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Application of the DNDC model to tile-drained Illinois agroecosystems: model comparison of conventional and diversified rotations

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Abstract Using the DeNitrification–DeComposition (DNDC) model we compare conventional, fertilizer-driven corn–soybean rotations to alternative management scenarios which include the management of cereal rye cover crops and corn–soybean–wheat–red clover rotations. We conduct our analysis for tile-drained, silty clay loam soils of Illinois. DNDC simulations suggest that, relative to conventional rotations, a nitrate leaching reduction of 30–50% under corn and of 15–50% under soybean crops can be achieved with diversified rotations, an outcome which corroborates results from a quantitative literature review we previously conducted using a meta-analysis framework. Additionally, over a 10-year simulation, legume-fertilized systems are predicted to result in 52% lower N_2O gas flux relative to fertilizer-driven systems. We identify soil organic carbon storage, legume N-fixation rate, and cereal rye cover crop growth as areas requiring further development to accurately apply DNDC to diversified cropping systems. Overall, DNDC simulation suggests diversified rotations that alternate winter and summer annuals have the potential to dramatically increase N retention in agroecosystems.

Keywords Nitrogen management · Agroecosystem model · Nitrate leaching · N trace gas · Cover crop · Legume · Corn · Soybean

Introduction

Humans introduce 170 Tg of reactive N into agroecosystems annually, with inorganic fertilizer additions to agroecosystems accounting for approximately 80 Tg N year^{-1} (Smil 1999). Nitrogen management presents a particular challenge because it is the nutrient which is most frequently limiting in agricultural systems and is also the most mobile nutrient with many potential pathways of loss. Recovery of applied N in crop biomass averages only 45–55% (Tilman 1999; Galloway 2000; Smil 1999; Galloway and Cowlings 2002); the inefficiency of N fertilization is a problem that must be addressed to significantly reduce anthropogenic forcing of the global N cycle. Nitrogen surplus is lost from agricultural

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landscapes through leaching, denitrification, ammonia volatilization, NO_x production during nitrification, and erosion. Current best estimates attribute denitrification with 26–60 Tg N year^{-1}, and leaching and erosion with 32–45 Tg N year^{-1} of N losses from agroecosystems (Smil 1999).

N export from corn–soybean systems of the mid-west

Aggregated budgets indicate that in the US and Europe, annual N and P inputs consistently exceed the amounts exported as harvested crops (Van der Molen and Boers 1999; David and Gentry 2000). As a result, the majority of lands under intensive agricultural management in industrialized countries tend to have nutrient surpluses. Increased nutrient loss from ecosystems following nutrient additions which saturate plant and microbial uptake has been documented for temperate forests (Fenn et al. 1998), other natural terrestrial ecosystems (Neff et al. 2002) and conventional (David and Gentry 2000) and organic agricultural systems (Oleson et al. 2004). Asynchrony in the availability of N in agricultural systems of the Mississippi basin resulted in N losses ranging from 30 to 50% of N applied (McIsaac et al. 2002). McIsaac and Hu (2004) show up to 100% of residual N can be lost to streams in these systems.

Water quality degradation as a result of agricultural management is observed at all scales, impacting both local and regional human water supplies as well as estuary and marine habitats important to domestic fisheries. Severe eutrophication was documented in 44 of the 139 domestic estuaries studied by Bricker et al. (1999), with an additional 36 estuaries demonstrating moderate eutrophication. The hypoxic zone off the coast of Louisiana is the most extreme manifestation of agricultural impact on water quality (Rabalais et al. 2002). Goolsby and Battaglin (2001) demonstrated that nitrate currently accounts for 62% of the N flux from the Mississippi Basin to the Gulf of Mexico, and that nitrate flux from 1980 to 1999 was three times the rate observed between 1955 and 1970. David et al. (2001) estimated 50% of surplus N was exported from the state of Illinois and attributed this high N loss rate to land management that is 64% row crop agricultural. Nitrogen contributions to the Mississippi drainage are dominated by fluxes from Minnesota, Iowa, Illinois, Indiana, and Ohio drainages, suggesting the need for social and economic policies which reduce the export of pollution across state boundaries.

Ecosystem approach to agricultural N management

Ecosystem management is a land-management approach that (1) takes into account the full suite of organisms and ecosystem processes, (2) applies the concept that ecosystem function depends on ecosystem structure and diversity, (3) recognizes that ecosystems are spatially and temporally dynamic, and (4) includes sustainability as a primary goal (Dale et al. 2000). Ecosystem-based management of N in agriculture entails the use of practices that influence ecosystem processes at a variety of temporal and spatial scales to reduce the need for chronic additions of surplus nutrients (Drinkwater 2004; Drinkwater and Snapp 2007). In previous work we quantitatively reviewed the agricultural literature to assess two alternative practices that impact both C and N cycling processes at multiple temporal and spatial scales but are not commonly used in intensified systems of the U.S. (Tonitto et al. 2006). Using a meta-analysis design, we quantified differences in yield and nitrate leaching across paired studies of conventional grain systems with a winter bare fallow compared to rotations with either leguminous (N-fixing) or non N-fixing cover crops. We found that yields in cover cropped systems receiving fertilizer were not significantly different from those in the conventional, bare fallow systems, while leaching was reduced by 70% on average. Relative to yields in N-fertilized systems, the legume-fertilized crops averaged 10% lower yields and a 40% reduction in nitrate leaching; no reduction in crop yield was observed when aboveground legume biomass contributed greater than 110 kg N ha^{-1}.

Here, we summarize ecosystem dynamics across a range of agroecosystem management approaches using the DeNitrification–DeComposition (DNDC) model (Li et al. 1992a, b, 1994, 2000). We focused on intensive, corn–soybean production in Illinois (IL) tile-drained lands, due to their significant contribution to nitrate loading in the Gulf of Mexico. We applied the DNDC model due to its biogeochemical rigor and its widespread use in management and policy studies. The DNDC model is a mechanistic, process based model of C and N dynamics (Li et al. 1992a, 2000) which includes descriptions of plant growth, litter decomposition, microbially mediated transformations of C and N in soil, C and N trace gas fluxes, and hydrology. In parallel work we calibrated the DNDC model for corn–soybean rotations grown on tile-drained silty loam Mollisol soils common to east-central Illinois (Tonitto et al. 2007). Here we apply our DNDC modifications to compare the impact of management decisions in these tile-drained Mollisol systems.

