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Application of the DNDC model to tile-drained Illinois agroecosystems: model calibration, validation, and uncertainty analysis

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Abstract We applied the Denitrification-Decomposition (DNDC) model to a typical corn–soybean rotation on silty clay loams with tile-drainage in east-central Illinois (IL). Model outcomes are compared to 10 years of observed drainage and nitrate leaching data aggregated across the Embarras River watershed. We found that accurate simulation of NO_3–N leaching and drainage dynamics required significant changes to key soil physical and chemical parameters relative to their default values. Overall, our calibration of DNDC resulted in a good statistical fit between model output and IL data for crop yield, NO_3–N leaching, and drainage. Our modifications to DNDC reduced the RMSE from 9.4 to a range of 1.3–2.9 for NO_3–N leaching and from 51.2 to a range of 13–23.6 for drainage. Modeling efficiency ranged from 0.25 to 0.85 in comparison with measured drainage and leachate values and from 0.65 to 1 in comparison with crop yield data. However, analysis of simulation results at a monthly time step indicated that DNDC consistently underpredicted peak drainage events. Underprediction ranged from 50 to 100 mm month^{-1} following three extreme precipitation events, a flux equivalent to 0.25–0.5 of the total measured monthly flux. Our simulations demonstrated high interannual variation in nitrate leaching with average annual NO_3–N loss of 24 kg N ha^{-1}, peak annual NO_3–N loss of 58 kg N ha^{-1} and low annual NO_3–N loss of 1–5 kg N ha^{-1}.

Keywords Nitrogen management · Agroecosystem model · Nitrate leaching · Tile-drainage · Corn · Soybean

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Introduction

Current estimates suggest human activities have doubled the global N fluxes of biologically active N (NH_3, NH_4^+, NO_3^-, NO_x, and N_2O) (Vitousek et al. 1997; Galloway et al. 2003, 2004), with agriculture accounting for 75% of the anthropogenic N forcing (Galloway and Cowling 2002). Ecosystem ecologists have used aggregated budgets at global, regional, and watershed scales to understand agricultural N cycling at these larger scales (Howarth et al. 1996; Vitousek et al. 1997; David and Gentry 2000; Galloway et al. 2004). 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). David et al. (2001) estimated 50% of surplus N was exported by rivers from the state of Illinois (IL) and attributed this high-transfer rate to the intensity of corn and soybean agriculture in the state, enhanced by artificial drainage from subterranean tiles. McIsaac and Hu (2004) showed that for tile-drained watersheds in central IL, 100% of residual N was exported to streams, illustrating the efficiency of nitrate leaching in tile-drained agricultural landscapes. Nitrate loss from agricultural landscapes can have important environmental impacts, such as the well documented hypoxia problem in the Gulf of Mexico (Turner and Rabalais 1991; Rabalais and Turner 2001).

Aggregated N budgets have demonstrated the extent of N imbalance, but alternative techniques are necessary to assess the impact of specific management practices on N loss from agricultural systems. Mechanistic models, which describe biogeochemistry and hydrology in agricultural systems are one tool for synthesizing the impact of land management. Due to its rigor in simulating C and N dynamics, the Denitrification-Decomposition model (DNDC), has been applied to a wide range of agricultural systems to asses the impact of land management and policy (e.g., Plant et al. 1998; Li et al. 2000, 2005a, b, 2006a, b; Brown et al. 2002; Zhang et al. 2002; Saggar et al. 2003; Grant et al. 2004). DNDC is a mechanistic, process based model of C and N dynamics (Li et al. 1992, 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. Simulations are conducted at a daily timestep, though it is often not possible to validate this level of temporal resolution for application in agricultural management.

The DNDC model has not been applied to examine corn and soybean agroecosystems on tile-drained soils in the mid-western US, a dominant landscape with large N export in streams (David et al. 1997, 2001; McIsaac and Hu 2004). Here, we apply DNDC to examine water and N fluxes in this type of system. Our objectives were to: (1) establish how well DNDC simulates NO_3^- leaching, drainage, and yield dynamics of corn–soybean rotations which dominate in tile-drained silty clay loam regions of IL; (2) determine the temporal resolution at which the model is accurate; and (3) examine how parameter variation effects model outcomes.

Methods

Field Site

We used aggregated data from the Embarras River watershed (48,100 ha) in east-central IL for our application of the DNDC model. We used aggregated data because this minimizes field-to-field variation, allows for long-term simulations, and integrates both corn and soybean fields each year. Although DNDC was developed as a field-scale model, our watershed-scale DNDC application is akin to the regional simulations currently supported by the DNDC model. While drainage and nitrate leaching are difficult to scale-up from lysimeter studies, drainage and nitrate leaching measurements from tile-drained systems are a relatively accurate integrator of watershed-scale ecosystem fluxes. These long-term, landscape-scale data afford us the unique opportunity to calibrate the DNDC model for tile-drained silty clay loam systems, which are common in the mid-western US. We use DNDC to simulate average conventional corn–soybean management across the watershed and compare model drainage and nitrate leaching outcomes to measured values. Both the watershed and specific field sites have been well studied and described previously (David et al. 1997, 2003; Gentry et al. 1998; Royer et al. 2004).

