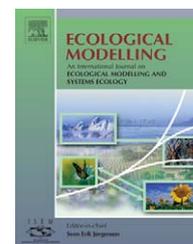


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## Modeling nitrate leaching with a biogeochemical model modified based on observations in a row-crop field in Iowa

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### ARTICLE INFO

#### Article history:

Received 16 December 2004

Received in revised form 10

December 2005

Accepted 1 February 2006

Published on line 20 March 2006

#### Keywords:

Agro-ecosystem modeling

Drainage flow

Nitrate leaching

DNDC model

### ABSTRACT

Prediction of nitrate leaching from cropland is crucial for preventing surface or ground water degradation. Accurate modeling of nitrate leaching requires simulations of both soil hydrological and biogeochemical processes. This paper reports an attempt to improve an existing biogeochemical model, Denitrification–Decomposition or DNDC, for estimation of nitrate leaching from crop fields with tile drainage system. DNDC was equipped with detailed biogeochemical processes of nitrogen turnover but a simple module for one-dimensional movement of soil water. Observations from nine drainage tiles with three different fertilizer treatments in 4 years (1996–1999) at an experimental field in Iowa were used for model modifications. Preliminary comparisons with observed tile discharge flow indicated that the original DNDC lacked the water leaching recession character. To correct this deviation, new water retention features were added to DNDC by: (1) adopting a recession curve to regulate the gravity drainage flow in the explicitly simulated soil profile (0–50 cm) and (2) introducing a virtual water pool for the space between the bottom of the modeled soil profile (50 cm) and the tile lines depth of placement (145 cm) to control the tile discharge flow. With these modifications, model prediction of water leaching fluxes from the tile drainage lines was improved. An adsorbed N pool was created in DNDC to simulate the buffering effect of soil on the amount of nitrate available for leaching. The Langmuir equation was adopted to simulate adsorption and desorption of ammonium ions on the soil absorbents. This modification enhanced the model capacity for simulating free ammonium dynamics, nitrification, and nitrate leaching. Sensitivity tests of the modified DNDC showed that the modeled impact of differences of precipitation, soil texture, soil organic carbon content, and fertilizer application rates on nitrate leaching rates were consistent with observations reported by other researchers. This study indicated that a biogeochemical model with limited modifications in hydrology could serve nitrate leaching prediction and be useful for sustainable agricultural management.

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doi:10.1016/j.ecolmodel.2006.02.007

## 1. Introduction

Modern agricultural practices are strongly linked to fertilizer application for maintaining optimum yields. However, inefficient fertilizer use has led to a significant portion of the nitrogen (N) applied to farm fields reaching surface or ground water systems (Karlen et al., 1998; Tilman et al., 2001). Surface and ground water quality in the Midwestern Corn Belt, the most productive region in the US, has been negatively affected by the increasing application of N fertilizers, particularly from 1950 to 1980s (Burkart and James, 1999). In this region it is common to have subsurface artificial drainage systems installed to improve the soil moisture conditions to allow for row-cropping operations, and hence create channels to lead the excess soil water rapidly into the surface water bodies. The intensive row-crop agricultural practices in the Midwestern Corn Belt are a significant source of N contamination of water resources in this region (Keeney and DeLuca, 1993; Cambardella et al., 1999; Jaynes et al., 2001; Dinnes et al., 2002). It is an increasing challenge to sustain agricultural production and the environmental quality by adopting best management practices including those for N management (Dinnes et al., 2002).

Nitrate ( $\text{NO}_3^-$ ) leaching from row-crop fields is directly controlled by water discharge flow and residual soil- $\text{NO}_3^-$  that is at risk for leaching, which are affected by numerous factors such as climate conditions, soil properties, and management (e.g., tillage, fertilization, irrigation, manure application, crop rotation, etc.). A large number of experiments have been conducted to observe the correlation between  $\text{NO}_3^-$  leaching and the environmental or management factors. However, with limited time and funding for field experiments, estimation of  $\text{NO}_3^-$  leaching, especially at regional scale, has to rely on mathematical models. Some of the models, such as MIKE SHE (DHI, 1999) and MODFLOW (Harbaugh et al., 2000) are hydrology-oriented with less details about N biogeochemical processes; and some, such as CENTURY and SOILN (Liu et al., 2000; Johnsson et al., 1987), have N turnover functions but with marginal hydrological features.

The goal of our project was to merge the two kinds of models for improving our modeling reliability. This paper reports how we adapted a biogeochemical model with limited modifications to serve as a  $\text{NO}_3^-$  leaching prediction tool that can be used for farm management planning.

## 2. Field observations

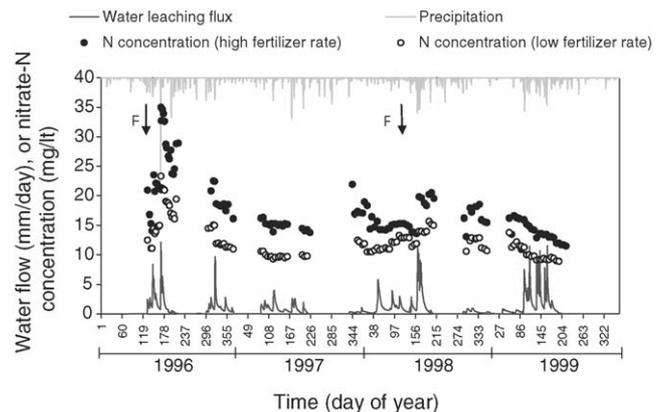
Field data used for this study were obtained from a 22 ha row-crop farm field near Story City in central Iowa (42.2°N latitude and 93.6°W longitude) with a 30-year average rainfall of 818 mm for this area (Hatfield et al., 1999). Jaynes et al. (2001) described the site as uniform for soil types and terrain. The local soils are in Kossuth-Ottosen-Bode association with high clay and organic carbon (C) content (45% and 2.9%, respectively, for the top 15 cm of soil) and poor drainage capacity (Brevik et al., 2003). Parallel drainage pipes or “tiles” were installed at an average depth of 1.45 m in 1992 (Jaynes et al., 2001). The study area contained nine tile lines, which are located in the mid-line of the areas they drain, and each of

the tile lines collected leachate from approximately 1.6 ha of the field and discharged to a drainage ditch.

Measurements of tile flow rates and  $\text{NO}_3^-$  concentrations were collected from 1996 through 1999. Flow from each tile was measured continuously. Flow-weighted composite water samples were collected from each tile on a weekly basis and were analyzed for nitrate nitrogen ( $\text{NO}_3^-$ -N). Details of the drainage and sampling systems were described by Jaynes et al. (2001) and Bakhsh et al. (2001). During the experimental period, corn [*Zea mays* L.] was planted in 1996 and 1998, and soybean [*Glycine max* (L.) Merr.] in 1997 and 1999.

For the corn-soybean rotated field, N fertilizer was only applied to the corn at three rates of low ( $67 \text{ kg ha}^{-1}$  in 1996 and  $57 \text{ kg ha}^{-1}$  in 1998), medium ( $135 \text{ kg ha}^{-1}$  in 1996 and  $114 \text{ kg ha}^{-1}$  in 1998), and high ( $202 \text{ kg ha}^{-1}$  in 1996 and  $172 \text{ kg ha}^{-1}$  in 1998). In 1996, corn was planted in April and harvested in November, and N fertilizer was applied as anhydrous ammonia 1 week before planting. In 1998, corn was planted in April and harvested in September, and N fertilizer was applied as urea ammonium-nitrate (UAN) 3 weeks after planting. No fertilizer was applied to soybean in 1997 and 1999.