Goals

We applied the DNDC model to assess yield, N, and C dynamics under diversified compared to conventional corn–soybean rotations in an Illinois tile-drained silty clay loam agroecosystem. We focused on these comparisons due to the significant potential of ecological management practices to reduce N losses from these agroecosystems. Given the limited spatial and temporal extent of diversified rotations in the Illinois landscape, application of ecosystem models is a necessary approach to quantifying management impacts at larger spatial and temporal scales. Here we address the following questions: (1) How do simulated yield, drainage, and nitrate leaching outcomes differ under diversified relative to conventional corn–soybean rotations in Illinois tile-drained Mollisol regions? (2) What are predicted trends in soil N, soil C, and N trace gas emissions under diversified relative to conventional management? (3) How do aggregate model dynamics differ under parameter variation?

Methods

DNDC application to diversified systems

In parallel work, we parameterized DNDC to describe an Illinois corn–soybean rotation on tile-drained silty clay loam soils (Tonitto et al. 2007). We assessed the predictive capacity of DNDC output using data from the Embarras River watershed near the city of Urbana, IL. We tested model predictions for bias, modeling efficiency, Theil's inequality, RMSE, and the correlation coefficient. Our calibration and validation research resulted in significant changes to four parameters which impact drainage and nitrate leaching below the root zone in the DNDC model. These parameter changes physically represent the feature of tile-drainage in these systems, a physical process not currently represented in the DNDC model. Due to the absence of diversified rotations in Illinois, there are no drainage, nitrate leaching or yield data for diversified rotations in tile-drained Mollisols. We conducted simulations of the diversified system using parameter ranges established for the conventional corn–soybean rotation. As a result, our DNDC application assumes the parameters calibrated to describe the conventional corn–soybean rotation apply to the diversified rotation. We consider this assumption applicable to diversified rotations because our parameter changes simulate the dynamics of tile-drainage.

We used the silty clay loam soils file for conventional and diversified simulations, with a clay fraction of 35%, porosity of 0.477, saturated conductivity of 0.025 cm min^{-1}, and field capacity and wilting points of 0.73 and 0.31 (as water-filled porosity or WFPS), respectively. In this application of DNDC we tested the following parameter values: (1) $0.025 < \text{DVD} < 0.05$, a parameter controlling loss of pore space water; (2) $0.05 < \text{DID} < 0.2$, a parameter controlling loss of freely available water, (3) $0.0002 < \text{PLN} < 0.5$, a parameter defining nitrate available for plant uptake, and (4) $200 < \text{DWL} < 700$, a parameter determining nitrate loss from a soil layer. See Tonitto et al. (2007) for a complete discussion of the impact of these parameters on DNDC outcomes.

Simulation structure

In this analysis, the conventional system is a corn–soybean rotation receiving inorganic N fertilizer and managed with a winter bare fallow. We chose a landscape distribution of 50% corn and 50% soybean coverage, because an even split between these two crops describes the average east-central Illinois landscape in a given year. We contrasted this management practice to five alternative rotations: (1) fertilizer-based corn–soybean with cereal rye cover crop management (corn–rye–soybean–rye), (2) fertilizer-based diversified corn–soybean–wheat rotation, (3) fertilizer-based diversified rotation with a rye cover crop (corn–rye–soybean–wheat), (4) legume-based diversified corn–soybean–wheat–red clover rotation, (5) legume-based diversified rotation with a rye cover crop (corn–rye–soybean–wheat–red clover). Management details are described in Table 1. For each simulated year, we model each crop considered in a rotation. We reduced the effect of initial conditions on element pool distributions by excluding the first simulated year from analysis.

In this analysis we compared the diversified rotations to a best-case corn–soybean rotation in which all fertilizer is applied in the spring. In practice east-central Illinois is averaging 80% fall N fertilizer application. Therefore, the results presented here represent a comparison of best-case conventional management to five potential alternative practices. Outcomes under current east-central Illinois management practices are detailed in Tonitto et al. (2007).

Our diversified management scenarios required the development of cereal rye and red clover crop input files. We edited the default non-legume hay (crop 5) and legume hay (crop 4) DNDC library files to reflect cereal rye and red clover physiology, respectively. Red clover physiology was represented in the crop 4 file using: total biomass C = 5000 kg C ha^{-1}, shoot proportion = 0.8, root proportion = 0.2, plant C:N = 17.8, root C:N = 20, shoot C:N = 10, N fix = 5 (N-fixation supplies up to 85% of legume N need). Cereal rye physiology was represented in the crop 5 file using: total biomass C = 5500 kg C ha^{-1}, shoot proportion = 0.6, root proportion = 0.4, plant C:N = 32, root C:N = 50, shoot C:N = 20, N fix = 1 (no fixation). In simulations, legume and non-legume cover crop biomass was incorporated into the soil prior to cash crop planting. We based our expectations for rye yield on results documented by Crandall et al. (2005). Modeled red clover yield was derived using field results from studies conducted under a range of soil and climate conditions (Drinkwater

Table 1 Management schedule for conventional and diversified rotations

	Cash crop	Tillage	Planting	Harvest	Winter cover	No-till planting	Fertilization	Amount	Type
Corn–soybean									
Year 1	Corn	4/21	5/1	10/21	None		5/1	190.00	NH_4NO_3
Year 2	Soybean	5/7	5/21	10/5	None		11/21		
Corn–rye–soybean–rye									
Year 1	Corn	4/21	5/1	10/21	Cereal rye	10/23	5/1	190.00	NH_4NO_3
Year 2	Soybean	5/7	5/21	10/5	Cereal rye	10/10			
Corn–soybean–wheat									
Year 1	Corn	4/21	5/1	10/21	None		5/1	190.00	NH_4NO_3
Year 2	Soybean	5/7	5/21	10/5	Wheat	10/10	10/10	20.00	NH_4HPO_4
Year 3	Wheat			6/21	None		3/21	60.00	Urea
Corn–soybean–wheat–red clover									
Year 1	Corn	4/21	5/1	10/21	None				
Year 2	Soybean	5/7	5/21	10/5	Wheat	10/10	10/10	20.00	NH_4HPO_4
Year 3	Wheat			6/21	Red clover	6/23	3/21	60.00	Urea
Corn–rye–soybean–wheat									
Year 1	Corn	4/21	5/1	10/21	Rye	10/23	5/1	190.00	NH_4NO_3
Year 2	Soybean	5/7	5/21	10/5	Wheat	10/10	10/10	20.00	NH_4HPO_4
Year 3	Wheat			6/21	None		3/21	60.00	Urea
Corn–rye–soybean–wheat–red clover									
Year 1	Corn	4/21	5/1	10/21	Rye	10/23			
Year 2	Soybean	5/7	5/21	10/5	Wheat	10/10	10/10	20.00	NH_4HPO_4
Year 3	Wheat			6/21	Red clover	6/23	3/21	60.00	Urea

et al. 2000; Vyn et al. 2000; Stute and Posner 1995).

