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Modelling nitrogen transport and turnover at the hillslope scale – a process oriented approach

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Abstract: Biogeochemical models used for simulating greenhouse gas (GHG) emissions and nutrient leaching are mainly designed for the plot scale. Lateral fluxes of nutrients such as nitrate, which may be important drivers for soil GHG emissions, are not or only scarcely considered and explored in such models. This is due to the complexity of microbiological, physico-chemical and plant processes which need to be investigated and simulated along one spatial dimension, a column. The introduction of a second (a hillslope) or third (entire landscapes) spatial dimension is likely to introduce additional complexity which can hardly be handled by most models. However, plot scale models, validated with data obtained from plot scale studies, will systematically under- or overestimate key GHG production and consumption processes if lateral in- or efflux of nutrients to or from a given site is of significant importance. E.g. in laterally connected environments, such as riparian zones denitrification will be fuelled by lateral influx of nitrate from uphill positioned fertilized land. Thus, landscape approaches are needed to identify and realistically simulate in particular indirect GHG emissions. From our view integrated model systems can help to identify processes and ecosystem conditions in connected ecosystems across a landscape, which may also be used as a tool guiding the design of new field studies to further quantify the importance of lateral nutrient transport for soil GHG emissions.

***Keywords**:* hillslope hydrology, nutrient turnover, model coupling, GHG emissions.

1 INTRODUCTION

The nutrient budget and turnover of a landscape is one of the key indicators for sustainability. Hydrological or biogeochemical transport and turnover processes in landscapes are well-represented in the literature and a variety of different model approaches from empirical-conceptual to process-oriented methods exist.
Landscapes are characterized through highly interwoven landscape components, different land uses, often a dynamic topography and most of all, lateral interaction within and between ecosystem components [Cellier et al., 2011; Durand et al., 2011]. This intrinsic interaction leads to the development of hot spots (in space) and hot moments (in time), where water, carbon and nitrogen gains or losses can be substantial, even dominating the overall budget of landscape nutrient turnover and losses [McClain et al., 2003; Groffman et al., 2009]. However, experimental

sites with long term measurements dealing with the lateral distribution of nutrients are still scarce. Experiments with shorter time horizons, where the lateral distribution is considered include the experiments by Hill [1994] and Grant and Pattey [2003].
Joint modeling of biogeochemical reactions and physical transport is hampered by the complexity to predict the path ways of water along the hillslope [Sivapalan, 2003] and the complexity of biogeochemical reactions with unknown lateral boundary fluxes in the subsurface zone. Therefore joined modelling approaches are developed and used scarcely and are often limited in their scope. Existing models can be distinguished into three different classes of connectivity: (1) Models without spatial explicit water transport in the subsurface, (2) models with spatial explicit water transport, but without solute transport and (3) models with explicit spatial water and solute transport. The first class includes lumped and semidistributed hydrological models, extended with biogeochemical routines which can either be empirical models like MONERIS [Behrendt et al., 2000] or simplified conceptional models like INCA [Whitehead et al., 1998], HBV-N [Arheimer and Brandt, 1998] or LASCAM [Sivapalan et al., 1996] and SWAT [Arnold et al., 1998] which uses a more complex approach for nitrogen cycling. However, applied in a multi-model ensemble framework SWAT showed less good performance than some of the simpler approaches mentioned above [Exbrayat et al., 2010, 2011]. Effort has been undertaken to improve the nitrogen turnover routines of SWAT by replacing the biogeochemical process descriptions with more sophisticated plot level models like DAYCENT by Li et al. [2004] and parts of DNDC by Pohlert et al. [2007]. Since both approaches still use the semi-distributed transport mechanism of SWAT, neither water nor solutes are explicit routed through the landscape. The second class of models consist mainly of studies, where the distribution of water is calculated using a spatial explicit approach first. The resulting distribution of soil water content is then used as input time series to run plot scale biogeochemical models. Examples of this approach are AHM/CENTURY [Meixner and Bales, 2003] and a combination of MIKE-SHE with DNDC [Cui et al., 2005]. With these approaches, effects of changes in the water regime on biogeochemical fluxes can be modelled including effects of a changed upslope water management on downslope areas. The RhesSYS model-system [Tague and Band, 2004] is one of the few approaches where water and solutes are transported from one spatial model unit to another, belonging to the third class of model structures. As a transport model, RhesSYS is using a DHSVM-like [Wigmosta et al., 1994] water and solute flux model. The biogeochemical model is process oriented and of intermediate complexity.