Water flux at the watershed outlet at Camargo (39°47′29″N, 88°11′08″W) is continuously gauged by the United States Geological Survey (USGS). This watershed is intensively drained by random tile systems (typically at depths of 1–1.5 m), has flashy hydrographs in response to precipitation events, and large exports of NO_3–N, typically

30 kg N ha^{-1} year^{-1} (David et al. 1997; Royer et al. 2004). Soils in this area are Mollisols formed in 100–150 cm of loess over medium to fine-textured till. Silty clay loam soils predominate, and when combined with nearly flat topography require tile drainage to remove subsurface water to allow agricultural activities in early spring. Drummer silty clay loam (fine-silty, mixed, superactive, mesic Typic Endoaquolls) is the dominant soil in this watershed, a typical poorly drained Mollisol that is highly productive with drainage. Annual precipitation during the study period of 1993 through 2002 was 102 cm (mean of three locations distributed around the watershed), and the annual mean temperature was 11.1°C (from Urbana, IL data). This watershed is typical of many counties in east-central IL in terms of soils, slopes, tile drainage systems, and cropping patterns.

We have long-term stream chemistry data for this watershed. Beginning in 1993 through 2002, water samples were collected weekly from the outlet, and more often during high-flow periods (as often as daily). Nitrate-N was measured using ion chromatography, and linear interpolation was used to calculate concentrations on days samples were not collected. By combining NO_3^- concentration data with daily flow, daily export of N as NO_3^- was then estimated. The watershed is dominantly (91%) in corn (*Zea mays* L.) and soybean [*Glycine max* (L.) Merr.] agriculture, with an equal area in each crop and rotating each year. For corn and soybean yields, we used county level estimates for Champaign County, IL (Illinois Agricultural Statistics 1993–2002), where the largest part of the watershed is located. Nitrogen fertilizer is typically applied in the fall or spring at rates of 160–200 kg N ha^{-1} year^{-1}, and was estimated from surveys to be 190 kg N ha^{-1} year^{-1} during the period simulated, with approximately 50% in the fall, and 50% in the spring.

Model application and parameter estimation

We parameterized DNDC version 82H to the system described above, which we term the IL corn–soybean system. Daily precipitation (mean of three sites) and temperature files were created to allow multi-year runs of the model. The silty clay loam soils file was used, with a clay fraction of 35%, porosity of 0.477, saturated conductivity of 0.025 cm per minute, and field capacity and wilting points of 0.73 and 0.31 (as water-filled porosity or WFPS), respectively. DNDC was calibrated and validated using the 10-year data set described previously for water and N export, and crop yields. The management schedule used was one typical for corn and soybean production in east-central IL. For corn, chisel tillage was on 21 April, with planting and fertilization on 1 May and harvest on 21 October. Fertilization was from 95 kg N ha^{-1} applied as ammonium-nitrate on 1 May, and from an additional 95 kg N ha^{-1} of anhydrous ammonium applied the previous 21 November, following the soybean harvest. Soybean tillage was conducted on 7 May, planting on 21 May, and harvest 5 October.

Because tile-drainage is not mechanistically represented in the DNDC model, our calibration focused on soil physical parameters, which affect the rate of drainage, and soil chemical parameters, which affect soil solute transport. To approximate tile-drainage, we specifically focused on understanding model response to variation in four parameters described in Table 1. To establish the appropriate parameter definitions for the IL corn and soybean agroecosystem, we systematically tested DNDC model outcomes over the entire realistic range of these parameter values. Water flux is determined by the parameters DID and DVD. Tile-drainage drastically increases water flux in silty clay loam soils. Changes to DID are necessary to adequately model the increased loss of freely available water between modeled soil layers, while changes to DVD are necessary to adequately model loss of soil pore water to the plant available water pool. Water loss from the soil porespace within each soil layer is modeled as a power function of percent clay. For the lowest values of DVD, extremely small quantities of porespace water are available in the system, with DVD = 0.01 allowing for only 0.02% of the porespace water to enter the freely available water pool. For intermediate values, DVD = 1, 1.5% of the porespace water becomes available in a given timestep, whereas for DVD = 2 more than 3% of the porespace

Table 1 Biophysical meaning of DNDC water and NO_3–N leaching parameters emphasized in calibration of the model to the IL corn–soybean system

Parameter	Description	DNDC default value	Range tested
DID	Proportion of water lost from freely available water pool	0.4	0.05–1
DVD	Power function coefficient describing the amount of water that is lost from the soil pore space	2	0.01–2
PLN	Defines the fraction of the leached NO_3 pool that is available for plant uptake	0.0002	0.0002–0.5
DLW	Power function coefficient, which determines the fraction of NO_3 that is leached from a given soil layer and ultimately leached from the system. The fraction is ultimately limited to ≤ 0.9	500	200–700

water is mobilized. Accurate simulation of nitrate leaching requires the modification of PLN to account for plant uptake of soil solute NO_3^- and of DLW to account for NO_3^- leaching from upper to lower soil layers, and ultimately out of the system. For low drainage (<5 mm per day) the amount of NO_3^- leaching from a soil layer will be greater for a larger DLW value.

