain purposes and to capture specific processes. For this reason, nearly no model can claim that it could describe all different processes well and satisfy all the requirements of the clients. For example, although DNDC is good at simulating N biogeochemical processes, it sometimes performs poorly in capturing soil water processes since it is based on the simple cascade approach instead of the Richards' equation (Kröbel et al., 2010). Conversely, although Hydrus simulates the percolation and SWC well, it yielded worse simulations of N uptake and N concentration than models addressing the crop growth and N dynamics (Doltra and Muñoz, 2010). Therefore, by coupling models with different purposes, weaknesses of these models can be minimized, and thus the soil water-N cycle can be better simulated. For example, to solve the deficits of DNDC, Kraus et al (2015) suggested coupling it with more complex soil hydrology models based on the Richards' equation.

Recently, Vereecken et al. (2016) proposed that a new generation of models based on a systemic approach should be developed to comprise relevant physical, chemical, and biological processes to address knowledge gaps in understanding soil processes and their interactions. Model improvements have also been attempted by revising the soil water module in N biogeochemistry models, revising the N biogeochemistry module in soil hydrology models, or constructing new models that integrate sophisticate hydrological and biogeochemical processes. For example, Li et al. (2007) built the water and N management model based on the processes of water dynamics, soil temperature, C and N cycles in soils and crops, crop growth, and agricultural management practices. Zhang et al. (2016) the extended the distributed time variant gain model by integrating detailed processes of soil biogeochemistry ecology. However, we prefer coupling existing models to improve the simulation of soil water-N cycle since it can be easier and more time-efficient than building new models and revising existing models (Jones et al. 2001). One model in this category is the Agricultural Productions Systems sIMulator (APSIM; Holzworth et al. 2014). It operates on a daily time step and has a modular platform, allowing users to add or remove submodels of various complexity. For example, SWC can be simulated with a relatively simple 'tipping bucket' model or with the SWIM model that is based on numerical solution of the Richards' equation and advection-dispersion equations (Stewart et al. 2006; Dietzel et al. 2016).

5. Summary

Soil water processes are critical controls of the soil N cycle. We reviewed the research progresses of SWC spatio-temporal variation and subsurface flow, the soil N cycle, and relationships between these two components. Bottlenecks to coupling the soil water-N cycles, include not considering soil water processes in the soil N cycle, treating soil water-N cycle as a black box, a lack of upscaling, and simplifying soil water parameters in N modeling. Based on these, we proposed possible solutions for coupling the soil water -N cycle. Possible solutions include the use hydrogeophysical tools to better detect soil water-N processes, upscaling the small scale monitoring and simulation based on hydropedological functional units, and coupling soil hydrology models with N cycle models.

This paper provides an alternative approach to studying the soil water-N cycles that will benefit and enhance our understanding of critical zone sciences. This approach will benefit efforts to better understand how soil and water interact to produce sources of greenhouse gas emission and water eutrophication. Specifically, by opening the black box of the soil water-N cycle across spatial scales, the temporal and spatial heterogeneities of N losses can be better predicted and explained. This information is critical to better manage the N cycle for food production and environmental quality.

An understanding of the coupled water-N cycling mechanisms of NO_3^- leaching and N_2O emissions can aid the development of strategies to reduce these N losses. The concepts of static and dynamic water properties could be used to guide precision N fertilizer (or manure) and irrigation managements that maintain the crop production while minimize the negative N environmental impacts. For example, farmers can apply N fertilizer in narrow concentrated ‘bands’ or homogenous ‘broadcast’ applications, and this decision could be informed by the importance of dynamic flow processes; irrigation could be planned around SWC thresholds that produce large N losses. In addition, by opening this black box, strategies (e.g., from different expertise like agricultural, engineering, ecological and sociological) to intercept non-point N contamination and to remove and immobilize excessive inorganic soil N can be targeted on the hot spots and hot moments of N losses. This will greatly improve the effectiveness and pertinence of these strategies.

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