The field data included measured tile water flow rates, N concentrations in the leachates, and N leaching rates for each of the nine tile lines. By analyzing the field data, we found that: (1) the water flow rates did not differ significantly across the nine tile lines; (2) the timing of the peak discharge water fluxes roughly matched the rainfall events across the entire 4-year period (Fig. 1); (3) the N concentrations measured in the leachates varied only slightly within a relatively small range ( $10\text{--}20 \text{ mg NO}_3^- \text{-N l}^{-1}$ ) and with no obvious correlation with the tile water flow rates (Fig. 1); (4) increase in fertilizer application rates did not proportionally increase  $\text{NO}_3^-$  concentrations in the leachate. The insignificant difference in water flow volume among the nine tile lines ( $P=0.05$ ) was assumed to be related to the relatively uniform soil texture and terrain at the site (Jaynes et al., 2001; Brevik et al., 2003). The fertilizer application rates at tile 1 ( $172\text{--}202 \text{ kg N ha}^{-1}$ ) were much higher than



**Fig. 1** – Field observed rainfall events (gray bars), water leaching fluxes (dark lines), nitrate concentrations in leachate (solid and open circles for high and low fertilizer treatments, respectively), and time of fertilizer applications (arrows) in a fertilized, corn-soybean rotated field with tile drainage system installed at depth of 145 cm near Story City in central Iowa.

that at tile 3 (57–67 kg N ha<sup>-1</sup>), but the average N concentrations in tile 1 (17.8 mg NO<sub>3</sub><sup>-</sup>-N l<sup>-1</sup>) was only 1.4 times higher than that in tile 3 (12.5 mg NO<sub>3</sub><sup>-</sup>-N l<sup>-1</sup>) (Fig. 1). The field observations demonstrated that the tile discharge water fluxes were dominated by the rainfall events, and there was apparently a buffering effect controlling N concentration in the discharge flow. The understandings gained from the field datasets were utilized to modify the DNDC model for this study.

### 3. The DNDC model

In comparison with several existing biogeochemical models, such as CASA, CENTURY or Roth-C (Potter et al., 1993; Johnsson et al., 1987; Jenkinson, 1990), DNDC possesses a relatively complete suite of N transformation processes under both aerobic and anaerobic conditions. In addition, a one-dimension water flow module has been developed in DNDC (Li et al., 1992; Zhang et al., 2002a,b). These existing routines provided a basis for further developing the model with new features such as N leaching.

DNDC was originally developed for estimating C sequestration in and trace gas emissions from the US agricultural soils (Li et al., 1992, 1994). DNDC consists of two compo-

nents bridging between ecological drivers (e.g., climate, soil, vegetation, anthropogenic activity, etc.) and soil environmental factors (e.g., temperature, moisture, pH, redox potential or Eh, substrate concentration gradients, etc.) on one hand, and between the soil environmental factors and soil biogeochemical reactions on the other hand. The first component, consisting of soil climate, crop growth and decomposition sub-models simulates soil temperature, moisture, pH, Eh, and substrate concentration profiles based on the ecological drivers. The second component consisting of nitrification, denitrification and fermentation sub-models predicts microbial activities and trace gas production based on the soil environmental variables (Fig. 2). Classic laws of physics, chemistry and biology or empirical equations derived from laboratory observations were used in the model to parameterize each specific reaction of C and N transformations. Driven by daily meteorological data, soil properties and agricultural management practices (e.g., tillage, fertilization, manure amendment, irrigation, flooding, weeding and grazing), DNDC predicts crop growth, soil organic carbon (SOC) dynamics and emissions of nitric oxide, nitrous oxide, dinitrogen, ammonia, carbon oxide and methane. DNDC has been independently tested by a wide range of researchers worldwide during the past decade (Wang et al., 1997; Smith et al., 1999; Butterbach-Bahl et al., 2001a,b,

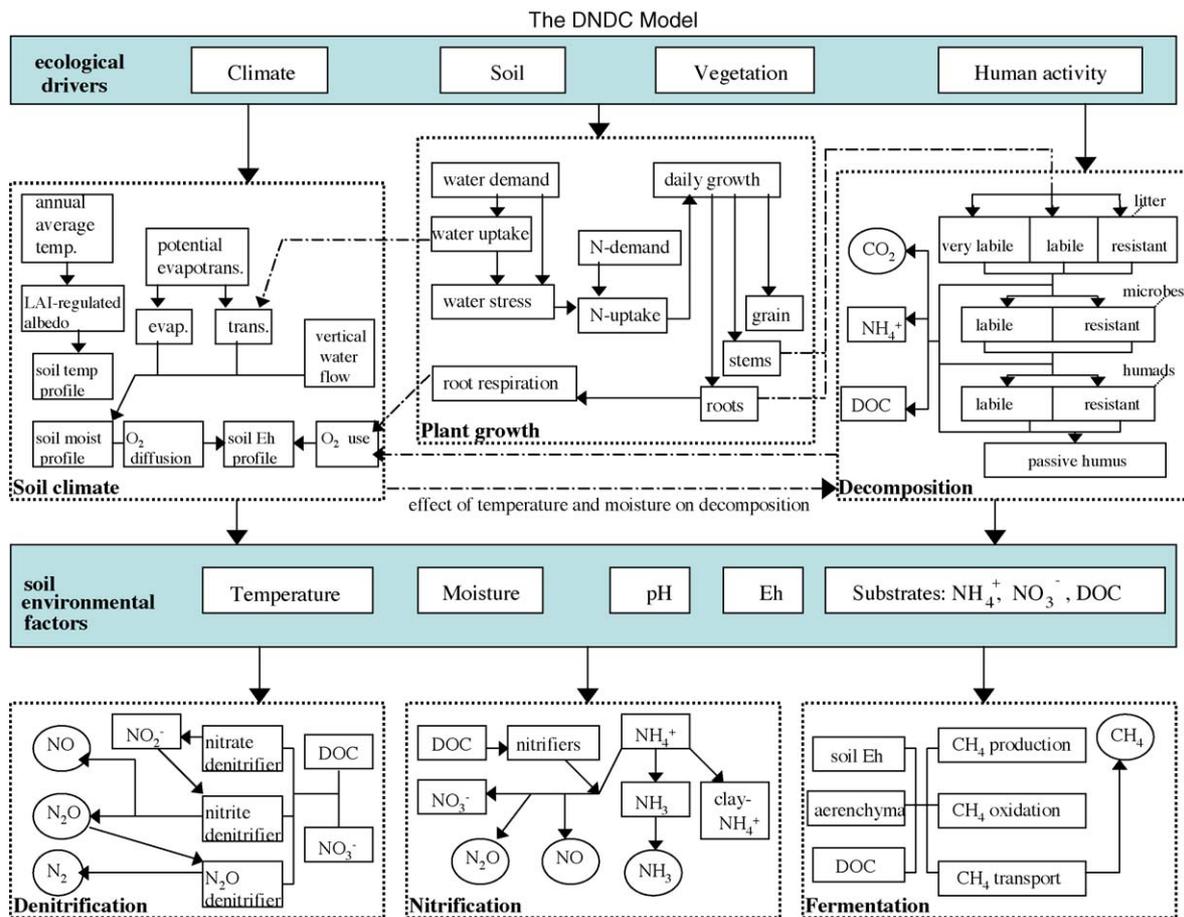
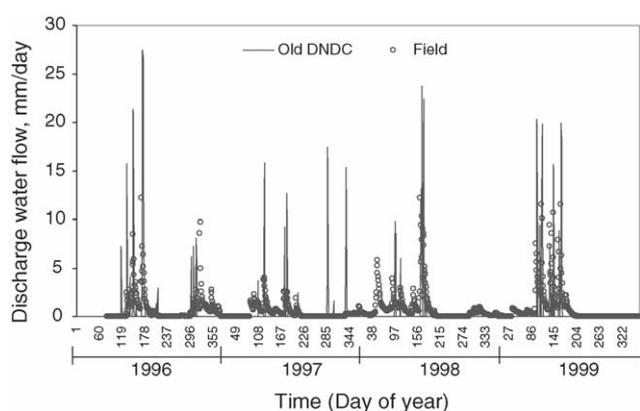