DHSVM is based on a large set of coupled hypotheses concerning the dominant flow paths in the subsurface. The base hypotheses in DHSVM include impervious bedrock, a strong decrease of conductivity with depth and topography as the only driver of lateral flow. The saturated as well as the unsaturated zone is assumed to be well mixed [Wigmosta and Lettenmaier, 1999; Wigmosta et al., 1994]. Such settings can be found in reality, however, for lowlands and rolling hills with deep soils, these assumptions can be completely wrong. Secondly, the biogeochemical model integrated into RhesSYS lacks the explicit modelling of trace gas emissions. The TNT2 model [Beaujouan et al., 2002] has a similar structure and scope. Although the fully distributed transport model is based on TOPMODEL, the base hypotheses are comparable to RhesSYS. For other hydrological settings, like in lowlands, completely different models need to be coupled with the biogeochemical model.

The question remains, whether the separate modelling of hydrological and biogeochemical fluxes in landscapes is still state-of-the-art or whether we need more models such as RhesSYS that explicitly consider the intrinsic interactions of C, N and water (or any other nutrient or pollutant). Due to the often variable complexity of landscape, a model that can reflect the different hydrological run off generation processes would be also favourable in contrast to the most often fixed model structure of today’s hydrological models. In this paper, we are presenting such a new concept of an integrated model, based on the modular hydrological modelling framework CMF [Kraft et al., 2011] coupled with the complex biogeochemical modelling framework LandscapeDNDC [Haas et al., 2011]. The models are wrapped as libraries of the Python language and exchange fluxes, states and parameters in a high frequency during runtime, as shown by Kraft et al. [2010].

2. METHODS

The catchment modelling framework CMF [Kraft, 2011; Kraft et al., 2010, 2011] is an open source library for the Python language to create a wide range of different hydrological models using model building blocks like water storages, boundary conditions and flux equations, based on the finite volume method as outlined by Qu and Duffy [2007]. These objects are used to create a network of water fluxes, using the boundary conditions and water storages as nodes of the network, and the flux equations as the edges. For this study, we set up a two dimensional hillslope model, using the Richards equation for subsurface flux and infiltration, and a kinematic wave equation for surface runoff.

The LandscapeDNDC model [Haas et al., 2011] is a modularized and advanced form of the DNDC-model [Li et al., 1992; Li, 2000]. The model is designed to model the C- and N-budget of ecosystems with a special focus on trace gas emissions. It consists of modules for plant growth, soil biogeochemistry, water and solute percolation (only vertical transport), microbiological processes like nitrification and denitrification as well as processes to calculate the in-canopy and soil energy fluxes. In this study, the water and solute transport module is not used. The transport process is instead modelled by CMF. In the virtual example shown, plant growth and biomass allocation, organic matter mineralisation, nitrification and denitrification processes play an important role.
Plant growth is simulated with a simple temperature sum based crop growth model as described in the original DNDC model [Li et al., 1992; Li, 2000]. Biomass allocation and harvest follows phenological states, and thus a yearly / seasonal cycle. Organic matter mineralization is modelled using first order kinetics triggered by organic matter quality like the carbon to nitrogen ratio, water content, temperature and size and activity of microbial biomass. Nitrification is modelled as a function of the ammonium concentration in the soil solution, soil temperature and size and activity of nitrifyer biomass. Most of the nitrified ammonium produces dissolved nitrate in the soil solution, however, small fractions are oxidised to nitric and nitrous oxide eventually degassed to the atmosphere depending on diffusion conditions and concentration gradients. Denitrification is driven by available carbon, the nitrate concentration, anaerobic soil fractions and denitrifier biomass and activity. By denitrification, nitrate is reduced to nitrite, nitric and nitrous oxide and finally to elementary nitrogen. The model divides any simulated soil layer in aerobic and anaerobic fractions using the concept of the anaerobic balloon. The size of the anaerobic balloon can change rapidly in dependence of soil respiration and diffusion of atmospheric oxygen into the soil, the latter mainly controlled by soil moisture.

