Sensitivity analysis of SWAT nitrogen simulations with and without in-stream processes

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The Soil and Water Assessment Tool (SWAT) has been widely used to estimate pollutant losses from various agricultural management practices. Although many studies have shown good performance in simulating total nitrogen (TN) and dissolved nitrogen (N), the model performed poorly in many other applications, particularly on dissolved N. Poor performance on dissolved N could be attributed to landscape (in-field) processes and/or in-stream N processes in the model. Therefore, the overall goal of this study was to evaluate SWAT N simulations with in-stream processes and without in-stream processes. Sensitivity analysis results showed that when in-stream processes were not simulated, denitrification threshold water content (SDNCO), nitrogen in rainfall (RCN) and N percolation coefficient (NPERCO) were the most sensitive parameters to dissolved N losses. However, when in-stream processes were simulated, the most sensitive parameters changed to initial organic N concentration in soil layers (SOLORGN) and organic N enrichment ratio (ERORGN); and the impact of SDNCO, RCN and NPERCO was greatly decreased. Furthermore, fertilizer timing and amount had little impact on N simulations. SWAT under-estimated dissolved N, but over-estimated organic N and TN. Further calibration could improve the simulation of dissolved N, but would degrade the simulations of organic N and TN.

Key Words: SWAT, nitrogen simulation; sensitivity analysis; in-field parameters; in-stream processes

Introduction

The Soil and Water Assessment Tool (Arnold et al. 1998; Arnold and Fohrer 2005; Gassman et al. 2007) has been developed to aid in the evaluation of watershed response to agricultural management practices. Conservation practices are evaluated through a continuous simulation of runoff, sediment and pollutant losses from watersheds. The model has been applied worldwide for solving all kinds of water quantity and quality related problems. Many studies including those summarized by Gassman et al. (2007) have demonstrated SWAT's capability in simulating N losses (Saleh et al. 2000; Santhi et al. 2001;

Saleh and Du 2004; Chu et al. 2004; White and Chaubey 2005; Arabi et al. 2006; Grunwald and Qi 2006; Plus et al. 2006; Hu et al. 2007; Jha et al. 2007; Niraula et al. 2012; Niraula et al. 2013; Wu and Liu 2014), and results from various studies indicated mixed success of SWAT N simulations. Although many studies reported good performance of SWAT in simulating N losses (Behera and Panda 2006; Gikas et al. 2006; Jha et al. 2007; Santhi et al. 2001; Stewart et al. 2006; Tripathi et al. 2003), quite a few other studies showed poor performance of SWAT in dissolved N simulations (Chu et al. 2004; Du et al. 2006; Grizzetti et al. 2003; Grunwald and Qi 2006; Gassman et al. 2007; Hu et al. 2007; White and Chaubey 2005). The poor performance of simulating dissolved N could be attributed to many factors, including inadequate simulation of landscape processes and/or stream processes. In addition, in some of those good TN performance, the good performance might be a result of smoothing or averaging poor simulations of different N species, including under- and/or over-estimation of individual N species.

After precipitation, overland flow forms first, then concentrated flow. Thus, watershed models generally include landscape processes (overland flow) which are also called in-field processes and stream channel processes (concentrated flow) which are also called in-stream processes. There is an increased recognition of the importance of integration of in-stream water quality processes in watershed models (Horn et al. 2004). The ability to simulate in-stream water quality dynamics is a strength of SWAT, but very few SWAT-related studies discuss whether the in-stream functions were used or not (Horn et al. 2004; Migliaccio et al. 2007). Santhi et al. (2001) opted to not use the in-stream functions for their SWAT analysis of the Bosque River in central Texas. Gassman et al. (2007) pointed out that all aspects of stream routing needed further testing and refinement, including in-stream water quality routines. Arnold and Fohrer (2005) also stated that further research and testing are needed with regard to SWAT in-stream water quality simulation.

Understanding the influence of SWAT parameters controlling the simulation of N losses from in-field processes and in-stream processes is very important. Moreover, understanding the different influence of in-field N related parameters from in-stream N related parameters on N losses is even more important because this would help model users and/or land planners to better understand the N processes. By understanding the different impacts of in-field parameters and in-stream parameters on N losses, the model could be applied to better evaluate the effectiveness of within field conservation practices and/or within channel conservation practices on improving water quality. Therefore, the overall goal of this study was to evaluate SWAT N simulations through sensitivity analysis of SWAT N-related in-field parameters on N losses and comparisons with field observed N losses. Specifically, we evaluated the sensitivity of in-field parameters on N losses with in-stream simulation and without in-stream simulation to understand the relative impact of in-field processes and in-stream processes on N losses at the watershed scale.

Method and Procedure

Study Sites (Wisconsin, USGS5431014)

The study area (Upper Rock Watershed) is one of the subwatersheds in the Jackson watershed in the southeastern part of Wisconsin (Figure 1). The USGS gauge at the Upper Rock Watershed outlet is located on Jackson Creek at Petrie Road near Elkhorn. This gauge draining 20.35 km^2 collects streamflow and water quality on a daily basis. Daily stream data are continuously available from 10/1/1983 to 9/30/1995. Daily total suspended sediment (TSS), dissolved N (NO_2^-+NO_3^-), organic N and TN are available for the periods 10/1/1983 – 9/30/1985 and 2/1/1993 – 9/30/1995. The watershed with elevation ranging from 292 to 348 m is dominated by crop lands, where corn-soybean rotation is practiced over 50% of the entire watershed (Figure 1 and Table 1). The predominant soil associations in the subwatershed include Kidder-McHenry-Pella (WI117, 55%) and Pella-Wacousta-Palms

(WI122, 45%) (Table 2). The Kidder and McHenry series (Fine-loamy, mixed, active, mesic Typic Hapludalfs) consist of well-drained soils, while the Pella, Wacousta and Palms series (Fine-silty, mixed, superactive, mesic Typic Endoaquolls) consist of poorly drained soils. Agricultural management information was obtained from the website of the NRCS database used for the RUSLE2 program (Revised Universal Soil Loss Equation, Version 2). The crop management templates for the Crop Management Zone 4 (CMZ4), where the watershed is located were downloaded (website: ftp://fargo.nserl.purdue.edu/pub/RUSLE2/Crop_Management_Templates/) and further processed by the Annualized Agricultural Nonpoint Source Pollutant Loading (AnnAGNPS) Input Editor (Table 3). Based on the general information for Crop Management Zone 4, the fertilizer application rates for corn are 11990 kg/km^2 of N and 4150 kg/ km^2 of phosphorus, and for soybean are 1680 kg/ km^2 of N and 3700 kg/ km^2 of phosphorus (Table 3).