Fig. 2 – Structure of the DNDC model consisting of two components to bridge among the ecological drivers, the soil environmental factors and the biogeochemical reactions including mineralization, nitrification, denitrification, ammonia volatilization, etc. The detailed N transformation processes embedded in DNDC provided a basis for developing new N-related features such as N leaching.



**Fig. 3 – Comparison of measured and modeled (with original DNDC) discharge water fluxes from tile drainage system in a fertilized crop field in Iowa in 1996–1999. The original version of DNDC overestimated peaks of the discharge flow but underestimated durations of the recession process.**

2004; Brown et al., 2002; Smith et al., 2002, 2004; Cai et al., 2003; Xu-Ri et al., 2003; Saggari et al., 2003, 2004; Grant et al., 2004; Kiese et al., 2004; Pathak and Wassmann, 2005). DNDC has recently been validated for predicting yields for several crops, cropping systems and sites including a corn-soybean farm field in Iowa with intensive spatial and temporal sampling of crop and soil parameters (Farahbakhshazad et al., 2002). Based on the widely tested processes embedded in DNDC, the model was modified to serve N leaching simulations in this study.

## 4. Model modifications

Based on the datasets from the tiled field in Iowa, we hypothesized that: (1) the observed tile drainage flow could be simulated with a one-dimension hydrological module by tracking the synchronal relation between the flow and rainfall events with a recession curve and (2) the observed stability of N concentration in leachate could be simulated with a buffering mechanism such as adsorption/desorption. The two hypotheses were implemented in DNDC by adding two new features upon the routines originally embedded in the model.

### 4.1. Modeling discharge recession

The field observations from the experimental site in Iowa demonstrated peaks of the discharge flow that were usually detected on days with rainfall; and then the discharge flow gradually decreased in the following several days after the rainfall ceased. By tracking gravity drainage driven by rainwater infiltration, the original DNDC captured the timing of start of the discharge fluxes but missed the recession. In contrast to the observations, the modeled discharge water fluxes had high peak values during the rainfall events, and then sharply decreased after the rainfall stopped (Fig. 3). This deviation in the simulated result was assumed to be related to the sim-

plified routine of water movement embedded in the original DNDC.

In the original version of DNDC, a one-dimensional soil water flow was used to calculate average hourly and daily soil moisture within a soil profile. The default thickness of the modeled soil profile is usually 50 cm but can be extended to 100 cm or deeper. DNDC characterizes soil physical properties by soil texture, following the work of Clapp and Hornberger (1978). The soil profile is divided into a series of horizontal layers. Typical vertical spatial resolution is 2 cm and time step is an hour. Each layer is assumed to have uniform texture and moisture. For each time step, water flow between layers is determined by the gradients of soil water potential (Ritchie et al., 1988). During a simulated rainfall event, rainwater is added on the surface of the soil and then infiltrates into the soil profile layer by layer to fill the soil pore. Gravity drainage occurs when the soil moisture is higher than the field capacity (i.e., 0.033 MPa for North American system, and 0.006 MPa for European soil system) in a layer. Water efflux from the bottom of the modeled profile is driven by gravity drainage only (Van Bavel et al., 1978). If the rainfall intensity, which is fixed as  $0.5 \text{ cm h}^{-1}$  in DNDC, is higher than the soil saturated hydraulic conductivity, water will pond on the soil surface and a surface runoff flow will be calculated based on the defined soil slope. Water withdrawal from the soil profile is calculated based on evaporation and transpiration. Potential evapotranspiration (ET) is calculated as a daily average value using the Thornthwaite formula, in which potential ET is determined by mean air temperature and then adjusted for daylight length relative to 12 h (Dunne and Leopold, 1978). Potential ET is separated into potential evaporation and transpiration. Daily potential transpiration is determined by daily water demand by plants, which is quantified based on the modeled daily increment of crop biomass. Actual plant transpiration is jointly determined by potential transpiration and soil water content. Potential evaporation is the difference of potential ET and actual transpiration. Evaporation is allowed to occur only for the top 20 cm of soil profile. By tracking precipitation, plant interception, surface ponding, surface runoff, infiltration, gravity drainage, transpiration, and evaporation, DNDC simulates water movement in the vertical dimension of soil profiles. A routine of heat transmission in soil has been built in DNDC to simulate soil freezing and thawing processes, which significantly affect water movement in the soil profile. The detailed descriptions about the hydrological equations and parameters have been reported in several former publications (e.g., Li et al., 1992; Zhang et al., 2002a,b). The major equations utilized for the soil climate sub-model are summarized in Appendix A.

In the original DNDC, water discharge from the bottom of soil profile was calculated based on the equation developed by Ritchie et al. (1988), in which drainage rate is linearly related to the water content above field capacity. DNDC discharged 50% of the water content above field capacity discharged from a layer at an hourly time step (Zhang et al., 2002a). With this linear control, DNDC produced sharp discharge flow following each rainfall event with almost no recession. To correct the deviation, we modified the soil hydraulic routines by: (1) replacing the linear function with a water discharge recession curve for the explicitly simulated soil profile (0–50 cm for this

case) and (2) adding a virtual deep water pool to imitate water storage in the space between the bottom of the simulated soil profile and the depth of the drainage tiles (145 cm for this case).

Based on Tallaksen's summary (1995), drainage of water from soil matrix can be generally described with a curve, which defines decrease of discharge rates along with decrease in the soil water content as a non-linear relation. According to the recession curve, drainage rate reaches its maximum when the soil is saturated during a rainfall event, and gradually decreases as the depth of saturation decreases when there is little or no precipitation. A simplified recession curve was implemented in DNDC to describe water discharge during and after rainfall events for each layer as follows:

$$\text{Discharge}[i] = a(\text{water}[i] - \text{fldcap}) \times 10^{-b/((\text{water}[i] - \text{fldcap})/(\text{spv} - \text{fldcap}))} \quad (1)$$

where Discharge[i] is the water flow (m h<sup>-1</sup>) discharged from bottom of soil layer i, water[i] the water content (m) in layer i, fldcap the soil field capacity (m), spv the soil pore volume in a layer (m), and a and b are the constant coefficients defining initial drainable water flux and the retention rate, respectively.