Uncertainty analysis

In this work, we applied (1) event validation and (2) traces (Rykiel 1996) to test the robustness of modeled N and C dynamics. Due to the limited availability of data, we emphasized trends in model uncertainty under parameter variation. Specifically, we examined how modeled yield, C, and N dynamics vary under a change in parameter values. Our broad test of drainage and nitrate leaching parameters identified 64 parameter combinations which produced statistically meaningful predictions for a conventional corn–soybean system on tile-drained Illinois Mollisols (Tonitto et al. 2007). Here we explored DNDC model outcomes under parameter variation for a suite of management practices. This analysis documents how model outcomes are influenced by parameter misestimation. Uncertainty analysis allows us to quantify our confidence in model application to specific land management protocols and bound model predictions to inform land management choices.

Event validation

Carbon, nitrogen, and water pools and transformations are modeled on a daily temporal scale. Though field data are not available at this resolution for all of the processes modeled, mechanistic biogeochemical studies demonstrate that C and N transformations are sensitive to the soil environment and that episodic events are important drivers of cumulative results (e.g., Leffelaar and Wessel 1988; Tanji 1982; Frissel and Van Veen 1981). Due to the lack of N trace gas field data, we tested model outcomes for relationships between N trace gas flux and the soil environment. Using the cross-correlation function (CCF, Eq. 1) we tested for pattern between predicted N_2 and N_2O flux and: (1) active soil C, (2) soil moisture, (3) soil NO_3^-, and (4) soil NH_4^+. Cross-correlation analysis allows us to assess whether predicted N gas flux events are correlated with predicted soil chemical and physical properties at a mechanistically relevant time scale. The CCF is not an even function; because we were interested in assessing whether past soil environment correlates to current N gas flux, we only considered the forward CCF. In our analysis we limited the lag, k, to a 30-day interval. Field and laboratory studies suggest that N_2 flux increases with increasing SOC and soil moisture (Bremner and Shaw 1958; Nommik 1956; Burford and Bremner 1975; Smith and Tiedje 1979; Focht and Verstraete 1977; Delwiche 1959). Additionally, we expected N gas flux rates to increase with increasing soil NO_3^- (McSwiney and Robertson 2005):

$$\mathrm{CCF}(k) = \frac{\sum_{t=1}^{N-k} \frac{(x_t-\bar{x})(y_{t+k}-\bar{y})}{N}}{\sum_{t=1}^{N} \frac{(x_t-\bar{x})(x_t-\bar{x})}{N} \sum_{t=1}^{N} \frac{(y_t-\bar{y})(y_t-\bar{y})}{N}} \qquad (1)$$

For x = time series 1, y = time series 2, N = number of observations, k = lag.

Trace analysis

Given that the daily time-step of DNDC biogeochemical outcomes exceeds biogeochemical observations in any ecosystem, we focused on temporally aggregated results to assess management scenarios. Trace analysis was used to assess the ability of DNDC simulations to track broad timescale patterns expected based on mechanistic and field studies. We aggregated daily modeled outcomes to understand model trends on annual to decadal time scales. Ultimately, we contrasted cumulative model outcomes across management scenarios to discuss the implications of management decisions. This long time scale approach complements the analysis of short time scale dynamics assessed with event validation.

Validation of diversified simulations

Due to the absence of data for diversified systems in Illinois, we compared temporally aggregated model results to quantitative results derived from our meta-analysis of diversified systems applied to annual rotations (Tonitto et al. 2006). Analysis of the literature comparing conventional to diversified rotations showed: (1) rotations managed with inorganic N fertilizer and winter cover crops had no significant cash crop yield decline and averaged 70% reductions in nitrate leaching, (2) rotations managed with legume-based N fertilization resulted in no cash crop yield declines when aboveground legume biomass provided at least 110 kg N ha^{-1} and averaged a 40% reduction in nitrate leaching.

Results and discussion

Annual model trends

Yield dynamics

Corn yield was significantly affected by variation in parameter values. Variation in modeled corn yield was observed for both conventional and diversified management scenarios. This is in contrast to model outcomes under current Illinois conventional management, which uses a higher percentage of fall fertilizer application (Tonitto et al. 2007). In our analysis of current Illinois practice, significant variation in corn yield as a result of parameter variation was limited to simulations of 1995 and 2000 yields. In the present study, conventional corn yield varied in 1995, 1999, and 2000, with 1999 and 2000 yield predictions ranging over 1,200 kg C ha^{-1}, a range much larger than that predicted under split fertilizer application. This result suggests that a subset of parameter combinations which were valid for DNDC simulation of current management do not reflect ecosystem processes under spring fertilization in dry years. Across all parameter sets 1999 and 2000 resulted in high spring loss of N_2O and N_2. Parameter sets which resulted in poor crop yield exhibited both increased periods of high N_2O and N_2 flux, as well as N trace gas flux which coincided with planting and early crop growth. The disadvantage to crop growth early on in the simulation prevented the crop from attaining expected yields. Increased instances of N trace gas flux were associated with low DVD values (reducing water loss from the soil pore space) and low PLN values (reducing the ability of plants to take up N).