Calibration and validation

We calibrated DNDC to simulate tile drainage in silty clay loam soils using the first 5 years of our data set. We began our calibration by testing the full range of possible parameter values for the four parameters we emphasized in our calibration (Table 1). Through simulation of 1800 parameter combinations, we isolated a range of soil physical and chemical parameters that produced statistically robust trends for tile-drained silty clay loams. Next, we validated our model calibration using the last 5 years of our data set. Separate model simulations were conducted for calibration and validation years. In order to reduce the residual effects of initial conditions, we conduct calibration for six consecutive years and validation simulations for six consecutive years, discarding the first year of each simulation. For model calibration and validation, we assessed goodness of fit between simulated and observed drainage, nitrate leaching, and crop yield using statistical metrics (Rykiel Jr 1996). Due to limited available data for model calibration and validation, we emphasize trends in model uncertainty under parameter variation.

Statistical metrics

Statistical analysis of the model is conducted by comparing model simulations (S) and field observations (O) over the course of simulation (t = time). We tested the fundamental applicability of the model to the IL corn–soybean system by testing the model for bias and autocorrelation (Power 1993). If there was statistical evidence of bias then the model makes systematic errors in simulating system behavior. We compute the bias as the mean difference between model simulations and field observations for drainage and nitrate leaching from the system, $\mathrm{BIAS} = \frac{\sum_{t=1}^{N}[(S(t)-O(t))]}{N}$. The existence of predictive bias is established by comparing the test statistic, $W = \frac{\sqrt{N}(\mathrm{BIAS})}{\sigma_{\mathrm{obs}}}$, to a t-table with n-g degrees of freedom, for n = number of data points and g = number of parameters estimated (Power 1993). Predictive bias exists if the absolute value of W is greater than the t statistic. Likewise, autocorrelation, $R_k = \frac{\sum_{t=k+1}^{N}\left[\left(S(t)-\overline{S}\right)\times\left(S(t-k)-\overline{S}\right)\right]}{\sum_{t=1}^{N}\left[\left(S(t)-\overline{S}\right)^2\right]}$, in the model errors is a sign of model inadequacy. Autocorrelation among the modeled errors exists if $\left(\sqrt{N}\right)|R_k| > 1.96$, for N = number of data points.

We assessed the predictive capacity of all parameter sets meeting the bias criteria using modeling efficiency $\left(\mathrm{EF} = \frac{\sum_{t=1}^{N}\left(O(t)-\overline{O}\right)^2 - \sum_{t=1}^{N}(S(t)-O(t))^2}{\sum_{t=1}^{N}\left(O(t)-\overline{O}\right)^2}\right)$, Theil's inequality coefficient $\left(U^2 = \frac{\sum_{t=1}^{N}(S(t)-O(t))^2}{\sum_{t=1}^{N}(O(t))^2}\right)$, the correlation coefficient $\left(r = \frac{\sum_{t=1}^{N}\left(S(t)-\overline{S}\right)\times\left(O(t)-\overline{O}\right)}{\sum_{t=1}^{N}\sqrt{\left(S(t)-\overline{S}\right)^2}\times\sum_{t=1}^{N}\sqrt{\left(O(t)-\overline{O}\right)^2}}\right)$, and the root mean square error $\left(\mathrm{RMSE} = \sqrt{\frac{\sum_{t=1}^{N}\left[(S(t)-O(t))^2\right]}{N}}\right)$ (Mayer and Butler 1993; Power 1993; Smith et al. 1997). Additionally, we break down Theil's inequality into its bias, variance, and covariance proportions (Power 1993). These techniques elucidate when model results provide more predictive power than using average field data. Best model performance results in EF = 1, while EF < 0 signifies the model performs worse than using the average of the observations. Conversely, $U = 0$ results when the best fit of the model to the observations has occurred, and $U > 1$ signifies the model performs worse than using past observations to describe future conditions. An r-value closest to 1 indicates the model matches the pattern of the observations. The RMSE is a measure of the deviation of the simulated values from observations, and is scaled relative to the units of measurement. A perfect simulation has a RMSE = 0, while the upper bound is infinity.

