Biogeochemistry (2009) 93:79–90
DOI 10.1007/s10533-008-9276-6

Modeling hydrologic controls on denitrification: sensitivity to parameter uncertainty and landscape representation

Christina Tague

Received: 20 February 2008 / Accepted: 21 July 2008 / Published online: 9 December 2008

Abstract This paper presents a general discussion of the interplay between model structure and hydrologic parameters in the context of denitrification estimation using coupled hydro-ecosystem models at a watershed scale. Given the key role played by hydrology in denitrification models, sensitivity analysis of hydrologic parameters is needed to determine both uncertainty in denitrification estimates and to suggest how measured data, such as streamflow, can be effectively used to reduce this uncertainty. This paper contributes to the broad goal of sensitivity analysis by examining the linkage between landscape tessellation, calibration, and the ability of models to capture hot-spot contributions to watershed scale denitrification across a range of N-loading. For a small mid-Atlantic forested watershed, denitrification estimates using RHESSys (regional hydro-ecologic simulation system) are compared across different strategies for calibration and landscape tessellation. Results demonstrate the utility of several potential approaches to account for hydrologically mediated hot-spots within landscapes.

Keywords Calibration · Denitrification · Eco-hydrology · RHESSys

C. Tague (✉)
Bren School of Environmental Science and Management, University of California, Santa Barbara, CA 93107, USA
e-mail: ctague@bren.ucsb.edu

Introduction

Denitrification is a significant pathway through which nitrogen is removed from the terrestrial environment. Models of terrestrial denitrification are widely used in estimating ecosystem N fluxes to the atmosphere and N export from terrestrial systems to river, lakes and coastal regions under different land management and climate scenarios. Recent reviews of denitrification models describe their application in a wide variety of research and land management settings ranging across plot to global scales (Boyer et al. 2006; Alexander et al. 2002; Shaffer and Ma 2001). These reviews summarize the many different types of terrestrial denitrification models, including simple regression based approaches and more complex models of coupled biogeochemical cycling and hydrologic processes. Previous reviews have emphasized differences in model structure or the basic equations used to estimate denitrification. Model applications, however, also differ in terms of procedures used to provide input data, assign or calibrate model parameters and evaluate uncertainty in model estimates. Evaluation of models and comparison between different models must be done in the context of a broader modeling framework—that includes issues of parameter uncertainty and sensitivity (Beven 2002, 2007).

Heinen (2006) performed a sensitivity analysis of parameters in the basic process equations used to estimate denitrification in a wide range of models, including widely used DNDC (Li et al. 2000) and

DayCent (Del Grosso et al. 2000) and others. Heinen's analysis included models of first-order decay kinetics and models that estimate denitrification as a function of soil chemical and physical conditions. In his analysis, Heinen used Monte-Carlo-based global sensitivity analysis (e.g., where parameters are simultaneously varied by random fluctuations within realistic ranges). His results show that the greatest parameter sensitivity occurred with parameters that influence soil moisture conditions, such as porosity, and denitrification responses to those soil moisture conditions. Heinen's analysis focused on the core denitrification equations in isolation. Many models, however, embed these equations within hydrologic and ecosystem models that are applied across a range of spatial scales. While there are a wealth of hydrologic modeling studies (reviewed by Wagener et al. 2004) that investigate the impact of hydrologic parameter calibration and uncertainty on streamflow estimates, fewer studies explicitly examine the implications for coupled biogeochemical cycling estimates. Estimation of denitrification at watershed scales will depend not only on sensitivity to local soil moisture as demonstrated by Heinen, but also on the distribution of the soil moisture conditions in space and time, and, in particular, the ability of the model to capture hot spots and hot moments.

The importance of hot-spot and hot moments in terrestrial nitrogen cycling has been well established in recent literature (McClain et al. 2003). Denitrification hot spots occur at multiple spatial scales, when there is a nexus of necessary substrates (nitrogen and carbon) and environmental conditions conducive to denitrification. For example, within a plot, high rates of denitrification have been localized in soil aggregates at sub-meter scales. At watershed scales, coarser scale topography can lead to elevated denitrification in wetter riparian zones; while at regional scales, spatial variation in land use and associated N-loading can generate hotspots. Hot moments occur when temporally varying conditions, such as increased soil wetness following rainfall, create opportunities for high rates of denitrification.

Given that local denitrification estimates are highly sensitive to soil moisture conditions, watershed scale denitrification estimates will be sensitive to the models and parameters that are used to estimate soil moisture over space and time. In particular, adequate representation of denitrification hot spots and hot moments is often tied to how models estimate hydrologic processes. One of the most important drivers of hot spots and hot moments is flux of water as both a control on environmental conditions (anaerobic vs. aerobic) and on the transport and accumulation of nitrogen and carbon through the convergence of hydrologic flowpaths. Models of the hydrologic controls that lead to hot spots and hot moments face two key challenges. Firstly the model structure must be able to resolve or account for spatial (or temporal) heterogeneity in moisture conditions that lead to hot-spots (or hot moments) and secondly, inputs and parameters must be available to effectively represent this spatial and temporal heterogeneity defined by the model structure. Model structures, inputs and parameters tend to facilitate the representation of hot-moments given that coupled eco-hydrologic models are often run at fine-time scales (hours–days) and hydrologic input data is often available at similarly fine-time scales. Capturing spatial heterogeneity of hot spots with these approaches is, however, less tractable.