In contrast to fertilized systems, 1995 and 2000 corn yield in the legume-fertilized system demonstrated little variation across parameter sets. In 1998, however, variation in corn yield in the legume-based system was larger than that of conventional systems. Parameter sets which resulted in low cash crop yields coincided with low gross mineralization rates in the early growing season. Simulated total legume biomass N ranged from 160 to 350 kg N ha^{-1}, resulting in gross mineralization ranging from 2 to 8 kg N ha^{-1} day^{-1} at crop planting and from 2 to 4 kg N ha^{-1} day^{-1} during the early growing season. Initially following planting, corn growth was similar across parameter sets, but growth rates declined due to N limitation in simulations with lower gross mineralization. Variation in soybean yield was large in conventional systems in 1994 and 1998. Soybean yield in diversified systems was similar or smaller than the range observed in conventional systems.

Model calibration and validation simulations of the split N fertilizer application which is practiced in tile-drained regions of Illinois showed good agreement between simulated and measured crop yield for 64 parameter sets (Tonitto et al. 2007). As described above, application of DNDC using these parameter sets for a conventional system with spring applied N results in high yield variability in some years. We sorted the parameter sets established through model calibration and validation such that simulated conventional spring applied N management compared to measured crop yield resulted in a modeling efficiency $EF > 0.8$. This analysis of simulation outcomes established four parameter sets which best simulated observed yields. Table 2 summarizes the mean annual percent deviation in yield of diversified rotations relative to the conventional, spring applied N simulation. A small reduction in corn yield was observed for both the corn–rye–soybean–rye and the legume-fertilized rotations, while fertilized corn–soybean–wheat rotations (with or without rye) enhanced corn production. Relative to the conventional system, soybean yield was slightly reduced in rotations which included a rye cover crop and slightly increased under corn–soybean–wheat and corn–soybean–wheat–red clover rotations.

Table 2 Average annual conventional crop yield and percent deviation of yield in diversified systems over a 10-year simulation

	Corn	Soybean
	Yield (kg C ha^{-1})	
Conventional		
Corn–soybean	3,890	1,550
	Yield (% deviation from conventional)	
Diversified		
Corn–rye–soybean–rye	–8.8	–9.0
Corn–soybean–wheat	2.1	1.2
Corn–rye–soybean–wheat	1.9	–8.5
Corn–soybean–wheat–legume	–6.7	3.5
Corn–rye–soybean–wheat–legume	–7.7	–6.7

Data from the top four parameter sets are presented

Overall, DNDC predicts yield in diversified systems to be within ±10% of conventional yield (Table 2), a result consistent with our meta-analysis (Tonitto et al. 2006). There were cases where the legume-based rotation produced significantly lower yields, for example the 2001 corn yield. In our simulations, legume biomass (above- and below-ground) contributed 160–390 kg N ha^{-1} year^{-1}, a range at the upper bound of above-ground biomass N values reported in field studies. Based on predictions from our meta-analysis, this level of N addition should maintain cash crop yields statistically comparable to the conventional system. The simulated 6–8% reduction in corn yield in our legume-fertilized rotations can reflect (1) the imprecise mineralization of legume biomass in the current DNDC model formulation, or (2) accurate simulation of grain yield with the yield reduction under legume-fertilization resulting because these diversified systems are being compared to the highest yielding corn systems in the United States. The 1999 soybean yield suggests that adding a rye cover crop to a corn–soybean–wheat rotation can lead to interference with crop yield in dry years, regardless of N management applied. The potential for some years to result in reduced yield caused by interference from cover crop management is consistent with field results quantified in our meta-analysis (Clark et al. 1997; Ranells and Wagger 1997). Though diversified management can produce cumulative crop yield comparable to conventional systems, in a specific year the interaction between management choices and abiotic conditions can result in a yield penalty (Thorup-Kristensen et al. 2003; Yadvinder-Singh et al. 1992). In this study, we used results from Crandall et al. (2005) to define our rye management schedule and rye biomass expectations. At this time, our modeled rye yields are consistently lower than those observed in field trials by Crandall et al. (2005). Currently, we plow down rye biomass two weeks prior to cash crop planting. In practice farmers may till rye cover as early as 4 weeks prior to planting. Given current limitations in DNDC's ability to model the winter growth of the rye cover crop, it is not possible to test best management practices for rye cover crops at this time.

Water flux and nitrate leaching dynamics

We compared cumulative annual drainage and nitrate leaching across management systems. Annual drainage was consistently reduced for diversified rotations relative to the conventional system (Table 3), with a higher proportional reduction in drainage in low flow years. Relative to conventional simulations, reduction in drainage under corn averaged 50% for legume-based rotations, 31% for fertilized corn–soybean–wheat rotations (with or without rye), and 42% for corn–rye–soybean–rye rotations. Reduction in drainage under soybean ranged from 25% to 30% in rotations with rye and averaged 10% in corn–soybean–wheat and corn–soybean–wheat–legume rotations. Overall, parameter variation resulted in small changes

Table 3 Cumulative trends in drainage across different rotations presented as total flux and as percent deviation from the conventional rotation

	Cumulative drainage (cm)		% Deviation from conventional	
	Corn	Soybean	Corn	Soybean
Conventional				
Corn–soybean	217	243		
Diversified				
Corn–rye–soybean–rye	169	187	–42.7	–26.6
Corn–soybean–wheat	203	231	–31.2	–9.4
Corn–rye–soybean–wheat	204	176	–30.8	–31.0
Corn–soybean–wheat–legume	145	229	–50.8	–10.2
Corn–rye–soybean–wheat–legume	146	175	–50.5	–31.3

Data for 10 simulated years are presented by cash crop for the top four parameter sets

in drainage, with variation spanning 5 cm in high flow years, and 2 cm in low flow years. Parameterization results in the largest range of drainage across parameter sets during low water flow under a wheat crop, suggesting accurate simulation of water dynamics of winter crops is sensitive to parameter choice.