Statistical tests of bias and model predictive capability were performed by comparing DNDC simulation results to IL corn–soybean observations for data grouped as: (1) monthly cumulative sum of NO_3–N leaching and drainage, (2) annual cumulative sum of NO_3–N leaching and drainage, and (3) annual crop yield. Due to variation in the maximum and minimum values observed for modeling efficiency and Theil's coefficient, respectively, we used different threshold values for these statistics when ranking model predictive capability for nitrate leaching versus drainage. For calibration simulations best case parameters where those which resulted in nitrate EF > 0.25 and water EF > 0.45. For validation simulations best case parameters where those which resulted in NO_3–N EF > 0.5 and water EF > 0.55. For the yield comparisons, EF > 0.65 was used to bound the best case parameter sets for both calibration and validation simulations. Criteria for establishing best case parameter set using Theil's inequality was set as $U^2 < 0.5$ for drainage and leaching outcomes, and $U^2 < 0.15$ for yield outcomes.

Uncertainty analysis

After we established parameter combinations that produced statistically meaningful simulation outcomes, we quantified the effect of parameter variation on simulation results. This uncertainty analysis bounds the error associated with a misestimation of these critical parameters. For parameter combinations which pass the bias criteria, we sorted parameter sets based on their predictive capabilities determined by modeling efficiency and Theil's inequality metrics. We selected parameter combinations that produced statistically meaningful outcomes for comparisons of modeled and measured (1) cumulative monthly drainage and leaching, (2) cumulative annual drainage and leaching, and (3) annual crop yield. We apply DNDC using this range of parameter sets and present the parameter-induced variation in outcomes using box plots which bound the 25th, 50th, and 75th percentiles of the model results. For comparisons of model outcomes under the new parameterization to simulations under the default DNDC parameter set, all DNDC simulations use our modified soil and crop library files.

Results and discussion

Calibration and validation

Of the 1,800 parameter sets tested, only a subset of the possible parameter space adequately depicted NO_3–N and water dynamics (Table 2). A limited number of parameter sets passed the bias criteria and fewer passed the modeling efficiency and Theil's inequality criteria. In contrast, modeled plant growth was not sensitive to the parameters varied. Compared to observed yield, most parameter combinations produced statistically significant simulated yields. Many parameter sets passing the bias criteria also passed the criteria for modeling efficiency and

Table 2 Summary of calibration and validation statistics from comparisons of DNDC model outcomes to 5-year calibration and validation data for the IL corn–soybean system

Data compared	% of DNDC model outcomes meeting criteria	
	Bias	Bias and $0 < EF < 1$ and $0 < U < 1$
Monthly NO_3 and H_2O calibration	20	7.4
Monthly NO_3 and H_2O validation	31	25
Annual yield calibration	99	84
Annual yield validation	85	76
Annual NO_3 and H_2O calibration	23	5.6
Annual NO_3 and H_2O validation	25	16.4

Percentage of total parameter sets tested which meet statistical criteria for model bias and performance

Theil's inequality. Although N and water availability do limit plant growth in DNDC, plant growth is also largely controlled by physiological parameters describing maximum yield and C : N partitioning. Daily variation in N and water availability directly affects drainage and NO_3–N leaching; in contrast, plant growth is not sensitive to daily time-scale variation. Other work validating DNDC against crop growth has likewise found favorable trends between model outputs and measurements (Zhang et al. 2002). Analysis of the components of Theil's inequality demonstrate that variance determines virtually all of a given Theil's inequality value.

Testing model outcomes for bias is one criteria used to test the basic soundness of applying DNDC to the IL corn–soybean system. Additionally, we tested model outcomes for autocorrelation of the errors (Power 1993). Using a lag of 12 months, we did not find significant autocorrelation. Although there is noise in the autocorrelation coefficient, analysis of the Rk function shows no trend in the pattern of variation.

Best case parameter sets

After establishing which parameter sets produced statistically meaningful results, we sorted the parameter sets to select those that produced the best approximations to the measured trends (Table 3). Again, we first emphasize trends in NO_3–N leaching and drainage because these model outcomes showed greatest deviation from field measurements for both monthly and annually averaged data. Comparisons of calibration outcomes for drainage and NO_3–N leaching at a monthly temporal resolution resulted in a maximum modeling efficiency of EF = 0.49 for NO_3–N data and EF = 0.62 for drainage data. Validation outcomes were more favorable, with a maximum modeling efficiency of EF = 0.83 for nitrate data and EF = 0.87 for drainage data comparisons. Although there were differences in EF-values between calibration and validation simulations, a parameter set that showed good calibration statistics generally performed well in the validation simulations. The converse was generally true for the top validation parameter sets. Parameter sets that passed the statistical criteria during the validation simulations, but not for the calibration period always failed the statistical metrics due to poor agreement with the IL NO_3–N data. Annual calibration outcomes demonstrated a maximum modeling efficiency of EF = 0.31 for nitrate leaching and EF = 0.62 for drainage, whereas validation simulations resulted in maximum nitrate leaching EF = 0.85 and maximum drainage EF = 0.88. A limited number of parameter sets produced an EF > 0 for annual leaching and drainage calibration simulations. As a result many of the favorable validation parameter sets result in negative calibration EF-values. Comparisons between measured and modeled crop yield resulted in a maximum EF = 0.98 for corn–soybean and EF = 0.97 for soybean–corn calibration simulations. Yield validation showed similarly good statistical outcomes.