The issue of providing a model structure that can capture hot-spots can be resolved through either explicit or implicit approaches. To explicitly represent hot spots, model spatial resolution must be commensurate with the scale of hydrologic variation that leads to the hot spot. For example, in models of watershed-scale denitrification, landscape tessellation may need to be fine enough to resolve upland versus riparian zone distinctions. Capturing very fine (sub-meter) scale heterogeneity within a riparian zone remains more challenging given that data to parameterize models at that scale are rarely available, particularly once the spatial extent of the model extends beyond an individual field plot. Hot spot characterization may also need to represent multiple scales of variation. For example, a fine scale nexus of carbon and nitrogen substrate availability may function as a hot spot only within a coarser scale hydrologic hot-spot such as a riparian zone. For explicit representations of hot-spots, these multiple and embedded scales must be resolved and appropriately parameterized.

In implicit representations, the impact of hot-spots is accounted for through the calibration of effective parameters. Because calibrated effective parameters do not necessarily represent physical or measurable quantities, they can account for disproportionate contributions of hot-spots to denitrification losses. For example, many local scale models of denitrification (Heinen 2006; Boyer et al. 2006) follow the form:

$$D = \alpha \times f_{H_2O} \times f_T \times f_C \times f_N \times f_{pH} \quad (1)$$

where D is the denitrification rate, α is a potential denitrification rate that is scaled by functional relationships with environmental conditions, specifically soil moisture (f_{H_2O}), temperature (f_T), carbon substrate availability (f_C), nitrate availability (f_N) and soil pH (f_{pH}).

Parameters within these various functional relationships are typically calibrated using field data. Thus extrapolation of the model beyond those conditions is questionable. Issues also arise with respect to the scale of application. When Eq. 1 is included in a watershed scale model, f_{H_2O} becomes a function of mean soil moisture of each modeling unit. In a coarse scale model, the model unit may be an entire watershed. Calibration of parameters within f_{H_2O} may account for soil moisture variance within the model unit and the resulting higher (or lower) overall rates of denitrification. If calibration of f_{H_2O} accounts for the effect of soil moisture variance within a modeling unit, application to other sites may be restricted to sites with similar soil moisture distributions, particularly if (a) soil moisture is the primary factor limiting denitrification and (b) f_{H_2O} is non-linear across the dominant range of soil moisture conditions within a modeling unit. Another possibility is to explicitly include a variance term within f_{H_2O}. Several hydrologic models have used this approach in estimating evapotranspiration for large scale patches that include heterogeneous land surface conditions (Giorgi and Avissar 1997; Zhenghui et al. 2003). This paper examines the use of variance terms for denitrification estimation.

The second issue and related issue in modeling hydrologic controls on denitrification is soil parameterization. Accounting for the spatial heterogeneity that gives rise to spatial patterns of soil moisture continues to be one of the core challenges in hydrologic modeling. While hydrologic processes are well understood, uncertainty in soil drainage parameters means that most hydrologic models require calibration, usually against streamflow data. Further, there are numerous examples of soil parameter equifinality in calibration against streamflow data, where streamflow data can only partially constrain soil parameters. Calibration equifinality leads to uncertainty in parameter estimation and consequently in the spatial patterns of soil moisture and drainage (Blazkova et al. 2002; Western et al. 1999). A broad literature recommends the use of additional measurement data such as tracers, arrays of soil moisture and groundwater measurements to improve hydrologic model calibration (Seibert and McDonnell 2002; Beven 2007). For many applications, however, measurement data are limited and the resulting uncertainty in soil hydrologic parameters and associated soil moisture conditions will have implications for denitrification estimates. How sensitive denitrification estimates are to soil parameter uncertainty, within the context of a watershed scale model, remains an important question.

Figure 1a summarizes the inter-related components of representing hydrologic controls on denitrification estimates in a coupled hydro-ecologic watershed model. This paper uses RHESSys (regional hydro-ecologic simulation system), a coupled hydro-ecological model, as an illustrative example of the role that different components—parameter calibration and explicit and implicit landscape representation—can play in developing estimates of denitrification. RHESSys was applied to a small forested watershed in the Mid Atlantic US and denitrification estimates compared across different model realizations and parameterizations.

Model description

Regional hydro-ecologic simulation system is a coupled model of hydrologic and ecosystem biogeochemical cycling processes. It is a spatially distributed model, which allows user specification of the size and shape of modeling units or patches. The hydrologic model comprises vertical moisture fluxes (interception, transpiration, soil, litter and canopy evaporation, infiltration and drainage through a rooting zone soil layer), as well as lateral moisture fluxes between patches as a function of topographic gradients and soil hydraulic parameters. Ecosystem biogeochemical cycling includes representation of carbon processes (photosynthesis and plant allocation, soil and vegetation respiration, litter and soil decomposition) and linked nitrogen cycling processes, including nitrification and denitrification. The denitrification model is based on the Century N-GAS model (Del Grosso et al. 2000).