Relative to the conventional corn–soybean system, corn–rye–soybean–rye and legume-based management resulted in significant reductions in nitrate leaching in years when corn is grown (Fig. 1a, Table 4). Reduction in nitrate loss in corn years averaged 34% in the corn–rye–soybean–rye rotation and 50% in legume-based rotations (Table 4). In soybean years, rotations which included a rye cover crop averaged a 46–54% reduction in leaching (Table 4). The reduction in nitrate leaching in diversified rotations relative to conventional management was controlled by reduced concentrations of inorganic N during the fall, winter, and spring. Additionally, a higher proportion of inorganic N occurred as NH_4^+ rather than NO_3^- in the legume-based relative to the conventional systems. The corn–soybean–wheat and corn–rye–soybean–wheat rotations under N fertilizer management had mixed results. Corn years in these systems showed nitrate leaching equivalent to the conventional system, while soybean years resulted in reduced nitrate leaching for the corn–rye–soybean–wheat rotation. Since the fertilized corn–soybean–wheat rotation had higher corn yields and higher nitrate leaching, simulation outcomes suggest the fertilization rate applied to conventional management is not optimal in this diversified system. Overall, model outcomes suggest that adding a rye cover crop to a corn–soybean rotation or converting to a legume-based corn–soybean–wheat–red clover diversified system will incur outstanding reductions in nitrate leaching (Table 4). The proportional change in nitrate leaching predicted by DNDC is of the same order as that quantified in our meta-analysis (Tonitto et al. 2006).

Cumulative N and C dynamics

Soil organic carbon dynamics

We conducted trace validation by comparing modeled C trends across conventional and diversified management. Trends in active C pools showed similar patterns in conventional and diversified systems, however conventional systems had higher active C pools in the majority of the years. In contrast, recalcitrant C pools were consistently larger in the diversified systems relative to the conventional. Modeled microbial biomass C was similar across the two management scenarios. Overall, the cumulative trajectory of C pools described conventional systems as accumulating active C pools, while diversified systems accumulated recalcitrant C pools (Table 5). Field data does not support significant C accumulation in conventional corn–soybean systems (Aref and Wander 1998; Darmody and Peck 1997; Drinkwater et al. 1998; McIsaac and David 2003). Given the importance of SOC processes for modeling diversified systems, SOC dynamics warrant further development.

Fig. 1 DNDC outcomes for NO_3^- leaching in years with a corn (**a**) or soybean (**b**) cash crop over the entire 10-year simulation for all 64 parameter sets. Leaching is tallied from January 1 until December 31 of the year the cash crop is harvested. The box plots show median (line in center of box), 25th and 75th percentiles (bottom and top of box respectively), 10th and 90th percentiles (bottom and top error bars, respectively) for the best 64 parameter sets. Data compare the conventional corn–soybean system to diversified systems including: (1) corn–rye–soybean–rye, (2) corn–rye–soybean–wheat, and (3) corn–rye–soybean–wheat–red clover

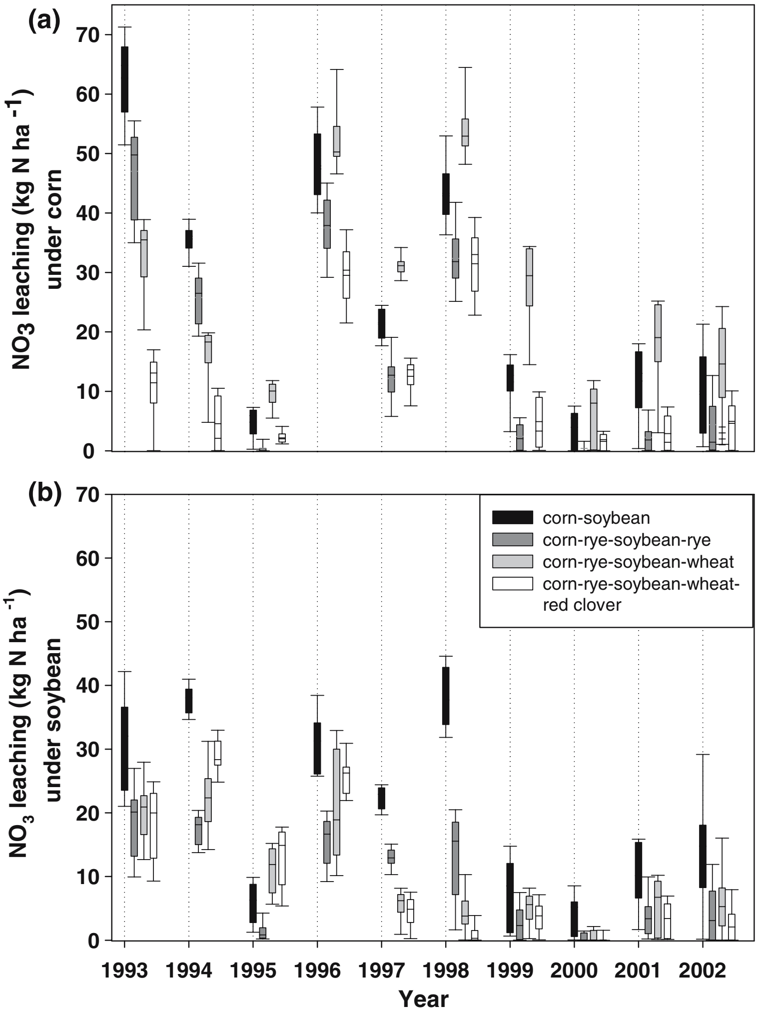

Table 4 Cumulative trends in nitrate leaching across different rotations presented as total N flux and as percent deviation from the conventional rotation

	Cumulative NO_3–N (kg N ha^{-1})		% Deviation from conventional	
	Corn	Soybean	Corn	Soybean
Conventional				
Corn–soybean	295	255		
Diversified				
Corn–rye–soybean–rye	196	119	–33.6	–53.3
Corn–soybean–wheat	296	251	0.4	–1.5
Corn–rye–soybean–wheat	297	136	0.7	–46.6
Corn–soybean–wheat–legume	149	218	–49.5	–14.5
Corn–rye–soybean–wheat–legume	148	130	–49.8	–49.0

Data for 10 simulated years are presented by cash crop for the top four parameter sets

N and C flux

Nitrogen losses were dominated by nitrate leaching, and N_2 and N_2O trace gas flux (Table 6). Cumulative simulation trends demonstrated that fertilizer-driven conventional and corn–soybean–wheat rotations experience equal N loss by nitrate leaching and from combined N_2 and N_2O flux.