<Table 1>

<Table 2>

<Table 3>

<Figure 1>

Nitrogen Simulation in SWAT

The SWAT model is designed to simulate long-term impacts of land use and management on water, sediment and agricultural chemical yields at various temporal and spatial scales in a watershed (Arnold et al. 1998; Arnold and Fohrer 2005; Gassman et al. 2007). More than 600 peer-reviewed journal articles have been published demonstrating the SWAT applications on sensitivity analyses, model calibration and validation, hydrologic analyses, pollutant load assessment, and evaluation of conservation practices (Gassman et al. 2007). SWAT theoretical documentation (Neitsch et al. 2009) provides a detailed description of model simulations of different processes.

The fate and transport of nutrients in a watershed depend on the nutrient transformations in the soil environment (in-field) and nutrient cycling in the stream water (in-stream). The SWAT models nitrogen cycle for fields, and it also models in-stream nutrient cycling. The nitrogen cycle is a dynamic system that includes atmosphere, soil and water. In summary, SWAT simulates five different pools of N in soil: two pools are inorganic forms of N, ammonium (NH_4^+) and nitrate (NO_3^-), and three pools are organic forms of N, which are active organic N, stable organic N associated with humic substances and fresh organic N associated with the crop residues. Nitrogen may be added into soil by fertilizer, manure or residue application, N_2 fixation by legumes and nitrate in rain deposition, while N can be removed by plant uptake, denitrification, erosion, leaching and volatilization. After the crop is harvested and the residue is left on the ground, decomposition and mineralization of the fresh organic N pool occur in the first soil layer. The N obtained by fixation is a function of soil water, soil nitrate content and growth stage of the plant; and nitrogen fixation stops as the soil dries out. Greater soil nitrate concentrations can inhibit N fixation and growth stage has the greatest impact on the ability of the plant to fix N. The actual N uptake is the minimum value of the nitrate content in the soil and the sum of potential N uptake and the N uptake demand not met by overlying soil layers. Denitrification is a function of water content, temperature, and presence of carbon and nitrate. The amount of organic N transported with sediment is associated with the sediment loss from the fields (HRUs) and the organic N enrichment ratio (ERORGN), which is the ratio of the concentration of organic N transported with the sediment to the concentration in the soil surface layer.

The SWAT models the in-stream nutrient process using kinetic routines from an in-stream water quality model, QUAL2E (Brown and Barnwell 1987). The transformation of different N species is governed by growth and decay of algae, water temperature, biological oxidation rates for conversion of different N species and settling of organic N with sediment.

The amount of organic N in the stream may be increased by the conversion of N in algae biomass to organic N and decreased by the conversion of organic N to NH_4^+ and by settling with sediment. The amount of ammonium may be increased by the mineralization of organic N and the diffusion of benthic ammonium N as a source and decreased by the conversion of NH_4^+ to nitrite (NO_2^-) or the uptake of NH_4^+ by algae. The conversion of nitrite to nitrate is faster than the conversion of ammonium to nitrite. Therefore, the amount of nitrite is usually very small in streams. The amount of nitrite can be increased by the conversion of NH_4^+ to NO_2^- and decreased by conversion of NO_2^- to NO_3^-. The amount of nitrate in streams can be increased by the conversion of NO_2^- to NO_3^- and decreased by algae uptake.

Input Preparation

The key geographic information system (GIS) input files to SWAT included a 30-m digital elevation model (DEM) downloaded from the National Elevation Dataset at a resolution of 1 arc-second (http://ned.usgs.gov/), an enhanced land cover/land use data layer based on the 2001 National Land Cover Database (NLCD), and State Soil Geographic Database (STATSGO) data from the USDA-NRCS. Based on the DEM and selected outlets, the watershed was delineated into several subbasins. Subsequently, the subbasins were partitioned into homogeneous units (HRUs), which shared the same land use, slope and soil type. In this study, a total of 106 subbasins were delineated and 918 HRUs were defined by using a 0% threshold which provided the most detailed information for the watershed. The enhanced land cover/land use data layer was an aggregate land cover classification created by combining the NLCD 2001 with the USDA-National Agriculture Statistical Survey Cropland Data Layer for the years 2004-2007. These land cover/land use data provided 18 different classes of agriculture rotation management, such as continuous (monoculture) corn and corn-soybean rotation (Mehaffey et al. 2011). Daily weather data (precipitation, minimum and maximum temperature) for 1980 through 2007 were acquired from the National Climatic

Data Center (NCDC). Missing records of daily observations were interpolated from weather data within a radius of 40 kilometers using the method developed by Di Luzio et al. (2008). Other weather information (solar radiation, relative humidity and wind speed) were generated by the WXGEN weather generator model (Sharpley and Williams 1990). Agricultural management information listed in Table 3 was used for SWAT simulations.

Since the objective of this study was to evaluate the SWAT N simulations, an attempt was made to better define N-related parameters wherever possible. The fraction of N in plant biomass (PLTNFR) for corn at emergence, 50% maturity and maturity were set as 0.047, 0.0177 and 0.0138, respectively (Neitsch et al. 2002). The N plant uptake for soybean at three plant growth stages were set as 0.0524, 0.0265 and 0.0258, respectively (Neitsch et al., 2002). The soil initial NO_3 (SOLNO3) was 3.23 mg/kg and organic N (SOLORGN) was 1000 mg/kg based on soil properties in the watershed (Table 2). The N content in fresh residue cover (RSDIN) was set as 10000 kg/ km^2. (http://www.agry.purdue.edu/ext/corn/pubs/agry9509.htm) and organic N enrichment ratio (ERORGN) was set as 2.5. More details regarding defining N-related parameters for SWAT simulations are described in the sensitivity analysis section.

Initial Model Simulation

After input was prepared, SWAT model was applied to simulate streamflow, TSS, dissolved N, organic N and TN losses from the Upper Rock Watershed. Simulation results were evaluated using observed data from the USGS gauge at the Upper Rock Watershed outlet before sensitivity analysis. Such an analysis would provide some insights on model's performance, which helps users better understand the model's processes. Due to discontinuity of available data, the evaluation of model performance consists of two parts: performance over the entire available data (10/1/1983 – 9/30/1985 and 2/1/1993 – 9/30/1995) and over a specific hydrological period (10/1/1993 – 9/30/1995) because many studies have concluded that the length or the number of streamflow measurements would have a significant effect on model performance and parameter uncertainty (Perrin et al. 2007; Seibert and Beven 2009; Tada and Beven 2012). Four widely used statistical criteria including Nash-Sutcliffe efficiency (NSE), coefficient of determination (R^2), Root Mean Square Error-observations standard deviation ratio (RSR) and percent bias (PBIAS) were used to evaluate model performance (Moriasi et al., 2007). The NSE is a normalized statistic indicating how well the observed and predicted data fit the 1:1 line (Nash and Sutcliffe 1970). The R^2 value describes the variance in measured data explained by the model. The PBIAS indicates the average tendency of the simulated data to be larger or smaller than the observed data (Gupta et al. 1999).