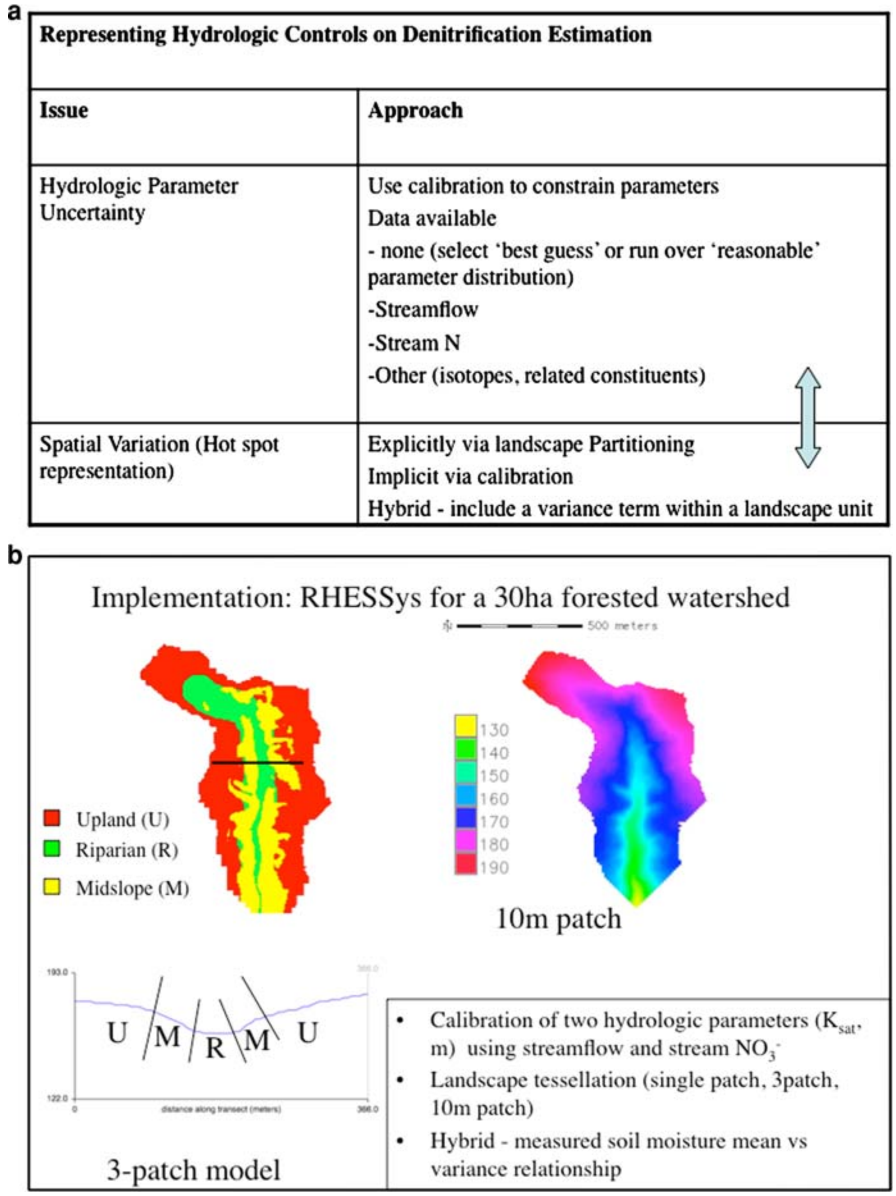

Fig. 1 Model implementation considerations for representing hydrologic controls on denitrification—summary of RHESSys case study

In RHESSys, denitrification (D) is a function of a maximum denitrification (R_{NO_3}) rate based on available soil nitrate (soil_NO3). The maximum denitrification rate is then modified by soil moisture (f_{H_2O}) and soil carbon availability (f_C), where soil respiration is used as an index of carbon availability.

$$D = f_{H_2O} \times f_C \times R_{NO_3} \tag{2}$$

$$f_{H_2O} = \frac{a}{b^{\left(\frac{c}{b^{(d \times \Theta)}}\right)}} \tag{3}$$

$$R_{NO_3} = 0.0011 + \frac{a\tan\left(\pi \times 0.002 \times \left(\frac{NO_3\_soil}{(N_{soil}+C_{soil})} - 180\right)\right)}{\pi} \tag{4}$$

$$f = \frac{0.0024}{\left(1 + \frac{200}{e^{(3.5 \times hr)}}\right)} - 0.00001 \quad (5)$$

where a, b, c, d are parameters set according to soil texture, Θ is soil moisture fraction, N_{soil} and C_{soil} are total soil nitrogen (kg N m^{-2}) and total soil carbon (kg C m^{-2}), respectively, and hr is total daily respiration (g C m^{-2} day^{-1}). Thus f_N, and α from Eq. 1 are combined within the R_{NO_3} term. Temperature sensitivity, f_T, is not explicitly included. However, it is assumed that soil respiration follows a similar sensitivity to temperature and thus the impact of temperature is accounted for. Denitrification responses to pH are not included.

RHESSys also supports anthropogenic nitrogen inputs, including elevated atmospheric N-deposition, fertilizer and septic loading. A full description of RHESSys process representation is given in Tague and Band (2004). RHESSys has been used for a wide variety of hydrologic and ecosystem biogeochemical cycling applications (e.g., Band et al. 2001; Zierl et al. 2006).