Analysis of the best case parameter sets for calibration and validation simulations showed the model performed best when DNDC default parameters are drastically changed (Table 3). Overall, the default DNDC parameter values did not produce statistically robust outcomes for drainage, leaching or yield. The consistently negative EF-values for simulations using the DNDC default parameters demonstrates that DNDC performed worse than using the average IL drainage, leaching and yield measurements.

Table 3 DNDC modeling efficiency under default and best case parameter ranges for calibration and validation simulations for the IL corn–soybean system

Data compared	Parameter range				EF range		RMSE range	
	DVD	DID	PLN	DLW	NO_3	H_2O	NO_3	H_2O
Monthly leaching calibration	0.025–0.05	0.05–0.2	0.0002–0.5	200–700	0.25 < EF < 0.49	0.45 < EF < 0.62	2.2–2.7	26–27.8
Monthly leaching validation	0.01–0.2	0.01–0.5	0.0002–0.5	200–700	0.5 < EF < 0.83	0.55 < EF < 0.87	1.3–2.9	13–23.6
DNDC default calibration	2	0.4	0.0002	500	–10.4	–1.57	10.50	60.30
DNDC default validation	2	0.4	0.0002	500	–7.3	–1.15	9.40	52.30
					Corn–soybean	Soybean–corn	Corn–soybean	Soybean–corn
Annual yield calibration	0.01–2	0.01–1	0.0002–0.5	200–700	0.65 < EF < 0.97	0.65 < EF < 0.98	209–800	166–617
Annual yield validation	0.01–2	0.01–1	0.001–0.5	200–700	0.65 < EF < 0.97	0.65 < EF < 0.98	103–805	231–695
DNDC default calibration	2	0.4	0.0002	500	–1.8	0.4	1466	784
DNDC default validation	2	0.4	0.0002	500	0.5	–0.8	997	1563

DVD and DID are interdependent. Not all combinations result in meaningful EF outcomes

For application to a silty clay loam tile-drained corn–soybean system in IL, the default DNDC model does not have statistically valid predictive capabilities. Smith et al. (1997) reported poor modeling efficiency outcomes for modeled soil organic carbon (SOC) dynamics for a broad range of models applied to agricultural data sets. These modeling efficiency results suggest that field data are needed to calibrate DNDC and other C and N models before these models can be reliably applied to predict a broad range of ecosystem management scenarios.

For PLN, the parameter controlling the ability of plants to access inorganic N, a broad range of parameter values produced statistically meaningful results. For calibration and validation simulations, good modeling efficiency for both nitrate leaching and drainage results was observed for the entire range tested, $0.0002 < \mathrm{PLN} < 0.5$, but the lowest value of $\mathrm{PLN} = 0.0002$ only represented 3% of statistically robust outcomes, and $\mathrm{PLN} = 0.001$ only accounted for 9% of robust outcomes. These results demonstrate the default DNDC-value, $\mathrm{PLN} = 0.0002$, may not be the best choice in the IL tile-drained corn–soybean system.

For DVD, the parameter controlling water retention in the soil pore space, calibration simulations required $\mathrm{DVD} < 0.2$ for statistically meaningful outcomes, whereas the best fit was for $0.025 \le \mathrm{DVD} \le 0.05$ (Table 3). Although $\mathrm{DVD} > 1$ accounted for 3% of the statistically meaningful validation parameter sets, overall validation simulations demonstrated that low-DVD produced the best fit to the IL drainage and leaching data (Table 3). Based on comparisons with drainage data, both calibration and validation simulations suggest low-values of DVD more reliably result in robust model outputs. This is in contrast to the default DNDC value of $\mathrm{DVD} = 2$, which never produced statistically robust model outcomes in the IL system studied.

For DID, the parameter regulating the loss of water not held in the soil pore space, calibration simulations required $\mathrm{DID} \le 0.4$ for statistically meaningful outcomes. Although validation simulations showed statistically meaningful outcomes over the full range, $0.01 \le \mathrm{DID} \le 1$, lower DID values produced higher EF statistics (Table 3). Silty clay loam soils are characterized by high-moisture retention. A low DVD-value reflects the high retention of water in the pore space of high-clay soils, whereas an intermediate value of DID approximates the faster drainage due to the presence of tiles.