For this study, we have chosen a scripting language approach to gain access to all states and parameters of the complex models in a short development time. While CMF was written as an extension to the Python language from scratch, LandscapeDNDC has been furnished with a Python interface to most of the internal states and parameters for this study. For more details see [Haas et al., 2011]. A Python script can alter the states and parameters of both LandscapeDNDC and CMF, and it can trigger the execution of the models for a single time step. Due to the modular structure of LandscapeDNDC, the realisation of the interface was possible in a few days.

Using the complete interface, the strategy which data are being exchanged needs to be considered. If the output of one model can be used as driving parameter of the other model, the steering script can simply update the parameter to let the joined model react accordingly. The leaf area index, calculated by LandscapeDNDC and used as a parameter for the CMF evapotranspiration routine is an example for this trivial case. Since all water related processes are disabled in LandscapeDNDC, the soil moisture can serve as a related example; the soil moisture is calculated by CMF and used as a driving parameter for LandscapeDNDC. However, not in all cases such a clear distinction concerning the affiliation of state variables to one of the model domains can be made, e.g. the concentration of dissolved matter in the soil. The concentrations are both affected by transport, calculated by CMF and biogeochemical reactions, calculated by LandscapeDNDC. In principle, two different strategies are possible to model shared system states: (a) the coupled models exchange fluxes only, and are responsible to update their own state variables in reaction to the external fluxes, and (b) the models overwrite their exposed state variables successively. Option (a) yields the benefit of a clearer and more modular approach. However, approach (b) has been proven in our experience to lead to higher stability and prevents inconsistent values for the shared state variables across the model domains. In this study, approach (b) has been used. This approach uses four steps: (1) LandscapeDNDC runs for one hour and changes internally the solute concentrations due to the biogeochemical reactions. (2) The steering script reads the concentrations from LandscapeDNDC and overwrites the concentrations in CMF. (3) CMF runs the same time step with updated concentrations and distributes the solutes in space, and (4) the steering script reads the new concentrations from CMF and overwrites the state variables in LandscapeDNDC. To maintain numerical stability of the coupling, LandscapeDNDC uses a time splitting scheme for the numerical integration. It integrates the involved processes of a time step in a fixed succession individually forward in time using already updated states when available. Most processes involved incorporate nonlinear stability controls. Therefore the perturbation of the soil water and nutrient concentrations due to the coupling can be seen as one of these split integration processes.

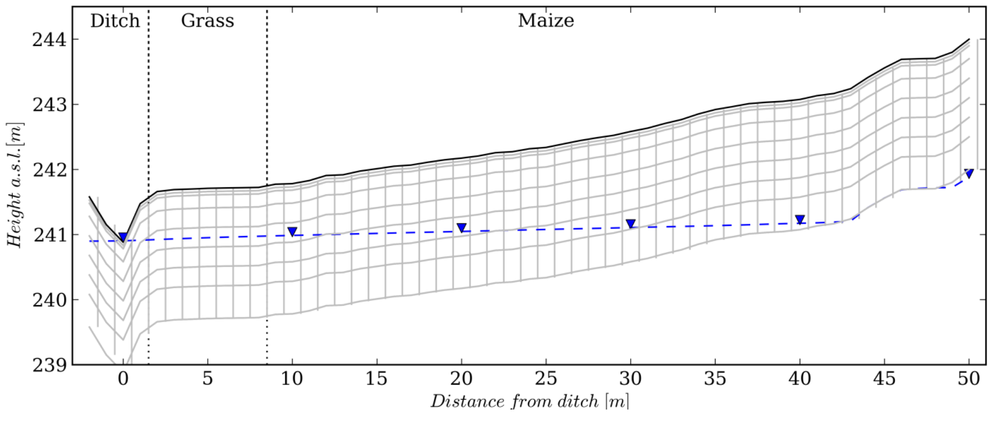

Figure 1: Model setup of the virtual hillslope. The hillslope consists of three zones: the ditch zone in direct vicinity to the outlet, the grass zone, an unfertilized buffer strip, and the maize zone, the intensively used upslope area. After 10 years of model run, the maize field is converted to extensive meadow. The grey lines indicate the discretization of the hillslope into finite volumes, the dashed line shows the groundwater table during base flow.