Study site

Regional hydro-ecologic simulation system was applied to the Pond Branch study watershed. Pond Branch is an 36 ha forested watershed, monitored as part of the Baltimore Long Term Ecological Research site. Vegetation in the watershed is dominated by a mature oak (*Quercus*) and hickory (*Carya*) forest. Soils are largely silt loams developed on deeply weathered schist, with more organic rich soil in the bottomlands. Topography of the catchment comprises gentle upper slopes, transitioning to steep side slopes leading to a broad riparian area. On the uplands, soils are typically 1–2 m deep, underlain by weathered saprolite greater 6 m in depth. Soils on the side slopes are thin (<0.5 m). The riparian valley zone comprises a deep layer of colluvial soils (U.S. Soil Conservation Service 1976). Continuous daily streamflow data is available from USGS (gauge 01583570) since 1999. Precipitation and meteorologic data were obtained from the Baltimore Washington International airport. Mean annual precipitation over the simulation period was 1,089 mm. Periodic sampling of NO_3^- concentration was done from 1998 to 2004 as described in Band et al. (2001). Weekly samples show a consistent elevation of streamflow NO_3^- during the summer, with NO_3^- concentrations near detection levels (0.01 mg N l^{-1}) throughout the remainder of year. Earlier modeling and field based analysis linked this elevated NO_3^- concentration with a switch from denitrification to nitrifying condition in the riparian zone during the summer (Band et al. 2001). The role of denitrification as a control on NO_3^- export in this watershed makes it an instructive site for investigation model denitrification estimates and their sensitivity to parameters and model landscape realizations.

Calibration approach

Two landscape tessellation strategies were implemented and the results compared—a lumped single patch representation and a simple representation where the study watershed is divided into upland, middle and riparian areas (Fig. 1b). Limited results are also shown for a fine-scale partitioning of the watershed as 30 m patches in the upland region and 10 m patches in the riparian zone. The focus, however, was primarily on coarse scale resolution patches, which reflect the scales typically used in estimating terrestrial denitrification for land management assessments. A 10 m patch realization is theoretically supportable by denitrification models given the availability of high resolution digital elevation models (DEM). However, the large number of resulting patches, input data requirements and accompanying computation cost often limit the applicability to broad spatial extents.

Implicit approaches to capture sub-patch fine scale variability in soil moisture controls on denitrification estimation were also considered and the RHESSys denitrification sub-model was revised to incorporate fine scale variance in soil moisture. Thus the soil moisture adjustment term (f_{H_2O}) for each patch was integrated over a normal distribution of soil moisture such that:

$$f_{H_2O} = \int_{\Theta-2\sigma}^{\Theta+2\sigma} \frac{a}{b^{\left(\frac{c}{b^{(d \times \Theta)}}\right)}} \quad (6)$$

.

Mean soil moisture, Θ, is the RHESSys daily estimate of soil moisture for that patch and standard deviation, σ, is parameterized using a previous field based assessment that found a linear relationship between mean soil moisture and soil moisture variance for the Pond Branch study site. Details on soil moisture monitoring and analysis are provided in Band et al. (2003).

Two soil hydrologic parameters were calibrated, using comparisons between observed and modeled streamflow. Hydrologic parameters are, K_{sat}, the saturated hydraulic conductivity at the surface, and m, the decay of this conductivity with depth. The calibration processes comprised a Monte-Carlo approach with 1,000 simulations for each model realization. Initial values of m and K_{sat} were selected using values in RHESSys soil default libraries (http://fiesta.bren.ucsb.edu/~rhessys/). For calibration, initial values ranged from 0.01 to 0.04 (dimensionless) for m and from 1 to 20 m day^{-1} for K_{sat}. These initial values were multiplied by a spatially uniform scale factor randomly selected from the following ranges for m and K_{sat}, respectively (0.0–2.28 and 1–200). Ranges are based on standard calibration procedures for RHESSys (e.g., Tague and Band 2001). Note that scale factors for K_{sat} are always greater than 1, reflecting results from most hydrologic modeling studies that find calibrated patch to landscape scale saturated hydraulic conductivity larger than conductivity based on soil type and pedotransfer functions. Higher conductivity at these scales reflects the role of macropore/preferential flowpaths (McDonnell 1990).

Calibration compared observed and modeled daily streamflow values. Performance metrics included Nash–Sutcliffe efficiency (NSE) between observed and modeled flow (Nash and Sutcliffe 1970), NSE of log transformed flows—to highlight low flow periods, R^2 of correlation between daily observed and modeled flow, and percent error in annual flow estimations. Note that NSE provides a measure of fit between observed and modeled flows that accounts for observed variance—a NSE value of 1 implies perfect correspondence between observed and modeled flows, NSE of 0 implies only a match between mean observed and modeled flow over the entire time period; NSE < 0 implies neither mean nor pattern are represented by the model. In addition to streamflow data, available stream NO_3^- concentrations were used to further constrain uncertainty in soil hydrologic parameters. Correlations between observed and modeled stream NO_3^- concentration were computed for weekly samples and R^2 reported.