Evaluation of the best parameter sets established based on EF and U criteria were also statistically significant when evaluated using the correlation coefficient, r. Nitrate leaching ranged from $0.54 < r < 0.76$ for calibration and $0.71 < r < 0.92$ for validation simulations. Drainage ranged from $0.55 < r < 0.8$ for calibration and $0.71 < r < 0.91$ for validation simulations. Yield correlation statistics also demonstrated a significant relationship between modeled and measured values. All but a few parameter sets resulted in $r > 0.95$ for calibration simulations. The majority of validation simulations resulted in $r > 0.95$, however a range of $0.75 < r < 0.95$ was also observed. These results demonstrate that the pattern of simulated values tracks the pattern of observations.

The reduction in deviation between model outcomes and field observations was also demonstrated by the RMSE results (Table 3). Our modifications to DNDC reduced the RMSE from 9.4 to a range of 1.3–2.9 for NO_3–N leaching and from 51.2 to a range of 13–23.6 for drainage. The RMSE for yield was reduced from 997 to 103–805 in corn–soybean simulations and from 1563 to 231–695 in soybean–corn simulations.

The preceding statistical analysis bounds a parameter space for which the DNDC model can adequately describe measured yield, drainage, and leaching dynamics. Here we describe in detail the aggregated yield, drainage, and leaching results, with emphasis on how model outcomes differ under parameter variation.

Annual dynamics

On an annual basis, the new parameterization of DNDC closely tracked IL drainage and NO_3–N leaching data (Fig. 1). For a 10-year simulation the top 64 parameter sets over-predicted NO_3–N leaching in 1 year and under-predicted NO_3–N leaching in 2 years. During this simulation period,

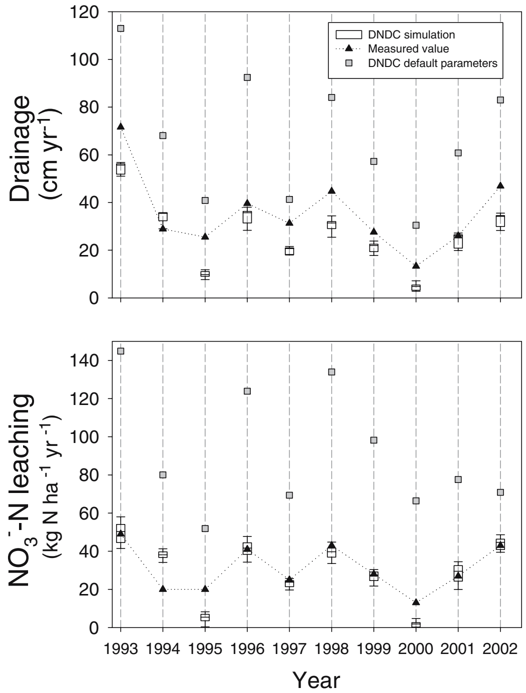

Fig. 1 DNDC simulated and measured annual drainage and NO_3–N leaching for calibration (1993–1997) and validation (1998–2002) years for the IL corn–soybean system. Shown are the measured values, simulation with DNDC default parameters, and *box plots* outlining median (*line in center of box*), 25th 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

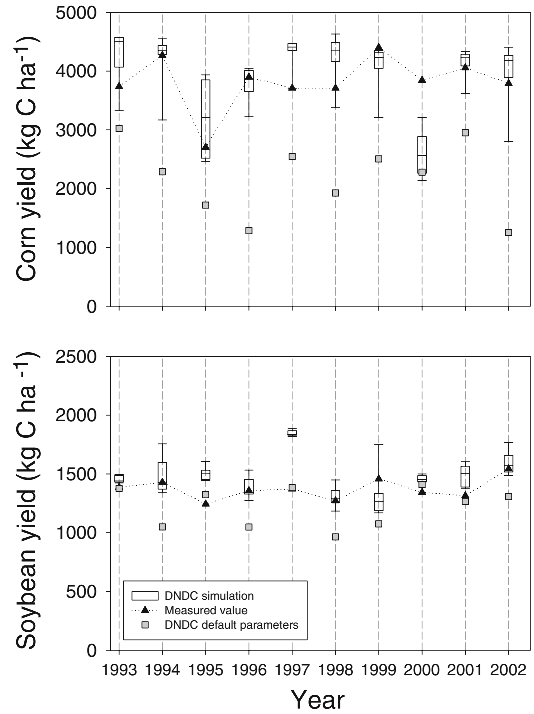

Fig. 2 DNDC simulated and measured annual corn and soybean yields for calibration (1993–1997) and validation (1998–2002) years for the IL corn–soybean system. Shown are the measured values, simulation with DNDC default parameters, and *box plots* for the best 64 parameter sets (see *box plot* description in Fig. 1)

the model under-predicted drainage in 7 years. Although there are slight under- or over-predictions of leaching and drainage on an annual basis, the new parameter range performed much better than that of the default DNDC model. Yield simulations likewise show good accordance with IL data (Fig. 2). Corn yield was slightly under-predicted in 4 years, and over-predicted in 1 year, whereas soybean yield was over-predicted in 4 years.