Table 5 Total C (kg C ha^{-1}) and N (kg N ha^{-1}) pools for all 64 parameter sets at the start and end of a 10-year simulation

Rotation			Active C	Recalcitrant C	SOC	Total N
Corn–soybean	Initial		**11,334**	**106,329**	**115,330**	**11,990**
	End	**Mean**	**29,540**	**105,503**	**135,043**	**12,018**
		Min	22,095	105,290	127,528	11,902
		Max	34,013	105,889	139,389	12,144
Corn–rye–soybean–rye	Initial		**11,344**	**106,325**	**115,337**	**12,058**
	End	**Mean**	**30,646**	**106,298**	**136,944**	**12,100**
		Min	25,647	106,004	132,153	11,918
		Max	33,807	106,763	139,885	12,281
Corn–soybean–wheat	Initial		**12,280**	**106,332**	**116,261**	**11,912**
	End	**Mean**	**25,252**	**105,051**	**130,303**	**11,924**
		Min	18,138	104,692	122,830	11,880
		Max	28,410	105,376	133,428	11,980
Corn–rye–soybean–wheat	Initial		**12,291**	**106,327**	**116,267**	**11,937**
	End	**Mean**	**26,411**	**105,359**	**131,769**	**11,956**
		Min	19,278	104,968	124,455	11,891
		Max	29,515	105,757	134,826	12,048
Corn–soybean–wheat–clover	Initial		**10,876**	**106,194**	**114,760**	**12,139**
	End	**Mean**	**20,819**	**111,840**	**132,658**	**12,232**
		Min	17,783	110,583	129,299	11,798
		Max	22,253	112,885	134,682	12,739
Corn–rye–soybean–wheat–clover	Initial		**10,888**	**106,188**	**114,764**	**12,165**
	End	**Mean**	**21,455**	**112,246**	**133,701**	**12,265**
		Min	18,368	111,001	130,549	11,810
		Max	22,923	113,302	135,763	12,808

SOC is separated into active C (very labile, labile, and recalcitrant litter), and recalcitrant C (humus and humads)

For the corn–rye–soybean–rye and legume-driven rotations, the significant reduction in nitrate leaching caused N_2 and N_2O to account for the largest proportion of system N loss. The legume-based rotations resulted in the lowest amount of N_2O flux. Flux of NO and NH_3 were minimal across all management protocols.

Legume-based rotations exhibited larger N fixation, gross N mineralization, and net N mineralization relative to the conventional system, as well as increased soil CO_2 flux (Table 6). Increases in these ecosystem processes are expected due to the increased duration of plant cover and the accompanying increase in C-fixation. Variation across parameter sets was small for CO_2 flux, N fixation, gross mineralization and net mineralization. In contrast, parameter variation resulted in significant differences for nitrate leaching and N_2O flux.

In most months, DNDC predicted similar N_2O flux in conventional and diversified systems. However when monthly flux differences were predicted the differences were large. During the past 15 years, DNDC has been tested against datasets of N_2O emissions observed worldwide (Wang et al. 1997; Smith et al. 1999; Butterbach-Bahl et al. 2001a, b; Brown et al. 2002; Smith et al. 2002, 2004; Cai et al. 2003; Xu-Ri et al. 2003; Saggar et al. 2003, 2004; Butterbach-Bahl et al. 2004; Grant et al. 2004; Kiese et al. 2004; Pathak et al. 2005, 2006; Kesik et al. 2005; Jagadeesh Babu et al. 2006). Results from these validation studies indicate that DNDC was capable of predicting N_2O emissions across climatic zones, soil types and management regimes although discrepancies existed for some cases. For example, DNDC could overpredict N_2O flux under dry conditions (Frolking et al. 1998) and under elevated soil NH_4^+ (Li et al. 1992a, b). In our application, modeled N_2 and N_2O flux demonstrated large interannual variability, resulting in extremely high values in some years. The 10-year cumulative results demonstrate a mean N_2 flux of 137–171 kg N ha^{-1} and a mean N_2O flux of 62–158 kg N ha^{-1} across the various management

Table 6 Cumulative flux of SOC, C and N trace gases, NO_3^-, and N process rates over a 10-year simulation for a corn–soybean compared to diversified rotations

	Mean cumulative C or N flux (kg C ha^{-1} or kg N ha^{-1})									
	SOC	CO_2	NO_3^-	N_2O	NO	N_2	NH_3	N fixation	Gross mineralization	Net mineralization
Corn–soybean										
Mean	**20,128**	**27,301**	**228**	**131**	**29**	**171**	**7.0**	**795**	**2,384**	**755**
Min	12,577	26,140	154	77	27	144	6.8	757	2,328	722
Max	24,514	27,783	284	203	32	216	7.1	879	2,430	792
Corn–rye–soybean–rye										
Mean	**22,061**	**28,856**	**128**	**158**	**30**	**137**	**6.9**	**724**	**2,502**	**776**
Min	17,269	28,347	82	123	29	118	6.9	699	2,474	743
Max	25,015	29,696	188	189	32	156	7.0	792	2,541	811
Corn–soybean–wheat										
Mean	**13,314**	**25,890**	**231**	**95**	**25**	**164**	**5.4**	**630**	**2,253**	**707**
Min	5,393	24,732	155	55	23	148	4.9	607	2,222	670
Max	16,152	26,363	284	185	29	197	6.0	698	2,281	749
Corn–soybean–wheat–legume										
Mean	**14,905**	**36,234**	**151**	**71**	**23**	**161**	**1.4**	**1,379**	**3,513**	**1,408**
Min	12,625	33,933	102	46	19	144	1.0	1,242	3,294	1,337
Max	16,446	38,044	204	115	29	181	1.9	1,499	3,692	1,466
Corn–rye–soybean–wheat										
Mean	**14,827**	**26,564**	**195**	**89**	**25**	**146**	**5.4**	**597**	**2,302**	**719**
Min	7,042	25,701	126	52	22	129	4.9	580	2,269	682
Max	17,606	27,144	245	181	29	182	6.4	667	2,332	751
Corn–rye–soybean–wheat–legume										
Mean	**16,089**	**37,033**	**121**	**62**	**23**	**140**	**1.4**	**1,344**	**3,559**	**1,405**
Min	13,768	34,756	72	43	18	128	1.0	1,216	3,342	1,336
Max	17,685	38,867	173	100	28	165	1.9	1,451	3,736	1,464