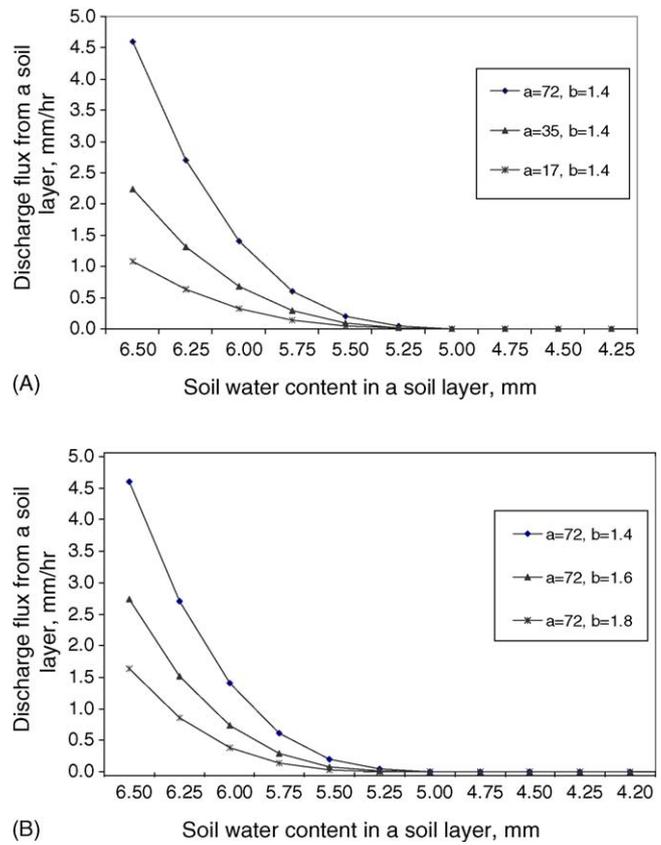
In the recession equation, a and b are two adjustable coefficients, which control the maximum discharge flow and the rate of decrease in discharge flow due to decrease in the soil water content. The magnitude of a or b is apparently related to soil texture and other physical properties (e.g., porosity, field capacity, wilting point, etc.). For example in soils with heavy texture, which usually have higher field capacity than lower textured soils, the value of a would decrease and the value of b would increase to allow a lower initial discharge flux with a longer recession process. Fig. 4A and B demonstrates how changes in value of a or b affects discharge flow rate. Equipped with the recession equation, DNDC was calibrated with the water flow data measured from tile 1 in 1998, and the coefficients a and b were determined to be 72 and 1.4, respectively.

As a biogeochemical model, DNDC routinely simulates a soil profile from 0 to 50 cm. This depth was assumed to be deep enough to cover the most important biogeochemical processes while minimizing computing time. It is inherently questionable that if the modeled discharge from the depth of 50 cm can represent the observed drainage flow from the tile lines that are installed at a deeper depth. To meet this gap, we created a deep water pool in DNDC. The pool is virtually located below the bottom of the modeled soil profile and above the drainage tiles. The capacity of the deep water pool (Vdwp) is a function of soil porosity and the distance between the soil profile bottom and the drainage tiles:

$$Vdwp = a \times \text{poro} \times (D_{\text{tile}} - D_{\text{spb}}) \quad (2)$$

where poro is the soil porosity, D<sub>tile</sub> the depth of tile (m), and D<sub>spb</sub> is the depth of soil profile bottom (m).

The initial water volume in the deep water pool is set to be equivalent to the field capacity. Whenever there is a discharge water flow modeled at the bottom of the explicitly simulated soil profile, the flow will be divided into two parts. A fraction (F1) of the water flow will be stored in the deep water pool; and the rest to be routed through tile drainage flow. If the water



**Fig. 4 – (A and B) Effects of coefficients a and b in the recession equation on rate of discharge water flow. Coefficient a determines the maximum water discharge rate and b defines the rate of decrease in water discharge flow after the rainfall ceases. Coefficients a and b are soil texture-related, and can be empirically determined by fitting to observations for a specific site.**

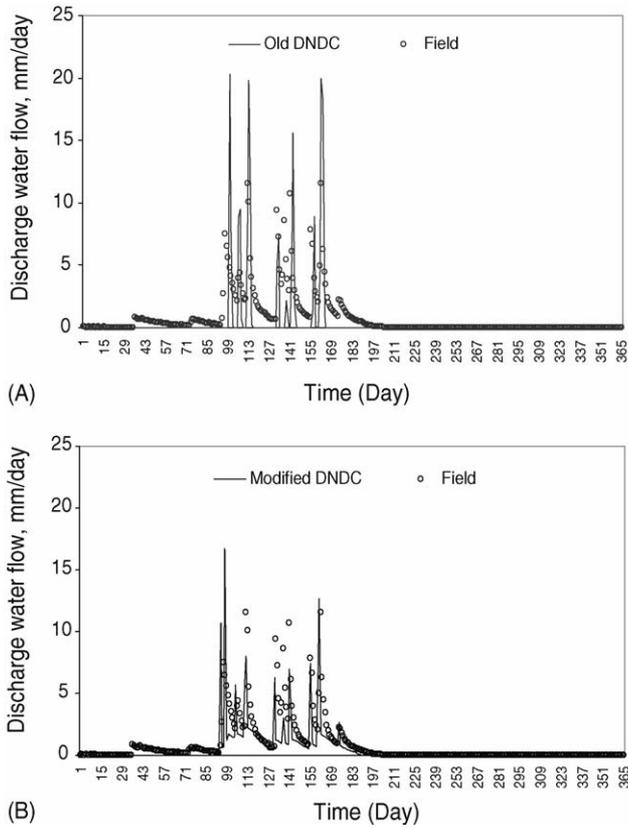
content in the deep water pool is higher than the field capacity, a fraction (F2) of the excess water will be released from the pool to the tile drainage flow. The fractions, F1 and F2, governing the water flow into and release from the deep water pool, respectively, were defined as functions of soil texture with clay content as an indicator. Through calibration against the observed tile discharge fluxes from tile 1 in 1998, F1 and F2 are calculated as:

$$F1 = 2.75\text{clay}^2 - 3.09\text{clay} + 1.16 \quad (3)$$

$$F2 = 0.0005\text{clay}^{-1.62} \quad (4)$$

where clay is the soil clay fraction.

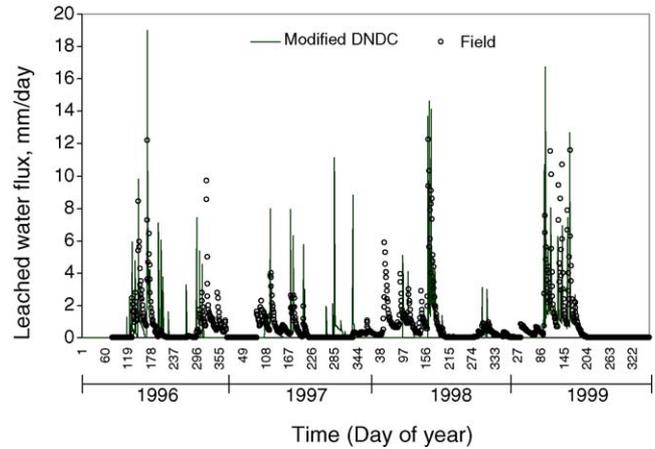
Equipped with these two modifications, we applied DNDC for all of the tile data from 1996 to 1999. The simulated results indicated that the modifications improved model performance. The modeled discharge fluxes had lower peaks with longer recession durations, which better matched the field observations. Fig. 5A and B provides zoom-in pictures for a 1-year discharge water fluxes simulated by the old and the new DNDC.