Sensitivity Analysis

The purpose of a sensitivity analysis is to investigate input parameters, especially those that are difficult to measure or whose expected effect on model output is unclear (Lane and Ferreira 1980). Therefore, the sensitivity analysis was performed to evaluate the influence of model input parameters on model output and decide if calibration is possible with user modification of selected input parameters.

In a study of Water Erosion Prediction Project (WEPP) model sensitivity, Nearing et al. (1990) used a single value to represent sensitivity of the output parameter over the entire range of the input parameter tested. Instead of using minimum and maximum values of selected parameters, the index used by Nearing et al. (1990) was amended using an interval of 20% of selected parameters. The index for sensitivity testing of the SWAT N component is shown as follows:

$$S = \frac{\frac{O_2 - O_1}{O_{12}}}{\frac{I_2 - I_1}{I_{12}}} \tag{1}$$

where:

I_1 and I_2 = the -20% and +20% values of input used, respectively;

I_{12} = the average of I_1 and I_2;

O_1 and O_2 = the output values for the two input values; and

O_{12} = the average of O_1 and O_2.

The index S represents the ratio of a relative normalized change in output to a normalized change in input. An index of one indicates a one-to-one relationship between the input and the output, such that a one percent relative change in the input leads to a one percent relative change in the output. A negative value indicates that input and output are inversely related. The greater the absolute value of the index, the greater the impact an input parameter has on a particular output. Because it is dimensionless, the index S provides a basis for comparison among input variables.

In this study, sensitivity analysis was conducted to determine the influence of input parameters on simulating dissolved N, organic N and TN losses. Parameters related to runoff and sediment simulation would also influence N simulations because N transport depends on runoff and sediment transport. In order to focus more on N processes, parameters related to runoff and sediment simulation were fixed as default since the model performed reasonably well on runoff and sediment during initial simulations. Thus, a total of 19 N-related parameters were selected (Table 4), of which eleven are in-field related and eight are in-stream related. The selection of those 19 N-related parameters was based on literature reviews of N processes and losses as well as used by other SWAT users in their N simulations. For sensitivity analysis, parameter values defined in the initial model simulations were used as default values; and the default values and their ranges, as shown in Table 4, were defined based on literature studies and suggested ranges for the sensitivity analysis tool in SWAT2005 (Neitsch et al., 2002).

<Table 4>

The sensitivity analysis was performed with existing land cover (Figure 1, Table 1) and one additional hypothetical scenario. For the hypothetical scenario, the existing 52% of the land cover in corn-soybean rotation was replaced by monoculture corn, resulting in a total of 66.5% of the watershed in monoculture corn (see Table 1). Simulation of this additional hypothetical scenario would provide some insights on how land cover changes would impact this sensitivity analysis. In order to differentiate the impact of N in-field related parameters from N in-stream related parameters, the model was first run with all in-stream N parameters that were turned off (in-stream processes not simulated) and then the model was rerun with all in-stream N-related parameters that were turned on (in-stream processes simulated). When the in-stream parameters were turned on, SWAT default values for in-stream parameters were used (Table 4). Starting with the initial values (default values in Table 4), the sensitivity analysis was performed with a simulation period from 1980 to 2007. The first three years were used for parameter initialization. The model was run with one specific parameter changed by 20% of the initial value at a time while the remaining parameters were held at the default values given in Table 4.

Sensitivity analysis was also performed to evaluate the impact of timing and rate of N application on N losses since studies have shown that N losses were affected by fertilizer application timing and rates (Moll et al., 1982). Fertilizer application timing and rate were modified for existing land cover (Figure 1, Table 1) and the additional hypothetical scenario (corn-soybean rotation was replaced by monoculture corn). In the baseline fertilizer scenario, N fertilizer was applied on April 20. To investigate the sensitivity of N losses to timing of fertilizer application, additional fertilizer timing scenarios were simulated using fertilizer application dates in June (6/20), August (8/20), October (10/10, due to harvest on 10/20) and December (12/20). Scenarios of fertilizer application in December may not be very realistic, but evaluating these less realistic scenarios provided results that served as benchmark information or helped in understanding model performance. For fertilizer rate scenarios, the fertilizer application date was fixed as April 20th and the fertilizer rate was increased or decreased by 20% and 50% of the amount listed in Table 3. Similar to the sensitivity analysis performed for N-related in-field parameters, the SWAT model was run with all in-stream N parameters that were turned off (in-stream processes not simulated) and on (in-stream processes simulated).

Results and Discussion

Sensitivity of in-field Parameters on Model Outputs without in-stream Processes

Dissolved N

The most sensitive variables for dissolved N were denitrification threshold water content (SDNCO), N percolation coefficient (NPERCO) and nitrogen in rainfall (RCN) (Figure 2). As expected, increasing the value of SDNCO resulted in higher dissolved N losses because a higher SDNCO means less potential for denitrification, thus more dissolved N available for loss through runoff as shown in many studies (Crumpton et al., 2007; Drury et al., 2009). Similarly, increasing the value of NPERCO resulted in higher dissolved N losses because a greater NPERCO value denotes a greater amount of dissolved N available from surface layer relative to the amount removed via percolation, thus a greater amount of dissolved N losses through surface and subsurface lateral flow (Evans et al. 1995; Drury et al. 2009). This is also consistent with the results from many previous model studies. In fact, many studies only adjusted the NPERCO value in the calibration for N losses (Behera and

Panda 2006; Gikas et al. 2006; Schilling and Wolter 2009) indicating the importance of NPERCO to N simulation. Finally, a higher value of RCN resulted in a greater amount of dissolved N losses as expected.

<Figure 2>

The secondary sensitive variables were the biological mixing efficiency (BIOMIX), mineralization of active organic nutrients (CMN) and N plant uptake (PLTNFR) (Figure 2). BIOMIX is a parameter describing how soil nutrients redistribute through biological activities (Neitsch et al. 2002). Although many studies have used BIOMIX in the calibration for different N losses (Chu et al. 2004; Santhi et al. 2001; Stewart et al. 2006; Jha et al. 2007), only Chu et al. (2004) showed that BIOMIX had much smaller impact than NPERCO on NO_3-N in surface water. Increasing the CMN value resulted in higher dissolved N losses because higher mineralization indicates a potentially higher amount of transformation from organic N to inorganic N, thus a potentially higher dissolved N to surface runoff losses. The sensitivity of CMN in the calibration for dissolved N losses was also found in other studies (Saleh and Du 2004; Du et al. 2006; Hu et al. 2007). Surprisingly, increasing the value of N plant uptake resulted in higher dissolved N losses although the impact was small. However, many field studies show that increasing plant uptake reduced dissolved N runoff potential because a higher value of PLTNFR resulted in less dissolved N available for loss through runoff (Mitsch et al. 2001; Vetsch and Randall 2004). Review of SWAT literature failed to find any studies reporting the sensitivity of this parameter.