Data represents the mean cumulative flux, as well as minimum and maximum flux observed for the top 64 parameter sets

scenarios (Table 6), a loss equivalent to 20–30% of recommended N fertilizer. This cumulative N flux is unevenly distributed across the simulated years. In low N gas flux years, DNDC predicts annual N_2 and N_2O flux ranging from 1 to 5 kg N ha^{-1}. In contrast, for high flux years DNDC predicted N_2 flux of 20–40 kg N ha^{-1} and N_2O flux of 10–35 kg N ha^{-1}. This is on the order of 10–35% of recommended N fertilizer. Though N gas flux field data is limited, a survey of the literature suggests an annual average N_2O flux of 1–10 kg N ha^{-1} in grain systems (Roelandt et al. 2005) and an average total loss of N from denitrification of 15 kg N ha^{-1} in corn systems (Tonitto, unpublished). While field data from temperate grain systems suggests average N_2O fluxes are below the upper range predicted by DNDC, measurement of denitrification and accurate spatial and temporal upscaling of denitrification estimates is severely limited by current field methods (Groffman et al. 2006). For example, it is likely that field sampling will miss extreme N flux events. Additionally, the literature survey covers a broad range of soil types and climate zones, and may not adequately characterize dynamics in tile-drained systems. Given the limitations of modeling and measuring denitrification, further analysis of differences between model predictions and aggregated field predictions is necessary to resolve for a complete understanding of agricultural N management.

Event validation of N trace gas flux

The time series generated as model output demonstrated a seasonal trend. As a result, the time series have non-stationary variance. To stabilize the variance, we used a Box-Cox square root transformation (Wei 1994). Though a logarithmic transformation is often appropriate to eliminate multiplicative seasonal trend (Chatfield 1996), we could not apply this transformation due to zero values in the time series. We applied time series techniques to assess whether short time scale (i.e., daily) model results were mechanistically correlated. For this reason, we did not emphasize the seasonal trend. Our application diverges from classic time series analysis which emphasizes long-term trends in order to forecast future outcomes. Using a Buys-Ballot analysis (Wei 1994), we sorted model years into low N gas flux years (years 4–6) and high N gas flux years (years 7–10) for further analysis. An autocorrelation analysis of modeled N_2 flux, N_2O flux, soil NH_4^+, soil NO_3^-, and soil moisture for the low and high N flux time series showed an exponentially decreasing trend and a partial autocorrelation analysis showed an initial large spike at lag 1, indicating that the data are best described using a first order autoregressive (AR(1)) model (Wei 1994). The autocorrelation and partial autocorrelation analysis indicated that these time series are suitable for cross-correlation analysis. Because the non-stationary mean in modeled SOC was a spurious model outcome, we eliminated the cross-correlation analysis between modeled N gas flux and SOC.

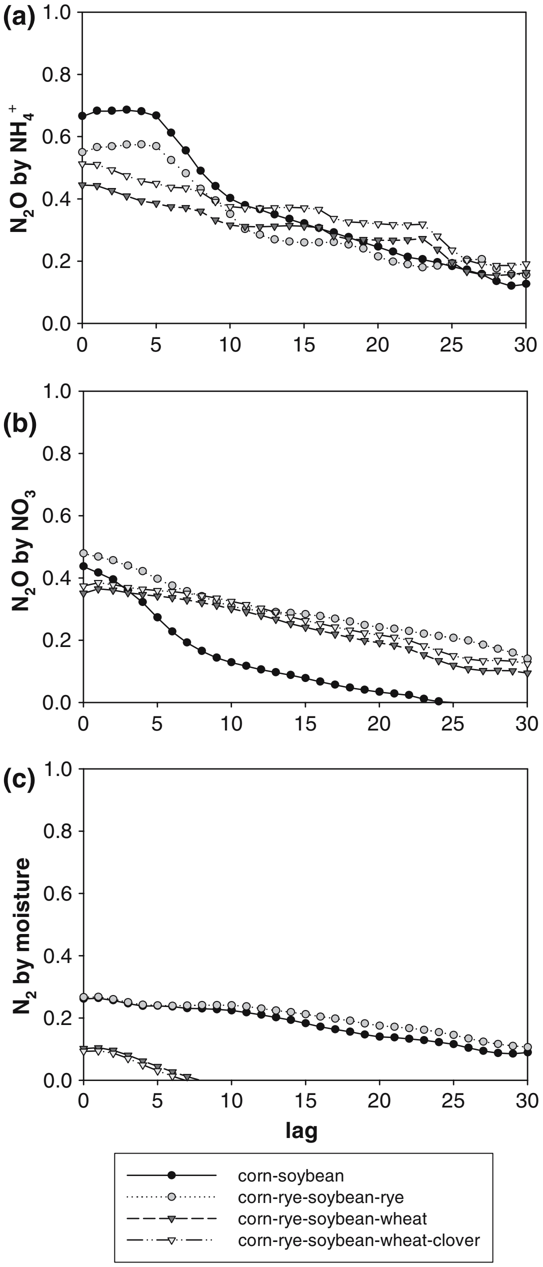

Fig. 2 Cross-correlation between soil environmental conditions and N trace gas flux. The cross-correlation coefficient (CCF) is calculated for lags of 0–30 days. The short time-scale relationship is shown for: (**a**) N_2O gas flux with soil NH_4^+ pools, (**b**) N_2O gas flux with soil NO_3^- pools, and (**c**) N_2 gas flux with soil moisture. All graphs are for the high-N gas flux time series

Cross-correlation analysis of N trace gas flux and soil environmental properties showed that modeled gas flux tracked modeled soil inorganic N pools. Both low and high N_2O flux time series showed the strongest cross-correlation between soil NH_4^+ and N_2O flux and this trend occurred in all rotations (Fig. 2a). Weak cross-correlation was seen between N_2O flux and soil NO_3^- in the corn–soybean and corn–rye–soybean–rye rotations in the low N_2O flux time series, while all rotations showed moderate cross-correlation between N_2O flux and NO_3^- in the high N_2O flux time series (Fig. 2b). No significant cross-correlation was seen between N_2O flux and soil moisture. Moderate cross-correlation was evident between N_2 flux and both soil NH_4^+ and soil NO_3^- across rotations and in both low and high N_2 flux time series. This cross-correlation did not significantly decrease after 5–10 days, suggesting inorganic N status is an important driver of modeled N_2 flux as a general soil property, rather than as a short time-scale, variable phenomenon. Weak cross-correlation was observed between N_2 flux and soil moisture (Fig. 2c). Field data suggest that soil moisture is an important driver of denitrification on short and long time scales. For application to an Illinois tile-drained system, the daily pattern of modeled N gas flux did not closely track trends in soil moisture, instead N gas flux more closely followed the pattern of soil inorganic N dynamics. However, at seasonal to annual temporal scales total N gas flux was strongly dependent on soil moisture status, with high precipitation years resulting in the highest N gas flux. Though there was high seasonal and interannual variation in N trace gas flux predictions, overall cross-correlation analysis demonstrated that simulated N trace gas flux captured important mechanistic relationships at short time scales.