**Fig. 5 – Comparison of observed tile drainage fluxes with modeled results with original and modified DNDC for 1999. The original DNDC overestimated the peak discharge fluxes with shorter discharge durations (A). After modification by adding a recession equation and a water buffer pool below the simulated soil profile, the new DNDC extended the discharge durations with lowered peak flow values (B).**

The model was tested with observed soil moisture data from sites in Canada and New Zealand, where there were water retention layers existing within the simulated soil profiles (i.e., at a depth <50 cm). The simulated discharge water flow substantially deviated from observations (Saggar et al., 2004). To correct this problem, we decreased the water conductivity by 90% at the depth where the water retention layer was located, and then the modeled results were significantly improved (Saggar et al., 2004; personal communication with Brian Grant). This test indicated that soil homogeneity was one of the key factors affecting the model’s performance.

With the above-described modifications, DNDC captured the magnitudes and patterns of tile discharge fluxes observed at the experimental field in Iowa although discrepancies still existed (Fig. 6). For example, the predicted discharge fluxes in October in 1997 were not observed in the field. We assumed the discrepancies could be related to lateral flow entering the tile lines, which is beyond the predictive capacity of DNDC. However, the results suggested that a simplified one-dimension model could be still useful for estimating discharge water flow from tiled drainage systems if the soil is homogeneous and the lateral flow is subdominant.



**Fig. 6 – Comparison of observed tile drainage water fluxes with modeled results with modified DNDC for 1996–1999. The model captured the recession processes although discrepancies existed.**

#### 4.2. Modeling nitrogen adsorption

Nitrate leaching is a part of N biogeochemical cycling in soils. Observations from the tiled field in Iowa indicated that the  $\text{NO}_3^-$  concentrations in leachate varied in a gentle manner neither increasing with fertilizer applications nor instantly decreasing with rainfall events (Fig. 1). Nitrate is highly soluble and readily subjected to leaching. The observed stability of N concentration in leachate could be interpreted with the soil buffering effect. Based on the general knowledge of soil biogeochemistry, this buffering effect can be constituted by several mechanisms including N assimilation/dissimilation by the soil microorganisms (O’Connel, 1988) and  $\text{NH}_4^+$  adsorption/desorption by the soil adsorbents such as clay minerals or organic matter (Hillel, 1998). As soon as  $\text{NH}_4^+$  ions are introduced into a soil through fertilization, atmospheric deposition or mineralization, the ions will be readily fixed by either assimilation or adsorption. The fixed  $\text{NH}_4^+$  in the living microbial pool can be released back into the soil liquid phase if the microbes die and the organic matter decomposes; and the  $\text{NH}_4^+$  fixed on the adsorbents can be released through chemical equilibrium. The  $\text{NH}_4^+$  released into the soil liquid phase can be quickly converted to  $\text{NO}_3^-$  by the nitrifiers. Although  $\text{NO}_3^-$  can be reused by the soil microbes again, the anion does not have affinity to the soil adsorbents. This creates a better chance for  $\text{NO}_3^-$  to move to the leaching water flow. So it is crucial to simulate the buffering effects of assimilation and adsorption for predicting  $\text{NO}_3^-$  leaching.

As a biogeochemical model, DNDC has a series of processes describing N transformations in soils, which include decomposition, nitrification, denitrification, urea hydrolysis, ammonium–ammonia equilibrium, ammonia volatilization, etc. (Li et al., 1992; Li, 2000). These processes enable DNDC to track N turnover mainly driven by microbial activities in the soil. Most of the above-listed processes involve growth and death of microorganisms, so that the microbial assimilation and dissimilation of N have been included in the model. In DNDC, these processes have been linked to soil environmental

factors (e.g., temperature, moisture, pH, Eh, and substrate concentration gradients) as well to farming management practices (crop rotation, tillage, fertilization, manure amendment, irrigation, grazing, etc.). In this study, the major effort was to build another buffering mechanism, i.e., N adsorption by the soil adsorbents. In contrast to the microbial buffering effect that is usually effective in the top soil, the existence of soil adsorbents can reach to deep soil layers. Cation exchange capacity (CEC) of clay minerals or organic matter can be very large. For example, a mere handful of clay may have an internal surface area of several hectares (Hillel, 1998). Laboratory experiments indicated that montmorillonite, illite and vermiculite adsorbed 170, 690 and 1800 mg N kg<sup>-1</sup> soil, respectively; and field measurements also showed agricultural soils, which contained mixture of clay minerals and organic matter, adsorbed NH<sub>4</sub><sup>+</sup> of 50–300 mg N kg<sup>-1</sup> soil (Zhu and Wen, 1992). Since these adsorbents, especially clay minerals, are basic components of soil profiles even in the deep soil, NH<sub>4</sub><sup>+</sup> adsorption by the adsorbents can create a buffering pool for most agricultural soils. In fact, some field measurements demonstrated that in contrast with the sharp decrease in NO<sub>3</sub><sup>-</sup> content as soil depth increased, NH<sub>4</sub><sup>+</sup> content decreased more slowly (Zhu and Wen, 1992). The measurements conducted at the Baker field, a site near our experimental field in Iowa, based on the 2M KCl-extracted NH<sub>4</sub><sup>+</sup> contents, showed that the profiles contained 215–455 kg N ha<sup>-1</sup> in the top 100 cm soil (calculated based on ISPAID, Iowa Soil Properties and Interpretations Database, 1996). The field observations imply that the role of adsorbed NH<sub>4</sub><sup>+</sup> pool in regulating soil N dynamics is not negligible.

To model the adsorption and desorption processes in DNDC, we adopted the Langmuir isotherm equation. The equation quantifies concentrations of adsorbate (e.g., NH<sub>4</sub><sup>+</sup>) distributed between its free ion phase and adsorbed phase based on the isotherm equilibrium (Stumm and Morgan, 1981). The Langmuir equation is expressed as follows:

$$\Gamma = \Gamma_{\max} K_{\text{ads}} [\text{NH}_4^+] / (1 + K_{\text{ads}} [\text{NH}_4^+]) \quad (5)$$

where  $\Gamma$  is the adsorbed NH<sub>4</sub><sup>+</sup> (kg N/layer),  $\Gamma_{\max}$  the potential maximum adsorbed NH<sub>4</sub><sup>+</sup> (kg N/layer),  $K_{\text{ads}}$  the adsorption constant, and  $[\text{NH}_4^+]$  is the NH<sub>4</sub><sup>+</sup> concentration in the liquid phase (kg N/layer).