There was little variation in modeled leaching outcomes across the 64 top parameter sets. In most years the range between minimum and maximum NO_3–N leaching was 10 kg N ha^{-1}, except for a 20 kg N ha^{-1} spread in 1993 and 2001. Drainage showed a similarly small range across parameter values, with variation in annual outcomes spanning 5–10 cm year^{-1}. Overall, 1995 stands out as the most difficult year to simulate in terms of both NO_3–N leaching and drainage. Variation in modeled yield was also generally small. Corn yield generally was within 100 kg C ha^{-1} for all parameter combinations, however 1995 and 2000 had significant yield variation depending on parameter values. Soybean yield likewise spanned a small range except for 1994 and 1999 results.

No dominant relationship across prediction errors for drainage, leaching, or yield outcomes was evident. The most extreme differences between model outcomes and the IL data, as well as variation across parameter combinations occurred in different simulation years for leaching and yield variables. One exception is 1995, which proved difficult to simulate in terms of NO_3–N leaching and drainage as well as corn yield.

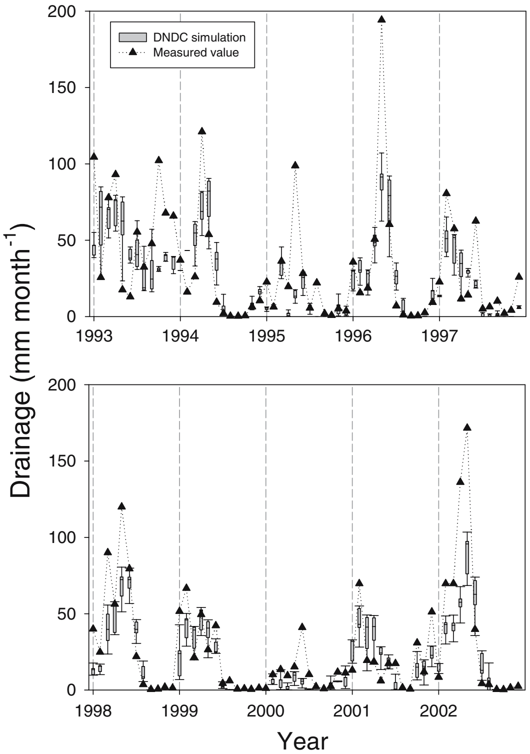

Fig. 3 DNDC simulated and observed monthly drainage. Monthly cumulative sums of drainage for calibration (1993–1997) and validation (1998–2002) years for the IL corn–soybean system. Shown are the measured values and box plots for the best 64 parameter sets (see *box plot* description in Fig. 1)

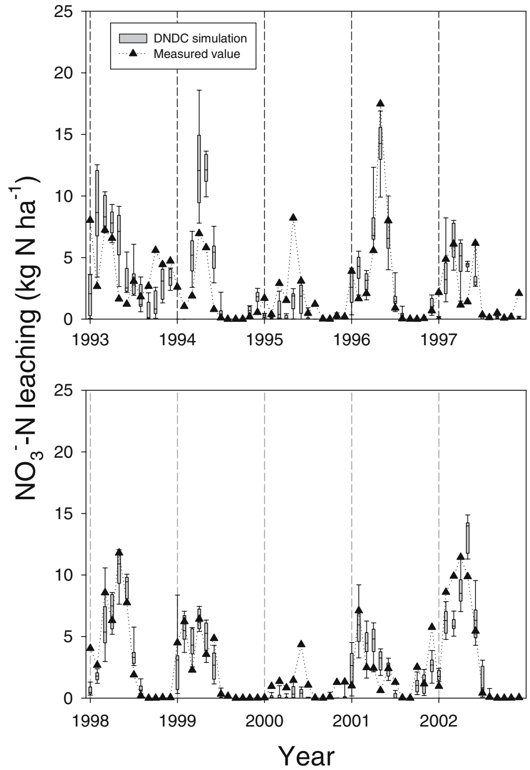

Fig. 4 DNDC simulated and observed monthly NO_3–N leaching. Monthly cumulative sums of NO_3–N leaching for calibration (1993–1997) and validation (1998–2002) years for the IL corn–soybean system. Shown are the measured values and box plots for the best 64 parameter sets (see *box plot* description in Fig. 1)

Monthly dynamics

Analysis of model outcomes at a monthly temporal resolution highlights the instances of disagreement between simulations and measurements. Graphs of monthly model output against data show the magnitude of model errors were large for only 1 or 2 months a year (Figs. 3, 4). For drainage, DNDC simulation consistently under-predicted the extreme peak flows. The model was never able to reproduce the most extreme monthly drainage measurements. Rather, in the model system, these extreme water fluxes where distributed as drainage in the following month(s).