The rest of the parameters barely contributed to dissolved N losses simulation. Dissolved N losses were not sensitive to initial organic N concentration in soil layers (SOLORGN), plant residue decomposition coefficient (RSDCO), organic N enrichment ratio (ERORGN) and N in fresh residue (RSDIN) because those parameters are not directly linked with the inorganic N pool in the soil (Neitsch et al. 2002). Surprisingly, the simulated dissolved N was not sensitive to the initial NO_3 concentration in soil layers (SOLNO3) (Figure 2). The reason may be due to the highly changeable characteristics of NO_3 in soil. After the 3-year warm-up period, the initial NO_3 concentration in soil diminishes with time and thus we do not see any impact on dissolved N losses (Ekanayake and Davie 2005). This also might be the reason why SOLNO3 was not selected for calibration in most reviewed literature (Santhi et al. 2001; Niraula et al. 2012).

Organic N

The SOLORGN and ERORGN were the most sensitive variables for organic N losses (Figure 2). As expected, increasing the value of SOLORGN or ERORGN resulted in higher organic N losses because a greater SOLORGN or ERORGN value denotes a greater amount of organic N transported with sediment, which results in greater organic N losses at the watershed outlet (Santhi et al. 2001). The secondary sensitive variables were SDNCO and BIOMIX (Figure 2). Contrary to the influence of SDNCO on dissolved N losses, a higher SDNCO value that resulted in less organic N losses as expected. A greater BIOMIX value results in higher organic N losses as in reduced and no-tillage practices, which have greater biological activity, can increase soil organic matter (Kladivoka 2001; Liang et al. 2004; Ullrich and Volk 2009), thus higher organic N losses.

The rest of the parameters had little or no impact on organic N simulation. Organic N was not sensitive to NPERCO, RCN and SOLNO3 because those three parameters are not directly linked with the organic N pool, but with the dissolved N pool (Neitsch et al. 2002). In addition, the impacts of N in fresh residue (RSDIN) and residue decomposition factor (RSDCO) on organic N were not detectable for a 20% change of parameter values in this study. Furthermore, increasing the value of mineralization of active organic nutrients (CMN) resulted in lower organic N losses as expected. Finally, organic N losses were sensitive to PLTNFR, and surprisingly a higher value of PLTNFR resulted in higher organic N losses.

Generally, a higher value of PLTNFR requires higher mineralization of soil N (Clarholm 1985), thus a lower organic N in the soil and transported in the sediment. Further research is needed to evaluate SWAT's organic N simulation to provide more insight in this parameter.

TN

The sensitivity of TN generally followed the pattern of organic N (Figure 2). The SOLORGN and ERORGN were the most sensitive variables for TN simulation (Figure 2). Increasing the value of SOLORGN or ERORGN resulted in higher TN losses, as observed in organic N losses. SDNCO and BIOMIX were the secondary sensitive variables to TN losses. Although SDNCO and BIOMIX had different impact on dissolved N and organic N losses, the combined impacts on TN losses were the same as their impacts on organic N losses.

The remaining parameters had little or no impact on TN losses. Although NPERCO and RCN were the most sensitive parameters to dissolved N losses, these two parameters had little impact on organic N losses. Thus, they had little impact on TN losses. A higher value of PLTNFR resulted in higher dissolved N and organic N losses, thus, a higher TN losses too. SOLNO3, CMN, RSDCO and RSDIN had little impact on TN losses because dissolved N and organic N losses were not sensitive to those parameters (Figure 2).

Sensitivity of in-field Parameters on Model Outputs with in-stream Processes

When in-stream processes were simulated, the most sensitive variables for dissolved N changed to SOLORGN and ERORGN (Figure 2 with in-stream modeling) from SDNCO, NPERCO and RCN (Figure 2 without in-stream modeling). The impact of NPERCO and RCN on dissolved N losses was greatly reduced. As a matter of fact, the NPERCO or RCN had almost no impact on dissolved N losses with in-stream processes simulated. Moreover, when in-stream processes were simulated, increasing the value of SDNCO decreased the dissolved N losses, which is opposite to the results of without in-stream simulation. These results of with in-stream simulation is also opposite to the results from field studies

(Crumpton et al. 2007; Drury et al. 2009). This shows that SWAT regroups N pools during in-stream simulation; the in-stream processes were so dominant that the impact of in-field parameters such as SDNCO, NPERCO and RCN on dissolved N was overridden. Therefore, model users should be cautious in applying the model in evaluating conservation practices. As we see from the simulation without in-stream processes, the focus of reducing dissolved N losses would be reducing percolation and increasing denitrification which are consistent with NRCS-recommended conservation practices such as drainage management, wetland and riparian buffers (Drury et al. 2009; Mitsch et al. 2001; Crumpton et al. 2007). However, when in-stream processes are simulated, the focus of reducing dissolved N losses is different since dissolved N losses are more sensitive to SOLORGN and ERORGN, not NPERCO and SDNCO. There is an urgent need to additionally evaluate SWAT in-stream processes in future studies.

When in-stream processes were simulated, the sensitivity of in-field parameters on organic N and TN was greatly decreased (Figure 2). As shown in Figure 2, the in-stream processes did not change the sensitivity of in-field parameters on organic N and TN qualitatively, but did change quantitatively.

Using in-stream parameters for nitrogen calibration is often seen in previous studies (Stewart et al. 2006; Jha et al. 2010; Niraula et al. 2012; Plus et al. 2006; White and Chaubey 2005). In these studies, biological oxidation of NH4 to NO2 (BC1), biological oxidation of NO2 to NO3 (BC2) and hydrolysis of organic N to NH4 (BC3) were mostly used for N calibration. In the study done by Jha et al. (2010), four in-stream parameters (BC1, BC2, BC3 and RS4) and one in-field parameter (ERORGN) were calibrated for nitrate simulation. Values of these parameters were adjusted to increase SWAT simulated nitrate to match the measured values, indicating the model underestimated nitrate loads prior to calibration and adjustment of in-stream parameters was needed in order to increase the simulated nitrate loads. Other in-stream parameters, such as organic N settling rate (RS4) and Algal preference for NH4 (P_N), were also used to increase the simulated N loads (Niraula et al. 2012; Plus et al. 2006). However, no discussion was made on the relative importance of in-stream parameters versus in-field parameters on N simulations in those studies.