In the Langmuir equation,  $\Gamma_{\max}$  and  $K_{\text{ads}}$  are functions of the surface property and total surface area of adsorbents in the soil. For a specific soil, the  $\Gamma_{\max}$  and  $K_{\text{ads}}$  values are constant and can be determined through adsorption experiments. Under natural conditions, the  $\Gamma$  value is usually much lower than the  $\Gamma_{\max}$  value. In the case, Eq. (5) can be simplified into (6):

$$[\text{NH}_4^+] = \Gamma / (K_{\text{ads}} \times \Gamma_{\max}) \text{ or } k \times \Gamma \quad (6)$$

In Eq. (6), NH<sub>4</sub><sup>+</sup> concentration in the soil liquid phase is linearly related to the amount of adsorbed NH<sub>4</sub><sup>+</sup> ( $\Gamma$ ). We assumed  $k$  was a function of cation exchange capacity (CEC), which is widely used to indicate the soil's potential for adsorption, and calculated  $k$  as follows:

$$k = a \times e^{0.0981\text{CEC}} \quad (7)$$

By applying Eqs. (6) and (7) for a randomly selected treatment (high fertilizer rate) in a random year (1998) of the observations, we empirically determined the coefficient  $a$  as 0.0144 for the soil in the experimental field in Iowa. After the calibration, DNDC was applied to all of the other tile lines with three different fertilizing rates across the 4-year time span. The modeled crop yield, crop removal N, fixed N and leached N were compared with the observations reported by Jaynes et al. (2001). Measured and modeled results are listed in Table 1 for comparison. The modeled crop yields, crop removal N rates, fixed N rates are in agreement with observations regarding their magnitudes and inter-annual patterns. A statistical analysis was conducted to quantify the correlations between the modeled and observed leached N fluxes. The  $P=0.95$  confidence limits for differences in the N leaching fluxes observed from the tiles were calculated and reported in Table 1. Simulated annual N leaching rates were mostly comparable with the observed values except for the low and medium fertilizer treatments in 1997 and 1999 where the model slightly overestimated leached N fluxes. In general, the modeled results are satisfied regarding the magnitudes and inter-annual patterns (Fig. 7a–c).

Our modifications on water recession and N adsorption were built upon the original routines of water movement and N biogeochemistry in DNDC, respectively. The original equations and parameters in DNDC have been reported in detail in several former publications (e.g., Li et al., 1992, 2004; Li, 2000; Zhang et al., 2002a,b). However, the major equations for the hydraulic and N biogeochemical processes embedded in DNDC are summarized in Appendices A and B for reference.

## 5. Sensitivity tests

Sensitivity tests were conducted to observe the general behavior of the modified DNDC. For the tests, a baseline scenario was composed for a corn field with the climate and soil conditions similar to that in the experimental site in Iowa. 1998 climate data with annual precipitation 896 mm from the same site were adopted for the baseline. The soil clay fraction was 43%, SOC content 3%, pH 6.5, initial ammonium content 0.6 mg N kg<sup>-1</sup>, and initial NO<sub>3</sub><sup>-</sup> content 3.0 mg N kg<sup>-1</sup>. The fertilizer application rate was 200 kg N ha<sup>-1</sup> in the baseline scenario. Alternative scenarios were constructed by varying each of the three selected factors, namely precipitation, N fertilizer application rate and SOC content, within the ranges of 360–1440 mm, 0–300 kg N ha<sup>-1</sup> and 0.1–6%, respectively. After the model runs with the scenarios, modeled plant N uptake rates, soil N mineralization rates, adsorbed N rates, and N leaching rates were recorded. By comparing the modeled results, we determined the relative sensitivities for the tested factors. In order to bring the comparison into a quantitative manner, based on Nearing et al. (1989) and Walker et al. (2000), a sensitivity index was calculated for quantifying the impacts of the input factors on the selected output items (Eq. (8)):

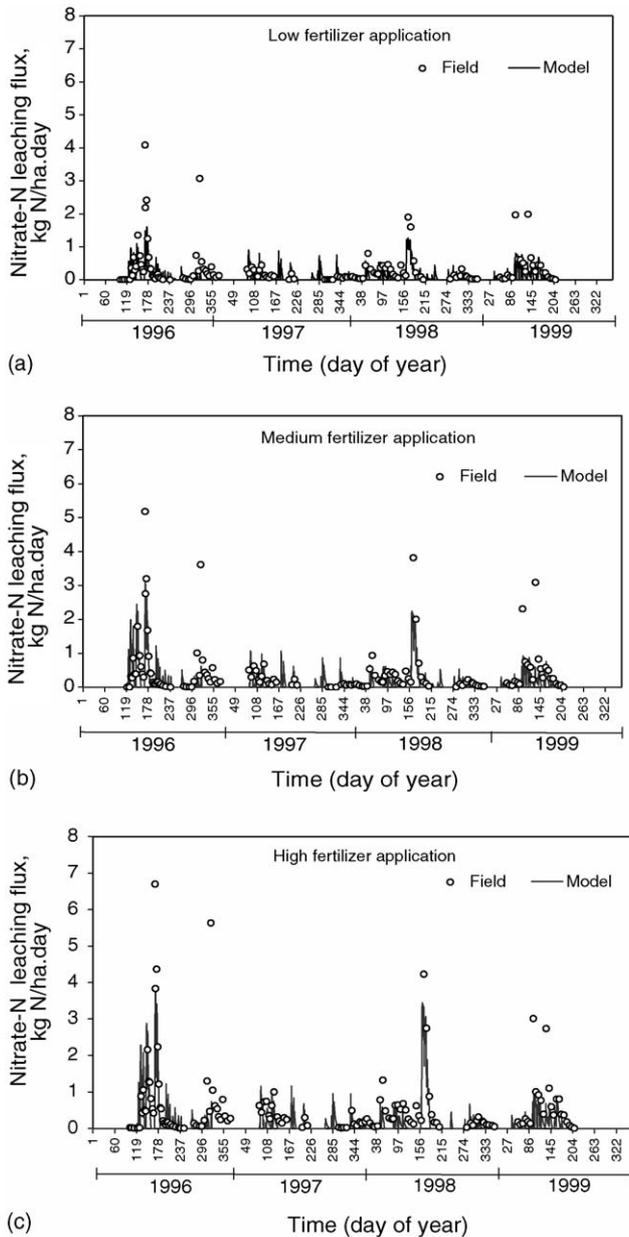
$$S = \frac{\left( \frac{O_2 - O_1}{O_{\text{avg}}} \right)}{\left( \frac{I_2 - I_1}{I_{\text{avg}}} \right)} \quad (8)$$

**Table 1 – Comparison between observed and modeled annual crop yields and N fluxes for the study field treated with three fertilization rates from 1996 to 1999**

Year and treatment	Fertilizer applied (kg ha <sup>-1</sup> yr <sup>-1</sup> )	Observed N fluxes (kg C or N ha <sup>-1</sup> yr <sup>-1</sup> )						Modeled N fluxes (kg C or N ha <sup>-1</sup> yr <sup>-1</sup> )				
		Crop yield (kg C ha <sup>-1</sup> )	N fixed (kg ha <sup>-1</sup> )	Crop removal (kg N ha <sup>-1</sup> )	N leached (kg ha <sup>-1</sup> )	S.D. <sup>a</sup>	0.95 confidence interval <sup>b</sup>		Crop yield (kg C ha <sup>-1</sup> )	N fixed (kg ha <sup>-1</sup> )	Crop removal (kg N ha <sup>-1</sup> )	N leached (kg ha <sup>-1</sup> )
							Lower limit	Higher limit				
1996 and corn												
L	67	2800	0	53	37	4.1	36	44	3063	0	79	36
M	135	4000	0	93	47	9.1	38	63	3877	0	86	45
H	202	4000	0	93	61	7.7	55	74	3877	0	86	55
1997 and soybean												
L	67	1440	187	196	13	1.2	10	13	1087	213	157	23
M	35	1440	195	198	16	1.1	15	17	1087	213	157	27
H	202	1440	191	197	26	6.9	17	32	1087	213	158	32
1998 and corn												
L	67	3200	0	69	38	5.1	30	41	2129	0	54	32
M	135	4000	0	96	43	4.4	37	47	2799	0	72	40
H	202	4080	0	108	59	11.4	44	70	3686	0	83	51
1999 and soybean												
L	67	1440	208	204	31	1.7	24	30	1053	206	151	34
M	35	1440	202	203	36	2.2	32	37	1053	206	152	39
H	202	1440	203	208	49	11.0	33	58	1053	206	151	48

<sup>a</sup> Standard deviation for observed N leaching fluxes based on three tile systems per treatment.