In order to assess the importance of including NO_3^- data in calibration, this paper considered how the range of denitrification estimates changes with the inclusion of this additional data to constrain model parameters. Model behavior for the two different partitioning strategies was also compared.

Results

Calibration of hydrologic parameters using streamflow data is sensitive to the spatial partitioning strategy used. Both model performance and the convergence of parameter values during calibration differ for model realizations using a single patch versus 3 patches. The optimal value for m, the decay of conductivity with depth is approximate 8 for the 3 patch realization versus 12 for the single patch (Fig. 2a). Similarly, optimal values for K_{sat} differ between the two realizations; although both show equifinality or a wide range of reasonable values for K_{sat} (Fig. 2b). The 3 patch strategy also leads to substantially improved hydrologic model performance using optimal parameter values, with peak NSE of 0.4 versus 0.1 for comparisons between log-transformed observed and modeled streamflow. Other streamflow performance metrics show less distinction between the two partitioning strategies, with maximum R^2 between observed and modeled flow of 0.47 and 0.43 for 3 patch and single patch, respectively, and bias in total mean annual streamflow of <10% for both realizations.

Initial calibration was based solely on hydrologic data. Using stream nitrate concentration data, R^2 between observed and modeled values were low ($R^2 < 0.1$) for all parameter values for the single patch realizations. Thus, the single patch realization was not able to capture the observed elevated summer stream nitrate concentrations. The 3 patch strategy showed better performance with maximum R^2 of 0.5 between observed and model stream nitrate concentrations. However, R^2 was reduced to 0.2 if parameter values were constrained to produce reasonable hydrologic performances (NSE > 0.1 for normal and log transformed flows).

For both landscape realizations, estimates of median annual denitrification losses vary by more

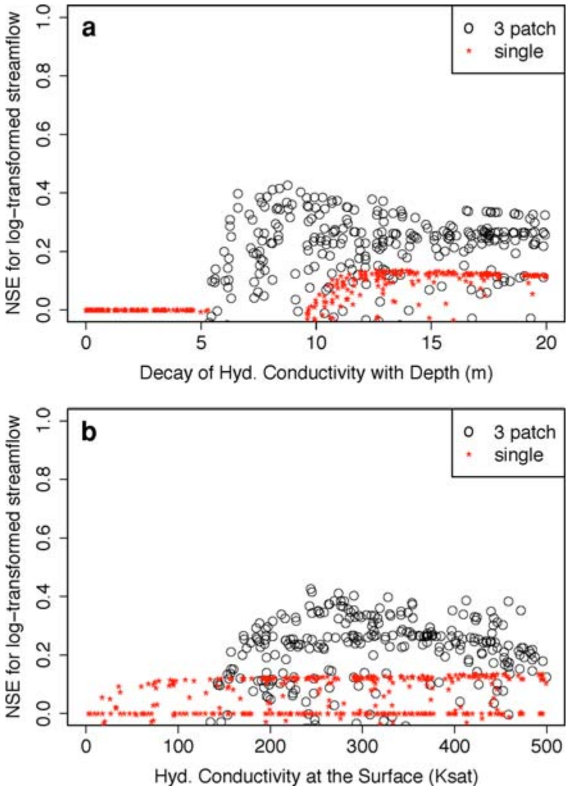

Fig. 2 Hydrologic model calibration results using Nash–Sutcliffe efficiency of log-transformed streamflow as the performance metric. Results are shown for a 3 patch landscape tessellation and a lumped single patch model. Sensitivity of the performance metric is shown for the two hydrologic parameters **a** the decay of saturated hydraulic conductivity with depth (m) and **b** saturated hydraulic conductivity at the soil surface (K_{sat})

than two orders of magnitude across the full range of soil drainage parameters (e.g., prior to calibration) (Fig. 3). If streamflow data is used to constrain soil parameters, the ranges of denitrification estimates are substantially reduced for both the single and 3 patch model realizations. For illustration, results are shown for simulations using all parameters and a subset of parameters that achieved a Nash–Sutcliffe efficiency of greater than 0.2 using both log-transformed and regular streamflow. For the 3 patch model, the range of denitrification estimates is further reduced if parameters are also constrained to those providing reasonable estimates of N-export. The median denitrification estimates is slightly higher, although within the same inter quartile range, when using only parameters providing reasonable N-export results. (Mean denitrification across parameter set follows patterns similar to median values.) As discussed above, for the single patch model, none of the soil hydrologic parameters produced a good match between observed and modeled streamflow NO_3^- export. When soil moisture variance is included in the model, the ranges of denitrification estimates are similar to those derived without soil moisture variance, for both single patch and 3 patch models.

Comparison between the two landscape representations suggests that differences are small for initial, low N input simulations. Median denitrification estimates (across all parameter sets) are similar for single patch and 3 patch models (Fig. 3) but differ slightly in the temporal patterns of year to year variation (Fig. 4). Median denitrification estimates, using parameters with acceptable hydrologic performance, are only slightly higher for the single patch realization (0.012 vs. 0.011 g N m^{-2} $year^{-1}$) in spite of a significant degradation in model hydrologic performance associated with the single patch realization.