Impact of Fertilizer Timing and Amount on N Losses

Studies show that the actual dissolved N losses depend on fertilizer timing and amount (Jaynes et al., 2001; Vetsch and Randall, 2004; van Es et al., 2006; Salvagiotti et al., 2008). Vetsch and Randall (2004) suggest that N should be applied in the spring because the risk of N loss is greater with fall application. When fertilizer is applied in April around planting time (April, June), it reduces the chances for losses from fields due to plant uptake. Therefore, it is expected that December application would result in greater dissolved N losses. When in-stream processes were not simulated, the annual average dissolved N loss was the highest for fertilizer application in December (Table 5). Secondly, the annual average dissolved N loss was the least for fertilizer application in June, followed by August, October and April which is the baseline; and the difference among the four dates was little (Table 5). Thirdly, the timing of fertilizer had greater impact on monoculture corn than on corn/soybean rotation. Finally, timing of fertilizer application had little impact on organic N and TN losses (Table 5, only TN is shown since the impact on organic N is similar to TN). When in-stream processes were simulated, the dissolved N and TN losses were greatly increased for all scenarios, but their relative changes from different scenarios were much decreased (Table 5). As a matter of fact, the changes from different application timing were almost negligible.

<Table 5>

When in-stream processes were not simulated, higher amounts of fertilizer application resulted in higher amounts of dissolved N losses, as expected, although changes from different scenarios were small (Table 5). Fertilizer application rate had more impact on monoculture corn than on corn/soybean rotation. The TN losses were not sensitive to the amount of fertilizer application (Table 5). However, when in-stream processes were simulated, increasing fertilization rates resulted in no changes on dissolved N losses due to much higher amount of dissolved N losses from in-stream processes (Table 5). This additionally shows the need to evaluate SWAT in-stream processes.

In summary, no difference was found with different timing of fertilizer application and/or different amount of fertilizer application when in-stream processes were simulated (Table 5).

Model Performance of N Simulations

The model performed better for the period of October 1993 – September 1995 than for the entire available monitoring period (10/1/1983 – 9/30/1985 and 2/1/1993 – 9/30/1995) when comparing model simulated results with measured data in terms of the four statistical criteria (Table 6). The model performed well on streamflow and TSS in terms of all four statistical criteria for the period of October 1993 – September 1995. Moreover, the PBIAS values of dissolved N and TN were within the suggested range of model satisfaction. While for the entire available monitoring period (10/1/1983 – 9/30/1985 and 2/1/1993 – 9/30/1995), the model only performed well on TSS and dissolved N in terms of smaller PBIAS values (Table 6a). The better model performance during October 1993 – September 1995 may indicate that the model inputs such as land use and management practices represented the watershed situation well during that period.

Generally, both the simulated streamflow and dissolved N followed the trend of observed streamflow and dissolved N (Figure 3). In April of 1995, the simulated dissolved N was much lower than the measured dissolved N (Figure 3b) as the simulated streamflow was lower than the measured streamflow (Figure 3a). In August of 1995, both the simulated streamflow and the dissolved N were higher than their measured counterparts due to higher rainfall in August of 1995 (Figure 3). Further calibration of fertilizer timing and amount would not make any difference as illustrated in Figure 3b and discussed previously. The lower simulated dissolved N was not caused by runoff simulation since runoff was over-predicted (Table 6). In contrast, comparison of simulated monthly organic N and TN with observed organic N and TN shows that the simulated organic N and TN were much higher than the observed organic N and TN, respectively (Table 6). The higher simulated organic N and TN were not caused by sediment simulation since the simulated sediment is close to the observed sediment (Table 6). To increase the simulated dissolved N losses, SOLORGN, and/or ERORGN need to be increased based on results of sensitivity analysis (Figure 2 with in-stream modeling); but this would make the already high simulated organic N and TN losses even higher (Figure 2 with in-stream modeling). Thus, there was an insurmountable barrier in calibrating SWAT to capture dissolved N simulation as well as organic N and TN simulation. This also explains why some studies only show good performance for TN (Arabi et al. 2006; Grunwald and Qi 2006; Saleh et al. 2000; Saleh and Du 2004; Santhi et al. 2001; White and Chaubey 2005; Hu et al. 2007; Niraula et al. 2013).

<Figure 3>

Conclusions

Sensitivity analysis of in-field N parameters on N losses with in-stream simulation and without in-stream simulation found that when in-stream processes were not simulated, denitrification threshold water content (SDNCO), N percolation coefficient (NPERCO) and nitrogen in rainfall (RCN) were the most sensitive in-field parameters for dissolved N losses. However, when in-stream processes were simulated, initial organic N concentration in soil layers (SOLORGN) and organic N enrichment ration (ERORGN) were the most sensitive in-field parameters for dissolved N losses. The impact of NPERCO and SDNCO on dissolved N losses was negligible. The sensitivity of in-field parameters for TN losses generally paralleled the results for organic N losses which were sensitive to SOLORGN, ERORGN, SDNCO and biological mixing efficiency (BIOMIX). Simulation of in-stream processes did not change the sensitivity of in-field parameters for organic N and total N qualitatively; however, the magnitude of impacts was much decreased with in-stream simulation.

When in-stream processes were simulated, the annual average dissolved N losses had little or no changes from different fertilizer application timing and amount. Compared with the monthly observed N losses, the SWAT simulated N losses with in-stream processes had lower dissolved N, but higher organic N and TN losses. Based on the sensitivity results, dissolved N losses could be adjusted by increasing the value of ERORGN or SOLORGN. However, this would also increase organic N and TN losses. Conflicts such as these demonstrated the importance of further evaluating SWAT's simulation of in-stream processes.

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Table 1. Land use in the subwatershed drained by gauge 5431014 in the Jackson watershed. This land use was an aggregate land cover classification created by combining the NLCD 2001 with the USDA-National Agriculture Statistical Survey Cropland Data Layer for the years 2004-2007.

Land use	Area (km^2)	% Watershed area
Corn-Soybean	10.58	52.0
Monoculture Corn	2.96	14.5
Other crops*	2.81	13.8
Forest	0.73	3.6
Pasture	1.43	7.0
Urban	1.77	8.7
Water	0.06	0.3
Total	20.35	100.0

*other crops include soybean-corn-wheat, corn-wheat, wheat, alfalfa, and grass.