<sup>b</sup> Confidence interval limits for observed N leaching based on three tile systems per treatment.



**Fig. 7** – Comparisons between observed and modeled leached nitrate fluxes for three treatments, i.e., low (a), medium (b) and high (c) fertilizer application rates for 1996–1999 (see quantified correlations in Table 1).

where  $S$  is the relative sensitivity index,  $I_1$ ,  $I_2$  the minimum and maximum input values tested for a given parameter,  $I_{avg}$  the average of  $I_1$  and  $I_2$ ,  $O_1$ ,  $O_2$  the model output values corresponding to  $I_1$  and  $I_2$ , and  $O_{avg}$  is the average of  $O_1$  and  $O_2$ .

Table 2 presents the calculated sensitivity indices for the impacts of precipitation, fertilizer rate and SOC content on plant N uptake, soil N mineralization, adsorbed N, and N leaching. The higher the absolute value of the index ( $S$ ), the greater the impact the input has on the output. A negative value indicates an inverse relationship between the input and the output.

The results listed in Table 2 indicated that annual precipitation had the greatest impact on soil N leaching and only slightly affected crop N uptake and soil N mineralization. Precipitation negatively affected the size of adsorbed N pool by elevating the release rate of  $\text{NH}_4^+$  from the soil solid phase for leaching. Fertilizer application rate had positive effects on all of the simulated N pools or fluxes. An increase in N fertilizer application rate had significant impacts on N leaching and soil N mineralization and also elevated crop N uptake and N storage in the adsorption pool. In DNDC, SOC plays a dual role in N biogeochemistry. SOC is a potential source of inorganic N through mineralization meanwhile SOC can temporarily fix  $\text{NH}_4^+$  through adsorption. In the sensitivity tests, increase in SOC content substantially increased the soil N mineralization rate and the adsorbed N pool but did not directly affect N leaching rates. In general, the tests indicated the soil N leaching rate was most sensitive to precipitation and fertilizer application rate. This result is basically in agreement with observations reported by other researchers (Bakhsh et al., 2000, 2001).

The sensitivity tests were designed only for observing several basic behaviors of the model but not for thoroughly evaluating impacts of all environmental or management factors on soil N leaching. For example, soil N mineralization rate can be affected by the type of fertilizer sources. Long-term application of animal manure or inclusion of legumes could increase N mineralization rates even without added synthetic fertilizer (Carpenter-Boggs et al., 2000; Davis et al., 2003).

## 6. Discussions

Over the past several decades, farmers have been subjected to ever shrinking profit margins (Blank, 2002). If a decision support model is to truly be of use to farmers or regulatory staff, it must be able to accurately predict outcomes on crop production and environmental impacts for a wide range of farming operations and climatic conditions. Requiring farm management to be based on models that have not been devel-

**Table 2** – Calculated sensitivity indices quantifying impact of the tested input parameters on output N pools or fluxes

Parameter	Range tested	Baseline	Sensitivity index ( $S$ )			
			N leaching	N uptake	Adsorbed N	N mineralization
Precipitation	360–1440 ( $\text{mm y}^{-1}$ )	900 ( $\text{mm y}^{-1}$ )	1.8	0.2	−0.7	0.2
Fertilizer rate	0–300 ( $\text{kg N ha}^{-1}$ )	200 ( $\text{kg N ha}^{-1}$ )	0.7	0.5	0.4	0.7
SOC content	0.1–6%	3.0%	0.1	0.04	0.9	1.2

<b>Table 3 – A comparison of DNDC with other models capable of simulating soil N leaching</b>							
	DNDC	CERES	ExpertN	ANIMO	Daycent	SWAT	RZWQM
<b>Hydrological processes</b>							
Surface runoff	✓	✓	✓	✓	✓	✓	✓
Percolation	✓	✓	✓	✓	✓	✓	✓
Bypass flow	✓			✓		✓	✓
Transpiration	✓	✓	✓	✓	✓	✓	✓
Evaporation	✓	✓	✓	✓	✓	✓	✓
Underground lateral flow			✓	✓		✓	✓
Tile drain	✓					✓	✓
<b>Nitrogen transformation processes</b>							
Mineralization	✓	✓	✓	✓	✓		✓
Microorganism-driven nitrification	✓						✓
Microorganism-driven denitrification	✓						✓
Empirical nitrification		✓	✓	✓	✓	✓	
Empirical denitrification		✓	✓	✓	✓	✓	
Ammonia volatilization	✓		✓	✓	✓	✓	✓
Ammonium adsorption	✓			✓			
Dissolved organic C/N	✓			✓	✓		✓
<b>Crop growth processes</b>							
Growth stage	✓	✓	✓			✓	✓
Water/nutrient stress	✓	✓	✓			✓	✓
Variable yield	✓	✓	✓		✓	✓	✓
<b>Management Processes</b>							
Planting date	✓	✓	✓	✓	✓	✓	✓
Tillage	✓	✓	✓	✓	✓	✓	✓
Irrigation	✓	✓	✓	✓		✓	✓
Fertilization	✓	✓	✓	✓	✓	✓	✓
<b>Other environmental concerns</b>							
Carbon sequestration	✓	✓	✓		✓		
NO emission	✓				✓		
N <sub>2</sub> O emission	✓	✓	✓		✓		
Anaerobic CH <sub>4</sub> production	✓						
CH <sub>4</sub> oxidation	✓				✓		
Reference	Li et al. (1992, 1994, 2004), Zhang et al. (2002a,b)	Quemada and Cabrera (1995)	Stenger et al. (1999)	Groenendijk and Kroes (1999)	Parton et al. (1998)	Neitsch et al. (2002)	RZWQM Development Team (1995), Ahuja et al. (1999)

oped to such a level could lead to financial failure. Nowadays modeling N leaching is attracting more attention, yet still is a complicated task. Nitrogen leaching is controlled not only by geological or hydrological processes but also by plant–soil processes. This requires a modeling capacity for both spatially distributed hydrological processes and detailed biogeochemical reactions. Our study tested the possibility that a site-scale biogeochemical model, which was intensively used for prediction of crop yield, C sequestration and trace gas emissions, could be utilized for predicting N leaching with limited modifications. Our goal is to develop a low-cost tool for farm managers or crop and environmental consultants to assess the comprehensive impacts of alternative cropping practices on agricultural production as well environmental safety for farmlands. A typical tile-drained corn-soybean rotated field in Iowa with intensive measured datasets was selected to test the biogeochemical model, DNDC. The initial discrepancies between the modeled and observed N leaching results led to two major model modifications namely discharge water recession and N adsorption. By adding the new features, the modified DNDC was substantially able to capture the magnitudes and patterns of both discharge flow and N leaching for the different fertilizer treatments across the 4-year time span. The results imply that a biogeochemical process-based model with one-dimension hydrology could serve for N leaching prediction, at least on a field-scale basis.