Limitations of model results

This analysis depends on the assumption that DNDC parameter calibration for a conventional corn–soybean rotation is applicable to the diversified systems studied here. This assumption was necessary due to the limited extent of diversified rotations in tile-drained Mollisols. We previously showed that statistically meaningful drainage and nitrate leaching results were attained by modifying DNDC soil physical and chemical parameters to simulate tile drainage. Given the fundamental hydrologic change that occurs following the installation of tile drainage, we expect broad hydrological dynamics will be determined by the presence of tiles, rather than changes in crop rotation. For this reason, we expect the parameters calibrated for the conventional system adequately described broad dynamics in the diversified systems.

Complex simulation models require large, resource-intensive spatial and temporal datasets for parameter calibration and model validation. Due to the limited availability of data for calibration, models cannot be readily applied as a simple policy or management tool. Rather model results must be viewed in the context of our empirical knowledge. Models cannot substitute for monitoring biophysical conditions, both tools are necessary to achieve sustainable policy and management.

Future directions

Our analysis demonstrated inconsistencies in DNDC predictions for diversified management practices. In order to extend the DNDC model for use in ecologically managed systems, simulation of diverse rotations and cover crop management need further refinement. In particular, the growth of both legume and non-legume cover crops requires further development. Despite significant manipulations of the cereal rye input file, we were unable to achieve cereal rye yields of similar magnitude to field observations (Crandall et al. 2005). Currently, DNDC does not allow for a field to grow two concurrent crops. For this reason, we were unable to seed cereal rye, wheat, or red clover into the previous crop, a practice commonly used by diversified grain farmers. The inability to accurately simulate these practices is a potential source of rye yield reductions, as there is little time for rye to grow following corn or soybean harvest. In contrast to the poor rye growth, simulated red clover growth consistently resulted in legume N biomass in the upper ranges of field observations. Refining N-fixation dynamics in DNDC is necessary to represent the feedback between soil N availability and N-fixation rate as well as the uncertainty farmers face when using legumes as an N source.

Modeled carbon dynamics in diversified systems was another area requiring refinement. Current DNDC outcomes predicted an accumulation of active carbon in conventional rotations, an ecosystem property which is not validated by field measurements. In contrast, DNDC predicted no accumulation in active C pools in diversified systems. DNDC does predict significant accumulation of recalcitrant soil C pools in diversified systems. Model partitioning of carbon between active and recalcitrant pools should be refined using experimental observations.

Diversified rotations as an N best management practice

Widely used tools for managing watershed N pollution can be broadly divided into internal techniques which reduce N losses from agricultural fields through crop management and external techniques which seek to intercept N from agricultural sources before it reaches sensitive aquatic ecosystems or ground water reservoirs (Drinkwater and Snapp 2007). The current approach to optimizing fertilizer management has been successful in terms of maximizing yields and has contributed to improvements in fertilizer N use efficiency however, mass balances indicate annual N and P inputs consistently exceed harvested exports by 40% to >100% resulting in substantial N and P losses to the environment (David and Gentry 2000; Galloway and Cowling 2002). The increasing extent and duration of hypoxic zones documents the severity of water quality degradation due to N pollution (Rabalais et al. 2002).

Best management practices (BMPs) that aim to intercept N losses receive the second-widest application (Mitsch et al. 2001). Landscape level strategies that integrate wetlands and other types of riparian buffers into agricultural landscapes are very effective in protecting sensitive natural ecosystems (Lowrance 1992; Mitsch et al. 2001), however, they offer less protection to groundwater resources. Recent work by Bracmort et al. (2004) documented that structural BMPs have a one third attrition rate over a 25–30 years time frame.

A holistic, ecosystem-based approach has yet to be systematically applied to nutrient management in agroecosystems. This approach includes diversifying rotations to replace bare fallows with cover crops, increasing the use of green manures, diversifying N sources, relay planting, or intercropping (Drinkwater and Snapp 2007). In contrast to techniques that specifically target improvements in the delivery of N-fertilizer, these practices operate at multiple spatial and temporal scales to re-couple C and N cycles, resulting in feedbacks affecting both the fate and supply of inorganic N and leading to improved agroecosystem-scale N use efficiency. Simulation of diversified management using the DNDC model suggests that adding diversified rotations to the nutrient management portfolio will complement BMPs that are widely practiced.

Conclusions

N management policy

Adoption of ecological management practices is more complex than techniques which aim to optimize fertilizer applications for a variety of reasons. First, these practices are knowledge intensive because they are targeting biologically complex processes such as decomposition and N cycling which are controlled jointly by plants and soil organisms. Second, development of ecological practices that are compatible with current cash crop rotations is complex because the outcome of modifications, such as the introduction of cover crops in place of bare fallows, impacts multiple, interacting processes. Finally, while many of these practices are compatible with existing management systems, they represent additional costs to farmers. Currently, with the exception of some very limited localities, farmers do not have any incentive for incurring these extra expenses. Through model simulation, we demonstrated that diversified rotations which minimize bare fallow periods have the potential to drastically reduce nitrate leaching. The DNDC simulations highlight that N loss in diversified rotations is complex, and that over-fertilized diversified systems are susceptible to N loss. Overall, our meta-analysis and DNDC modeling assessment suggests that ecological management practices represent an opportunity to significantly reduce N loss from agroecosystems. Expanding our ability to adopt ecological management practices should be a research priority.

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