Table 2. Soil physical content and estimated chemical content in SWAT

Soil type	Kidder (WI117)			Pella (WI122)			
Layer	1	2	3	1	2	3	4
Depth from the soil surface (mm)	279.4	711.2	1524	330.2	787.4	965.2	1524
Organic carbon content (% soil weight)	1.16	0.39	0.13	3.2	1.07	0.36	0.12
Moist bulk density (Mg/m^3)	1.45	1.58	1.5	1.25	1.33	1.48	1.55
Nitrate concentration (mg/kg)	5.3	3.4	1.5	5	3.2	2.7	1.5
Humic organic N concentration (mg/kg)	828.6	278.6	92.9	2285.7	764.3	257.1	85.7
Total nitrogen concentration ($10^2 kg/km^2$)	3378.2	1924	1150.7	9455.1	4666.8	683.7	755.6

Table 3. Management applied on major crop plantation types (corn-soybean, continuous corn and soybean)

Rotation	Date	Management
Corn-Soybean		
Year1	4/20	Fertilization (4150 P kg/km^2, 11990 N kg/ km^2)
	5/10	Corn planting
	10/20	Harvest & kill
	11/1	Tillage (Chisel)
Year2	5/15	Soybean planting
	5/15	Tillage (Cultivator)
	10/10	Harvest & kill
Corn		
Year1	10/25	Fertilization (4150 P kg/km^2, 11990 N kg/ km^2)
Year2	5/1	Corn planting
	10/20	Harvest & kill
Soybean		
Year1	5/14	Fertilization (3700 P kg/ km^2, 1680 N kg/ km^2)
	5/15	Tillage (Chisel)
	5/15	Soybean planting
	10/10	Harvest & kill

Table 4. The range, default, minimum, maximum and average values of selected SWAT N-related parameters. (: Minimum, maximum and average values of the parameters were used for sensitivity analysis.)

Parameter Name	Description	Process	Parameter Range[a]	Default Value	20% decrease.	20% increase
BIOMIX	Biological mixing efficiency	Soil	0 - 1	0.2	0.16	0.24
CMN	Rate factor for mineralization of active organic nutrients	Nutrient	0.001 - 0.003	0.0003	0.00024	0.00036
ERORGN	Organic N enrichment ratio	Nutrient	0 - 5	0 (2.5)	2	3
NPERCO	Nitrogen percolation coefficient	N in groundwater	0.001 - 1	0.2	0.16	0.24
PLTNFR	Fraction of N in plant biomass (kg N/kg biomass)	Plant N uptake	-	0.0305[b]	0.0244[b]	0.0366[b]
RCN	Concentration of nitrogen in rainfall (mg/l)	Nutrient	0.001 -15	1	0.8	1.2
RSDCO_PL	Residue decomposition factor	Crop residue	0.01 – 0.099	0.05	0.04	0.06
RSDIN	Initial residue cover (kg/ha)	N in fresh residue	0-10000	0 (100)	80	120
SDNCO	Denitrification threshold water content	Soil	0.001-1	0.8	0.64	0.96
SOLNO3	Initial NO3 concentration in soil layers (mg/kg)	Soil	-	0 (3.23[c])	2.58[c]	3.87[c]
SOLORGN	Initial organic N concentration in soil layers (mg/kg)	Soil	-	0 (1000)	800	1200
BC1	Biological oxidation of NH4 to NO2	In-stream	0.1 - 1	0.55	-	-
BC2	Biological oxidation of NO2 to NO3	In-stream	0.2 - 2	1.1	-	-
BC3	Hydrolysis of organic N to NH4	In-stream	0.2 - 0.4	0.21	-	-
MUMAX	Maximum specific algal growth rate at 20 °C (day^{-1})	In-stream	1 – 3	2	-	-
P_N	Algal preference factor for ammonia nitrogen	In-stream	0.01 – 1	0.5	-	-
RHOQ	Algal respiration rate at 20 °C (day^{-1})	In-stream	0.05 - 0.5	0.3	-	-
RS3	Sediment source rate for ammonium N at 20 °C (mg NH4-N/m2-day)	In-stream	0.1 – 5	0.5	-	-
RS4	Organic N settling rate at 20 °C (day^{-1})	In-stream	0.01 - 0.1	0.05	-	-

a: the range of parameter values are suggested in SWAT2005.mdb (Neitsch et al., 2002).
b: the value is an average of PLTNFR at 3 different plant growth stages for corn and soybean.
c: the value is an average of NO3 values in all layers of WI117 and WI122 soil.

Table 5. Average annual (1983-2007) dissolved N and TN losses at the watershed outlet and their relative changes to baseline with various fertilizer timing and rate scenarios. (Note: remaining model parameters at default values shown in Table 4).

		Without in-stream modeling				**With in-stream modeling**			
Parameter	Model value	Dissolved N (kg/km^2)	Relative Changes (%)	TN (kg/km^2)	Relative Changes (%)	Dissolved N (kg/km^2)	Relative Changes (%)	TN (kg/km^2)	Relative Changes (%)
Corn-soybean									
Baseline		56.7		1163.5		714.2		2852.3	
Fertilizer timing	Jun. (6/20)	51.3	-9.5	1055	-9.3	682.9	-4.4	2738.7	-4.0
	Aug. (8/20)	55.7	-1.8	1172.1	0.7	718.5	0.6	2863.6	0.4
	Oct. (10/10)	53.8	-5.1	1171.7	0.7	721.4	1.0	2867.4	0.5
	Dec. (12/20)	156	175.1	1273.8	9.5	743.6	4.1	2898.1	1.6
Fertilizer rate	-50%	54.3	-4.2	1165.8	0.2	718	0.5	2859.6	0.3
	-20%	55.7	-1.8	1164.1	0.1	716.5	0.3	2855.6	0.1
	20%	57.6	1.6	1162.8	-0.1	713.4	-0.1	2851.1	0.0
	50%	59	4.1	1161.9	-0.1	712.8	-0.2	2848.4	-0.1
Corn									
Baseline		62.8		1144.1		752.8		2977.7	
Fertilizer timing	Jun. (6/20)	56	-10.8	1137.4	-0.6	750.9	-0.3	2975.5	-0.1
	Aug. (8/20)	57	-9.2	1138.4	-0.5	750.5	-0.3	2973.7	-0.1
	Oct. (10/10)	58.5	-6.8	1139.7	-0.4	751.9	-0.1	2975.6	-0.1
	Dec. (12/20)	196.7	213.2	1273.9	11.3	784.2	4.2	3014.3	1.2
Fertilizer rate	-50%	58.8	-6.4	1140	-0.4	756.9	0.5	2982.6	0.2
	-20%	61.2	-2.5	1142.5	-0.1	754.3	0.2	2978.9	0.0
	20%	64.4	2.5	1145.8	0.1	751	-0.2	2976.5	0.0
	50%	66.9	6.5	1148.2	0.4	749.1	-0.5	2975.5	-0.1

Table 6. SWAT model performance on monthly simulations of flow, TSS and nitrogen during (a) entire available period and (b) October 1993 – September 1995. (Note: NSE denotes Nash Sutcliffe coefficient; R^2 denotes coefficient of determination; RSR denotes RMSE-Observations Standard Deviation Ratio; PBIAS denotes percent bias.)