To study the importance of incorporating lateral fluxes in a complex biogeochemical model, a virtual hillslope of 50 m length has been created (Figure 1). Water enters the system as rainfall, and leaves the system through a ditch at the foot of the slope. Nitrogen input is through fertilization only, and output of nitrogen and carbon is possible via dissolved transport (NO_3, NH_4, DON, DOC) out of the system, gaseous losses (CO_2, N_2O, N_2, NO, NH_3) and export by harvest. The model is run for 20 years, with a land use change from moderate nitrogen initial conditions (2 % organic carbon in the ploughing horizon with a C/N ratio of 22.3) over a ten year periode of intensive maize cultivation to extensive meadow in the upslope area. The lower part of the slope (up to 7 m from the ditch) is used as unfertilized grassland for the whole model period. The grassland and the ditch receive reactive nitrogen only by lateral, waterbound transport from the upslope. During the first 10 years a total amount of 233 kg N/(ha a) fertilizer is applied in the maize zone, as manure and inorganic fertilizer. The soil type is a very well drained, macro pore rich, loamy sand. The soil solution is initialized with 10^{-4} mgN/l for each of the nitrogen components. Since this study focusses on the transition from nitrogen poor to nitrogen rich conditions and back to unfertilized conditions, no spin-up runs have been applied. The total height difference between ditch and shoulder is 3 m, with a slight slope at the hillfoot (1-2%) and steeper slopes in the upper area (7-15%). The meteorological input data has been taken from a south German observation site with a precipitation average of 926 mm/a and a mean annual temperature of 8.5 °C.

3. RESULTS

Although only a single hillslope is modelled, the produced data set is large, therefore only a limited set of the results can be presented. To separate stochastic effects from climatic trends, the model runtime is divided into 5-year periods: the initial phase 1994-1998, the mature cropping phase 1999-2003, the early transition phase 2004-2008 directly after the land use change and fertilization stop at the upslope area, and the extensive phase 2009-2013. In this study we will use modelled nitrous oxide emissions from the different zones as an indicator for complex nitrogen turnover processes.

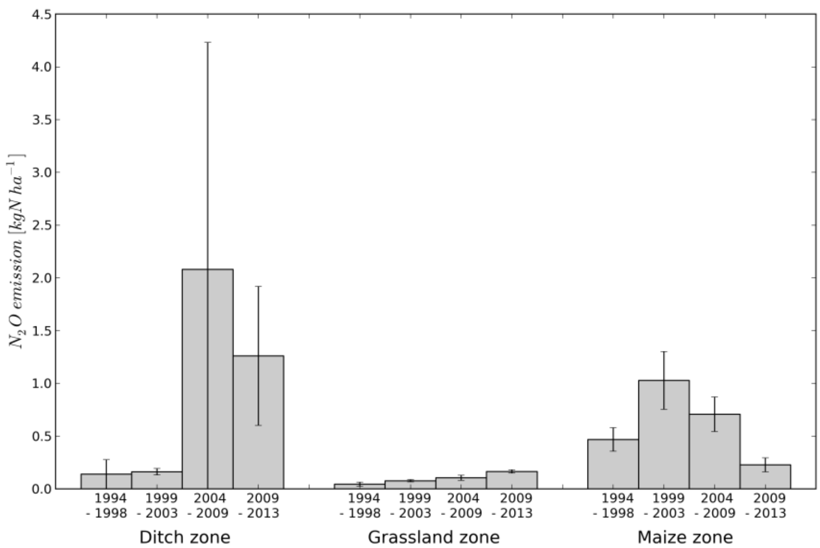

Figure 2: Emission of N_2O from the 3 zones of the hillslope during the 4 runtime phases. The error whiskers show the standard deviation in the 5 years of each phase for the mean of the whole zone.

During the initial phase (1994-1998), C and N stocks are build up in the upslope zone and depleted in the grassland zone. In this phase, the ditch zone and the grassland zone emit only marginal amounts of nitrous oxide, while the fertilized upslope zone emits N_2O at a moderate level (Figure 2). During the second phase (1999-2003) the ongoing high fertilization rates and rising mineralization of maize residuals are resulting in generally higher nitrate and ammonia concentrations in the soil solution. As a consequence, both dissolved nitrogen seeps from the rooting zone and N_2O production and emission in the maize zone increase. The ditch zone and the grassland zone are still unaffected. Despite the land use change in the upslope area to unfertilized fallow land in the year 2004, N stocks are still large. The high mineralisation rate in combination with marginal uptake, leads to elevated concentrations of nitrate in the upslope region, which are then – together with the already existent nitrate stocks in the deeper soil layers – washed out towards the ditch (Figure 3). The highest nitrate concentrations in the ditch are therefore found during this phase. The nitrous oxide emission in the ditch zone is up to 4 kg N/(ha a), while emissions in the maize zone are declining. However, depending on the timing of the availability of reactive nitrogen and the saturation of nitrogen in the stream bank, formation of nitrous oxide varies widely over time. In the extensive phase without fertilizer application also mineralization of N stocks is declining, and thus, less nitrate and ammonia is transported downslope and leached to the groundwater. The stream concentrations remain high, but are also declining (Figure 3).