Atmospheric N-inputs for the low N model scenarios were $\sim$0.4 g N m^{-2} $year^{-1}$. Median denitrification estimates for all scenarios suggest $\sim$3% of this input was lost as denitrification. Most of the remaining input was incorporated into organic material. To examine model sensitivity when N-inputs are higher, simulations were repeated with the addition of fertilizer inputs (10 g N m^{-2} $year^{-1}$) (Fig. 5). With additional N inputs, the differences between the single patch and 3 patch models were significant, such that median denitrification was an order of magnitude lower for the single patch model (1.2 vs. 0.01 g N m^{-2} $year^{-1}$ or 12 vs. much less than 1% of N-input, for parameters that gave reasonable hydrologic performance). As before, including fine scale variance in the 3 patch model had little impact on median annual denitrification estimates. Including soil moisture variance in the single patch model, however, increases denitrification to values more similar to those obtained with the 3 patch model (Fig. 5). Median value using the single patch model with soil moisture variance included was 2.9 g N m^{-2} $year^{-1}$ or 27% of N input. For the single patch model, with soil moisture variance included, the range of denitrification estimates is within the range for the 3 patch model; when soil moisture variance is not included estimates are all outside 3 patch model range. It is also important to

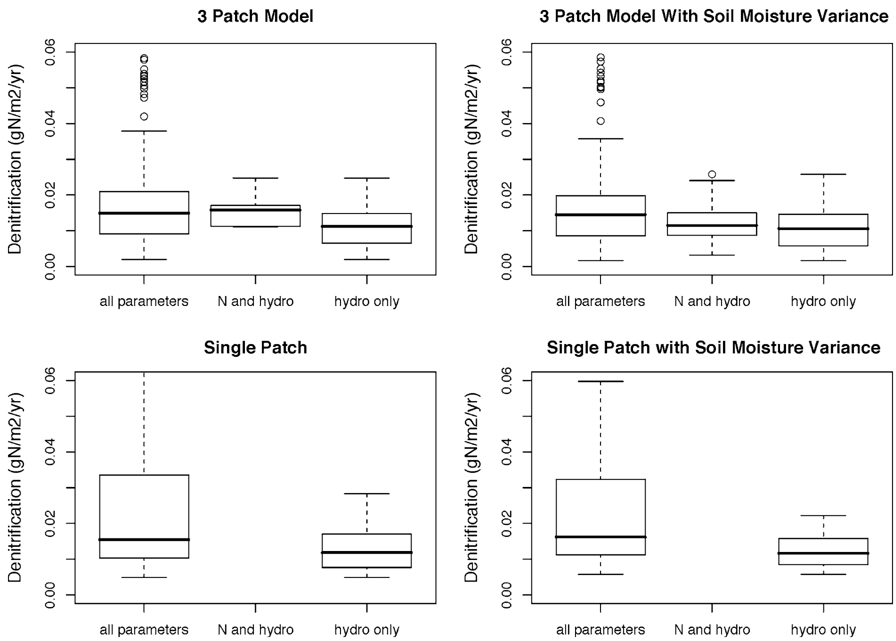

Fig. 3 Model estimates of mean annual denitrification over the simulation period (water years 2000–2003). *Box-plots* show results across all parameter values, for parameters giving acceptable hydrologic performance and parameters giving both acceptable hydrologic performance and a good correspondence between modeled and observed stream nitrate. Results are shown for a 3 patch landscape tessellation and a lumped single patch model with and without a soil moisture variance term included in denitrification submodel. Atmospheric nitrogen deposition is the only N input to the system

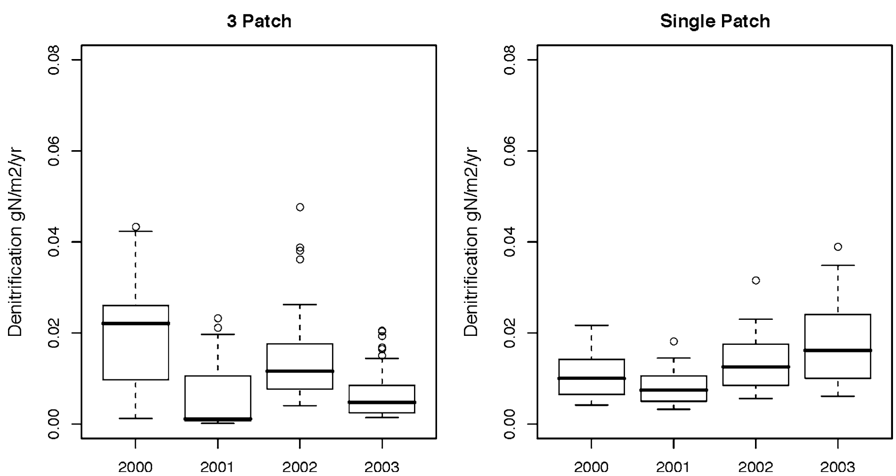

Fig. 4 Model estimates of mean annual denitrification for water years 2000–2003. Results are shown for a 3 patch landscape tessellation and a lumped single patch model and for baseline nitrogen inputs. *Box-plots* summarize results for all parameters giving acceptable hydrologic performance

note that for the high N input scenarios, the implications of constraining hydrologic parameters are more significant. Within original N inputs, constraining hydrologic parameters with streamflow data significant reduced the range of denitrification estimates but did not substantially alter median values. With higher N input, constraining hydrologic parameters with available streamflow data, lowers the median denitrification estimate in addition to constraining the estimate range. Note that this is also true for mean denitrification estimates, which reduced from 5.3 to 2.8 g N m^{-2} year^{-1} when streamflow is used to constrain parameters. As with the original N inputs, the impact of including N-export data on the range of denitrification estimates is small relative to reduction in uncertainty associated with calibration using streamflow data.