Simulated NO_3–N leaching was most accurate when monthly nitrate loss was less then 2 kg N ha^{-1}, a nitrate loss rate representative of the second half of the growing season in most years (Fig. 4). Simulations tended to under-predict NO_3–N leaching in late fall and winter. Over-prediction of NO_3–N leaching generally occurred in the spring. In some years, measured peak flows of NO_3–N were accurately simulated.

A monthly temporal resolution demonstrates when the range of parameters tested result in a wide range in drainage and leaching outcomes. During seasons with high drainage, model results could vary across a range of 25–50 mm month^{-1}. At a monthly time resolution the parameter range tested resulted in up to a 5 kg N ha^{-1} month^{-1} range in modeled nitrate leaching in the first half of a simulation year.

Comparison with other model studies of corn–soybean agroecosystems

The Root Zone Water Quality Model (RZWQM) (RZWQM Team 1992, 1996) has been prominently applied at the field-scale to study short-term N dynamics of corn–soybean agroecosystems (Hanson et al. 1999; Ghidey et al. 1999; Jaynes and Miller 1999; Landa et al. 1999; Bakhsh et al. 2001, 2004). Similar to our DNDC results, comparison between field measurements and model outcomes demonstrated better agreement for water balance than for N dynamics in RZWQM applications (Ghidey et al. 1999; Jaynes and Miller 1999; Landa et al. 1999), highlighting the difficulty in simulating N dynamics. Model outcomes for corn–soybean systems demonstrated slight over- or underprediction of annual nitrate leaching on well drained loam soils of Iowa (Jaynes and Miller 1999), up to 400% overprediction of soil nitrate under corn and 85% underprediction under soybean on silt loam soils of Ohio (Landa et al. 1999), overprediction of soil nitrate in post-harvest corn systems and pre-planting soybean systems, underprediction of soil nitrate in post-harvest soybean systems, and overprediction of nitrate leaching in claypan soils of Missouri (Ghidey et al. 1999). Application of RZWQM in tile-drained regions of Iowa resulted in underprediction of peak water flux and nitrate leaching events followed by the re-distribution of these losses over the weeks proceeding a peak precipitation event (Bakhsh et al. 2001, 2004), results paralleling our DNDC findings.

The difficulty of modeling peak water and nitrate flow events in agroecosystems was likewise observed in an application of the Erosion Productivity Impact Calculator (EPIC) model to corn–soybean systems of Minnesota (Chung et al. 2001). In a comparison of the Soil and Water Assessment Tool (SWAT2000 and SWAT-M) Du et al. (2005) find the absence of tile drainage in SWAT2000 results in extreme underprediction of water flow; while tile drainage in SWAT-M allowed model simulations to track measured water flux. Although SWAT-M represents a significant improvement over SWAT2000 for tile-drained systems, simulations in densely tiled subbasins resulted in $EF < 0$, indicating SWAT-M does not capture all water flow dynamics.

Overall, results from RZWQM, EPIC, SWAT, and DNDC demonstrate that simulation of water and nitrate dynamics from peak flow events remains a challenge for model application. This highlights the need to monitor nutrient and hydrologic cycles for model development and application to policy. Here, we identified changes to parameters governing drainage and nitrate leaching which allow DNDC outcomes to achieve $EF > 0$ for comparisons of measured and simulated drainage and leaching over an entire decade; this relatively long temporal comparison suggests DNDC is an appropriate tool for exploring the impact of management in tile-drained corn–soybean agroecosystems. We find that though DNDC does not explicitly model tile drainage, our parameterization of DNDC produces drainage and nitrate leaching results with modeling efficiency values comparable to those documented by Du et al. (2005). Furthermore, our expansive test of parameter space outlines a range of parameter combinations, which produce statistically valid model simulations, suggesting parameter uncertainty does not preclude model application beyond the temporal extent of our data.

Conclusions

Comparison of modeled fluxes with field measurements demonstrated DNDC can be calibrated to represent corn–soybean systems in tile-drained regions of IL. By calibrating the model to physical and chemical parameters that controlled soil water and N, we were able to greatly improve model fit to observed data for drainage and NO_3–N leaching, as well as corn and soybean yields. While the default DNDC model resulted in consistently negative modeling efficiency values, our modifications to DNDC resulted in modeling efficiency ranging from 0.25 to 0.85 in comparison with measured drainage and leachate values and from 0.65 to 1 in comparison with crop yield data. Calibration of the DNDC model to tile-drained corn and soybean agroecosystems is a significant step toward understanding N fluxes in these important systems. Models such as DNDC cannot alone substitute for monitoring biophysical conditions. The applicability of a simulation model is governed by the availability of measurements for calibration and validation. Our statistically robust calibration of the DNDC model for application to tile-drained regions of IL was possible due to the availability of long-term drainage, leaching, and yield data. For these reasons, modeling must be coupled to biophysical data collection to achieve sustainable policy and management.

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