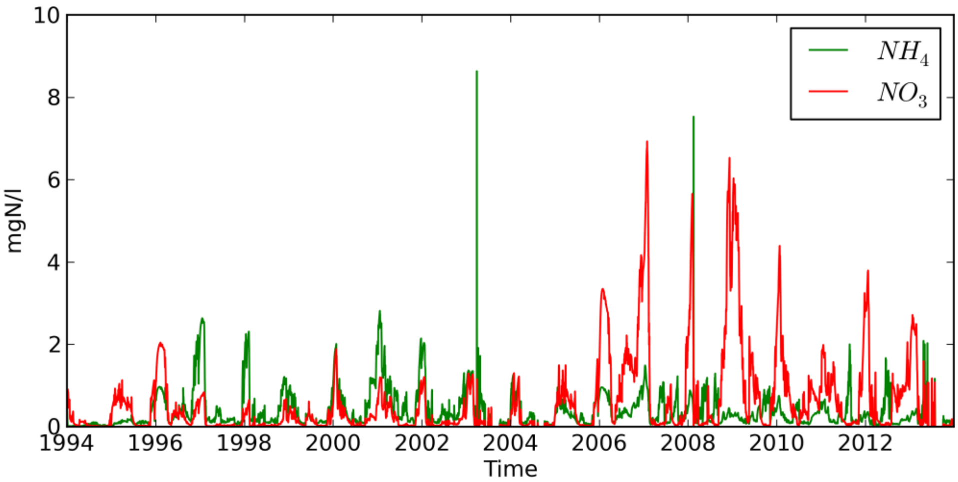

Figure 3: Concentration of nitrogen compounds in the water leached from the virtual hillslope into the ditch. DON is of minor importance and does not significantly contribute to leaching.

4. DISCUSSION

The most important finding from this virtual joined model application are twofold: First it describes the C & N cycling of a coupled biosphere – hydrosphere system reproducing indirect N_2O emissions at the riparian zone due to lateral nutrient transport from a fertilized upland soil. Second, it presents the time lag between the application of fertilization to the upslope zone and its effect on elevated nitrous oxide emissions and discharge concentration at the ditch. Local emissions in the upslope zone start immediately with fertilization during maize cropping and occur at a relative constant rate after a few years of continuous cropping. However, indirect emissions start more than ten years after the first cropping year and after the land use change in the year 2004. It could be assumed that results shown here are representative only for the selected hillslope type and soil parameterization. However, we also tested various other hillslope topographies and forms as well as soil types which resulted in comparable time lags (data not shown here). However, a systematic assessment of the time lag influencing factors is still missing and will be carried out in a later study.

But the main question is: can such time lags be observed in reality? Most experimental setups focus on the plot scale. They are carefully chosen to prevent strong lateral effects to constrain the number of unknown boundary conditions. And many field experiments are carried for the length of typical funding period of 3 years. Lacking a full dataset of the landuse history, at least climatic driving data and knowledge concerning crop rotation and estimated fertilizer use of the last decade needs to be available for a consistent spin-up phase. However, including the dominant flow paths of a hillslope in a biogeochemical study involves good knowledge of hillslope hydrology. Field experimentalists and modellers from both biogeochemistry and hydrology need to work in an interdisciplinary setup to design such an experiment. The comparison of breakthrough curves of conservative tracers and highly bioreactive tracers like nitrogen and other nutrients may help to understand the dynamics of nutrients in the hillslope, by separating transport and turnover processes. The design of such costly experiments can be guided by virtual experiments using the presented modelling approach before and during the experiment, while the results from the careful "model-compatible" experiments help to improve the models.
We think that our understanding of nutrient turnover on the landscape scale with dominant lateral transport is still poor. Further investigation of the spatio-temporal effects by using the coupled model can guide the formulation of hypotheses to test in real field applications.

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