(a) Entire available periods (10/1/1983 – 9/30/1985 and 2/1/1993 – 9/30/1995)

	Flow	TSS	Dissolved N	Organic N	TN
Measured mean*	3.96	19.56	0.94	0.18	1.13
Simulated mean*	5.18	19.00	0.48	0.93	2.10
NSE	0.34	0.36	0.21	-11.22	-0.50
R^2	0.46	0.39	0.37	0.87	0.53
RSR	0.81	0.80	0.89	3.50	1.22
PBIAS	-30.83	2.87	48.78	-413.97	-86.08

(b) October 1993 – September 1995

	Flow	TSS	Dissolved N	Organic N	TN
Measured mean*	2.56	10.54	0.65	0.10	0.76
Simulated mean*	2.81	11.45	0.26	0.70	1.24
NSE	0.72	0.65	0.09	-19.73	-0.18
R^2	0.74	0.75	0.24	0.82	0.47
RSR	0.53	0.59	0.95	4.55	1.09
PBIAS	-9.49	-8.68	60.49	-623.21	-64.24

* Unit for flow is cms, and unit for TSS, dissolved N, organic N and TN is 10^2 kg/ km^2

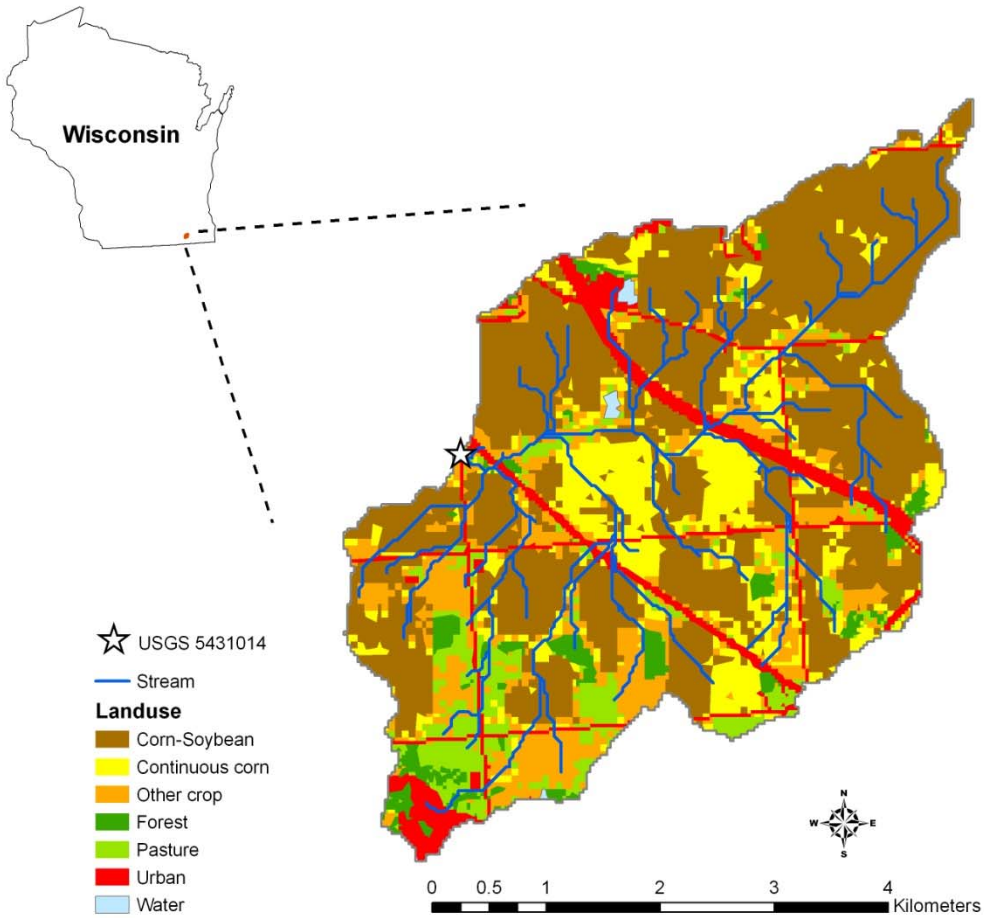

Figure 1. Land use distribution and location of gauging station in the Upper Rock subwatershed