Finally, results from a single simulation using a finer landscape representation (10 m) were examined. Hydrologic performance was somewhat improved with higher resolution patches (NSE 0.5), although only limited calibration (20 trials) was undertaken. For baseline atmospheric N input scenarios, median annual denitrification fluxes using this higher resolution model were slightly higher (0.04 g N m^{-2} year^{-1}) than those obtained with the 3 patch model

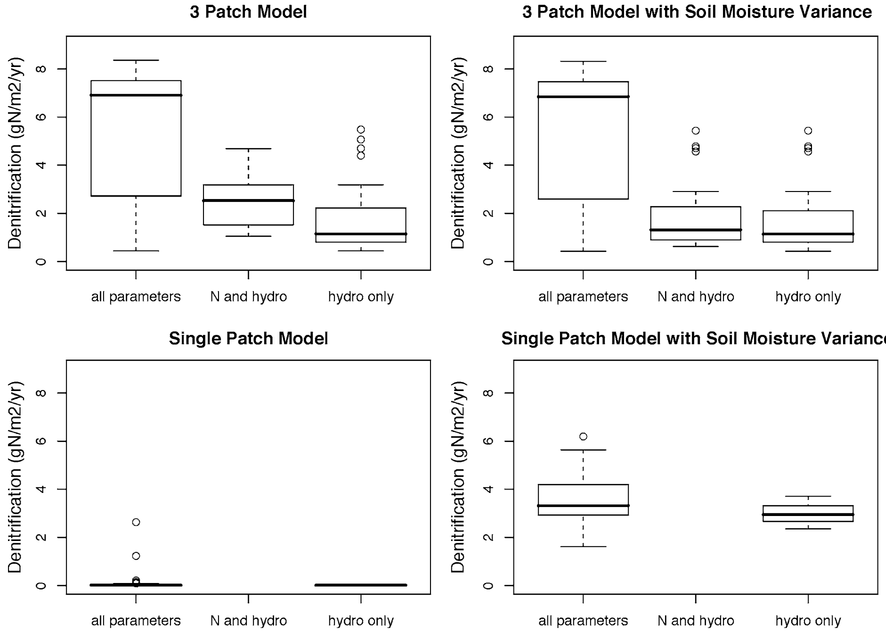

Fig. 5 Model estimates of mean annual denitrification over the simulation period (water years 2000–2003) for simulations with added fertilizer (10 g N m^{-2} year^{-1}). Results are shown for a 3 patch landscape tessellation and a lumped single patch model with and without a soil moisture variance term included in denitrification submodel

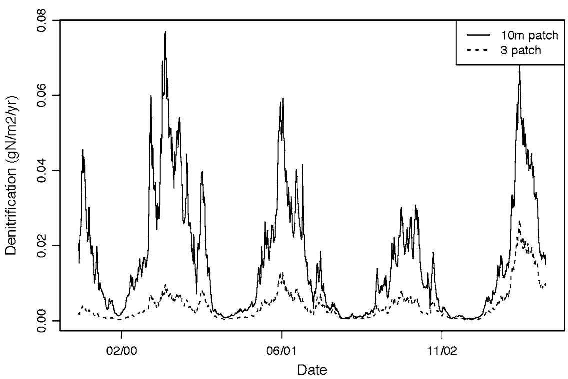

Fig. 6 Daily denitrification for a 3 patch model and a high resolution landscape tessellation (30 m in uplands and 10 m riparian areas). Results are shown for high N-loading simulations with fertilizer additions of 10 g N m^{-2} year^{-1}

(mean across acceptable parameters of 0.01 g N m^{-2} year^{-1}). With elevated N-inputs, the finer landscape representation produces significantly higher denitrification (7.6 g N m^{-2} year^{-1}) versus results from the 3 patch model (1.5 g N m^{-2} year^{-1}) although seasonal and inter-annual patterns of denitrification are similar (Fig. 6).

Discussion

Results from this case study show that, at the watershed scale, the availability of streamflow data for calibration substantially reduces the uncertainty in hydrologic parameters and leads to a significant reduction in the range (across soil parameter uncertainty) of denitrification estimates. These results suggest that application of RHESSys, using a single parameter set selected without streamflow data for calibration, could lead to an order of magnitude error in denitrification estimation. In cases where streamflow data is not available, it is worth noting that if the model was run over the full distribution of parameter sets, median estimates would be similar to that obtained using calibrated parameters for the low N case but somewhat higher for the high N case. Thus even in the high N case, running simulations over a distribution of parameters is likely to lead to substantially better estimates of denitrification. The inclusion of stream nitrate data in calibration in some cases further reduced the range of denitrification estimates; however, the reduction was small relative to reduction associated with hydrologic calibration.