Without in-stream modeling With in-stream modeling

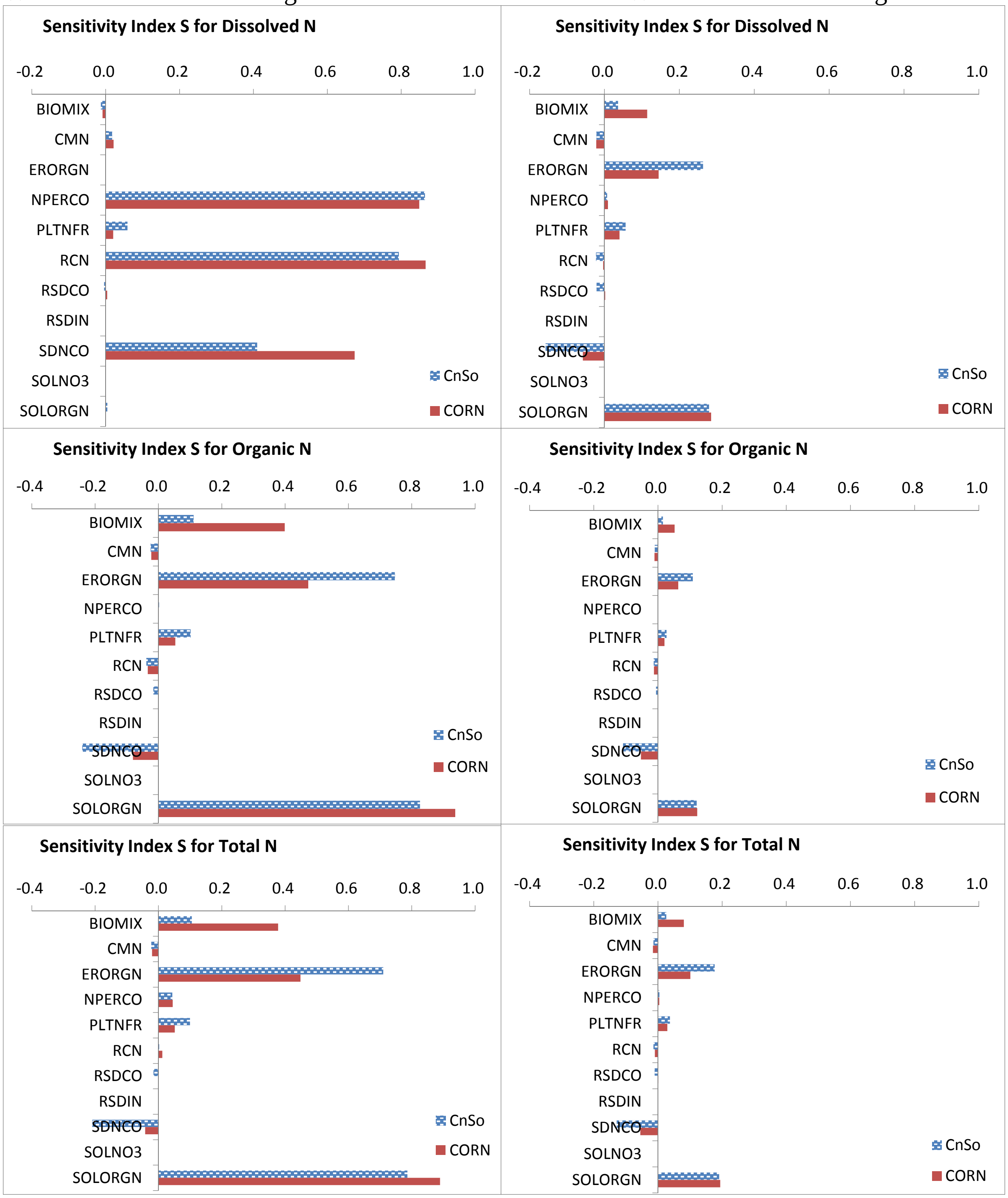

Figure 2. Sensitivity of in-field parameters to dissolved N, organic N and TN losses at watershed outlet (Left: without in-stream simulation; right: with in-stream simulation; red: corn; blue pattern: corn/soybean). Please see Table 4 for parameter description.

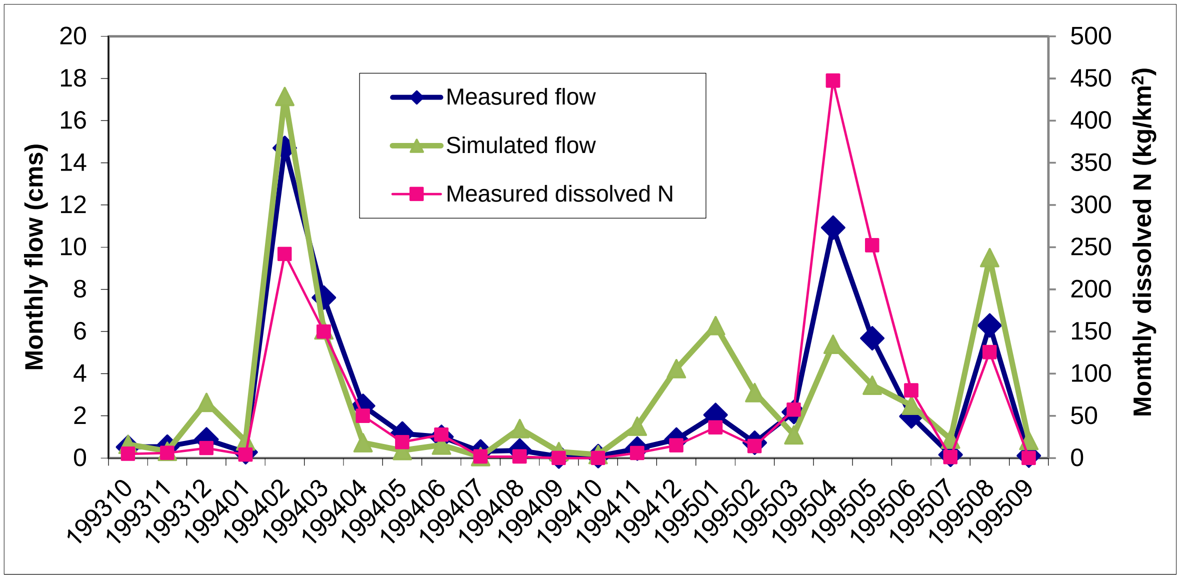

Figure 3a. Comparison of measured and simulated streamflow

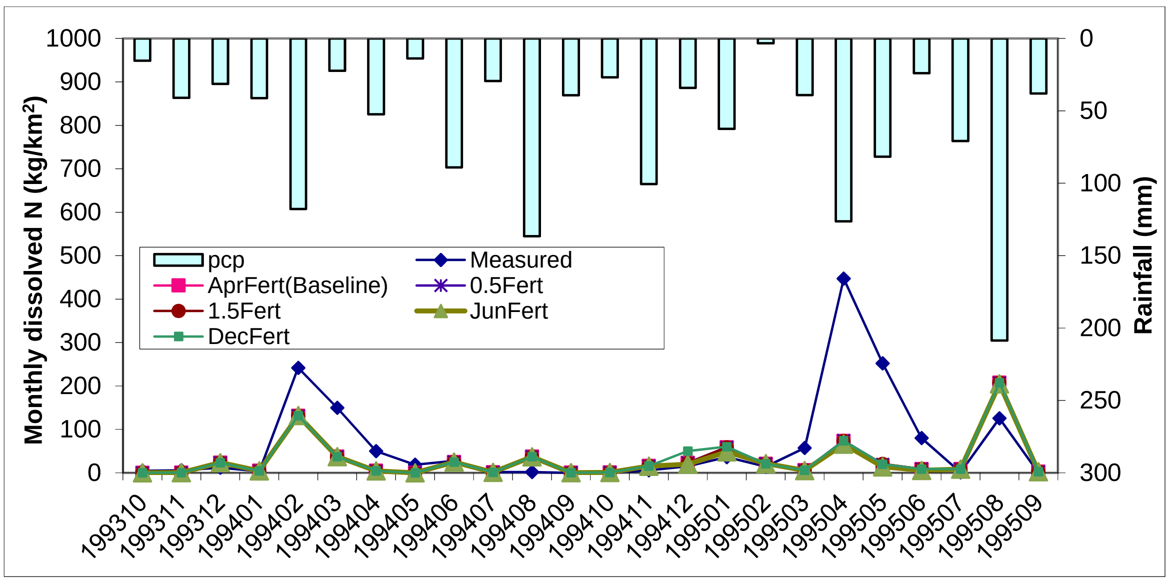

Figure 3b. Comparison of measured and simulated dissolved N losses of baseline scenario (corn/soybean rotation; fertilizer was applied in April), two fertilizer timing scenarios (Applied in June and December) and two fertilizer amount scenarios (increased and decreased by 50% of the initial fertilizer rate) for periods of October 1993-September 1995