While these results highlight the importance of streamflow measurements for constraining watershed scale denitrification estimates, it is also worth noting that the single patch model had relatively poor hydrologic performance as measured by the NSE metric. The 3 patch model performance was better but still only moderate (peak NSE of 0.4). Nonetheless denitrification estimates were similar for both models and close to those obtained using the fine resolution patch structure. Thus, although limiting the parameter set through comparison between observed and modeled streamflow was critical for constraining denitrification estimates (e.g., reducing the range by two orders of magnitude in some cases), a fairly general level of correspondence was sufficient (such as that measured by general metrics, such as R^2, rather than more precise metrics such as NSE).

Landscape tessellation often determines the ability of the model to capture hot spot behavior. In comparing a single with a 3 patch model, at a watershed scale, this paper focused on hot-spots that can be linked with topographic features such as riparian zones, which occur at scales of 10s of meters. It is important to recognize that the 3 patch implementation includes the redistribution of water between patches. Simply partitioning the watershed into finer resolution, but hydrologically independent patches would not account for the riparian hot-spot. Many denitrification models resolve spatial differences in inputs through partitioning the landscape into spatial units, but unless model units are connected, riparian hot spots are not necessarily accounted for. Result here show difference in behavior for different model partitioning strategies, where landscape patches are hydrologically connected. For the case study watershed used here, the importance of landscape partitioning varies with N limitation, such that the need for resolution of riparian hot-spot increases for higher levels of available N. For the high N case, the importance of resolving the riparian zone hotspot is clearly demonstrated by the substantially lower estimates using the lumped single patch representation. It is important to recognize that the implications of landscape tessellation were not apparent under the low N case, suggesting that model evaluation under low N inputs may be misleading.

In simulations over large spatial extents it may not be feasible to include an explicit representation of riparian hot spots as was done for this study site. In these cases, inclusion of a variance term (hybrid approach in Fig. 1) offers an alternative. For this case study, the inclusion of a soil moisture variance term within Eq. 1 demonstrated some success for including the effect of the riparian hot-spots in a single patch model. Particularly for the high N simulations, inclusion of the variance term lead to substantially higher denitrification estimates that were much closer to estimates generated using finer landscape tessellations (explicit approach). It is important to note, however, that implementation of this approach required additional parameterization, specifically an estimate of soil moisture variance. This may limit the broad applicability of this approach. Further testing of sensitivity to uncertainty in the soil moisture variance term is needed to assess whether simply including a regionally defined variance term might improve watershed scale denitrification estimates for single patch models. Nonetheless including a soil moisture variance term within ecosystem models that compute denitrification at coarser scale may offer an improvement, particularly when the scale of application or model structure does not support the routing of water between patches nor the isolation of riparian hotpots. Similar approaches have been successfully applied in regional rainfall-runoff models (e.g., Giorgi and Avissar 1997).

This paper focused largely on hydrologically mediated hot spots in riparian zones. There are also likely to be finer scale hot spots within riparian zones and other landscape locations. Higher denitrification estimates using the 10 m patch representation are evidence of this effect; although it is worth noting that the increase in denitrification estimates with this finer scale tessellation (relative to the 3 patch model) are substantially smaller than increases associated with including the riparian zone (3 patch vs. single patch).

Finally, it is important to recognize that this paper focuses only on model sensitivity to soil moisture parameterization. Other components of the denitrification model, including parameterization of other controls in Eq. 1, were not varied as part of this study. While Heinen (2006) found that parameterization of soil moisture is often the most sensitive component of denitrification models, uncertainty in other parameters and model input may also contribute to model error and may have synergistic effects with soil moisture parameterization. A full, global sensitivity analysis, where parameters are varied simultaneously would offer a more complete picture—although this process can be computationally challenging in a fully coupled model such as RHESSys. The hydrologic and denitrification sub-models in RHESSys are similar to those used in many other models and thus results from this paper may have broader implications for other models and study sites. Generalizability to other models and study sites, however, would require additional analysis.

Conclusions

Previous sensitivity analysis of local scale denitrification equations suggests that hydrologic conditions will play a key role in determining uncertainty in denitrification estimates. In watershed scale models, denitrification equations are often linked with hydrologic models. In this paper, an application of RHESSys was used to illustrate the importance of model set-up—including hydrologic parameter calibration and landscape tessellation in using coupled models to estimate denitrification. Calibration and landscape tessellation are not independent—and calibration of effective parameters is often used to compensate for spatially averaging effects of landscape tessellation. Results from this paper show that while calibration does substantially reduce uncertainty in denitrification estimates, it is not sufficient to compensate for the loss of riparian zone hotspots in coarser scale calibrations, particularly under high levels of N-input. Fine scale landscape tessellation is not always feasible for large scale simulations—thus alternative approaches are needed. Incorporation of soil moisture variance terms does improve denitrification estimates of coarse scale model but additional research is needed to develop techniques for calibrating soil moisture variance term under a range of geographic settings.

Acknowledgments This paper is a product of a workshop on Denitrification Modeling Across Terrestrial, Freshwater, and Marine Systems, held November 28–30, 2006, at the Institute of Ecosystem Studies, Millbrook, NY, with support from the Denitrification Research Coordination Network of the National Science Foundation, award DEB0443439 and the Northeastern States Research Cooperative (Grant # 02-CA-11242343-105).

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