In comparison with several existing models capable of simulating N leaching, DNDC has an advantage due to its more detailed processes of N transformation embedded in the model. Theoretically, any model that possesses both hydrological and N transformation features should be able to predict N leaching. In fact, many models, such as CERES, Expert-N, ANIMO, Daycent, RZWQM, SWAT, DNDC, etc., do possess the basic hydrological and biogeochemical processes and produce simulated N leaching fluxes. For example, most of the above-listed models declare their ability for simulating denitrification, an important process causing N loss from the soils into the atmosphere and a reduction of N available for leaching. However, a careful comparison finds that denitrification is simulated in different ways across the models. Denitrification consists of sequential conversions of nitrate to nitrite, nitric oxide, nitrous oxide, and finally dinitrogen. The amount of soil N lost to denitrification is determined by the conversion kinetics among the N species. The complex processes are highly simplified in many models. For example, the SWAT (Soil and Water Assessment Tool) model quantifies denitrification rate as a linear function of nitrate concentration subject to organic carbon content in the soil (Neitsch et al., 2002). By ignoring many other factors such as soil redox potential, pH, etc., the simplification could limit the applicability of the model across a wide range of natural or management conditions. This argument is valid for most models capable of modeling N leaching (Table 3). DNDC tracks activities of the soil microbes driving

the sequential reactions of denitrification, and hence is able to provide reliable estimates of the N gas emissions across climate, soil and management regimes. Equipped with the detailed processes of N transformation such as denitrification, DNDC is able to precisely simulate the wide range of N transformations and thereby close the N budget for most agricultural soils. The comprehensive set of N transformation provides a sound basis for the model to quantify the residual N available for leaching.

While we are encouraged by the recent improvement to DNDC for nitrate leaching estimation, we realize there are still limitations for widespread application of this tool. We anticipate that soil heterogeneity would be the major obstacle for applying the model across sites. For example, we empirically determined the values of coefficients in the recession equation and the Langmuir equation through calibrating procedure for the selected field. We suspect the values may not be applicable to other sites with different soil conditions. If the model is applied to a new site, we suggest carrying out tests to verify or modify the coefficients. To eliminate this inconvenience in the future, we will continue testing the model against more observations across climate zones, soil types, and management regimes. We expect the empirical coefficient constants to be gradually replaced with functions that would make the model more process-based. For example, the coefficients  $a$  and  $b$  in the recession equation, and  $k$  in the Langmuir equation, very likely can be expressed as functions of soil texture or other soil physical properties. We hope that the tests reported in this paper have taken an initial step towards this direction.

As shown in Table 3, in comparison with other models, the major disadvantage of DNDC is its inability of simulating lateral flow in the soil. DNDC was developed as a site or field-scale model with a one-dimension routine to track the vertical movement of water in the soil profile. To predict N transport in the horizontal dimension at watershed or landscape scales, DNDC will need the information of horizontal water flow across the simulated grid cells, which can be produced by the spatially distributed hydrological models such as SWAT or MIKE SHE. In fact, this method for linking DNDC to the spatial hydrological models is being tested through several other projects (Zhang et al., 2002b; Cui et al., 2005; Sun et al., submitted for publication). We expect these efforts will enhance the applicability of DNDC for predicting N leaching at regional scales.

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## Acknowledgements

This research was supported by the following Swedish research foundations: Knut and Alice Wallenberg Foundation, WennerGren Foundation and Sweden-America Foundation. We thank Mr. Qingyuan Zhang for advice about statistical analysis and Dr. Liwang Ma for useful information about model comparisons.

**Appendix A. Major equations of soil climate sub-model in DNDC**

Equations	Description
$SM_{max} = 0.07T$	Daily maximum snow melt (cm)
$C_{soil} = a \frac{3450000V_{org} + 2350000V_{min} + 4180000V_{water}}{V_{soil}}$	Soil volumetric heat capacity (J/K per layer)
$K_{soil} = 86400(1 - poro)(0.0025F_{org} + 0.029F_{min}) + 0.0057poro \times wfps$	Thermal conductivity (J/cm s K)
$Q[i] = b \times K_{ave}(T[i] - T[i + 1]) / (Z[i + 1] - Z[i])$	Heat flux from layer i to layer i + 1 (J/s)
$dT = \frac{dQ[i]}{C_{soil}}$	Change in soil temperature (CircC)
$dQ_w = (4100000 - 2100000)V_{water}$	Heat release due to water freezing (J/layer)
$PI_{max} = 0.02LAI$	Daily maximum crop interception (cm)
$PET = DAY(1.6/NM)(10 \times T_m/I)^a$	Potential evapotranspiration (m/day)
$I = \sum_{n=1}^{12} (T_m/5)^{1.5}$	Coefficient for PET
$a = 0.49 + 0.07I - 7.71e^{-5}I^2 + 6.75e^{-7}I^3$	Coefficient for PET
$PT = dB \times WUE$	Potential transpiration (m/day)
$U_w = c(wfps - wiltpt)$	Actual transpiration (m/day)
$EV = PE \frac{D/0.2}{D/0.2 + e^{-2.92 - 1.43D/0.2}}$	Evaporation of soil water (m/day)
$Fd[i] = k1(water[i] - fldcap) \times 10^{(-k2/((water[i]) - fldcap)/(poro - fldcap))}$	Discharge water flow from layer i (m h <sup>-1</sup> )
$LEACHw = F1 \times Fd[bottom]$	Discharge water flow from tile system, when Fd[bottom] > 0 (m h <sup>-1</sup> )
$dPOOLi = (1 - F1) \times Fd[bottom]$	Water divided into a deep water pool when Fd[bottom] > 0 (m h <sup>-1</sup> )
$dPOOLo = F2 \times POOL[deep]$	Water released from deep water pool to tile system if FLOWd[bottom] = 0 (m h <sup>-1</sup> )
$LEACHw2 = dPOOLo$	Discharge water from tile system, when FLOWd[bottom] = 0 (m h <sup>-1</sup> )
$F1 = 2.7533clay^2 - 3.0935clay + 1.1561$	Coefficient for water distribution in deep water pool
$F2 = 0.0028clay^{-1.6216}$	Coefficient for water release from deep water pool
T	Daily temperature (°C)
V <sub>org</sub>	Volume of organic matter (m <sup>3</sup> /layer)
V <sub>min</sub>	Volume of mineral matter (m <sup>3</sup> /layer)
V <sub>water</sub>	Volume of water (m <sup>3</sup> /layer)
V <sub>soil</sub>	Volume of soil (m <sup>3</sup> /layer)
poro	Soil porosity
F <sub>org</sub>	Organic fraction of soil
F <sub>min</sub>	Mineral fraction of soil
Wfps	Water filled porosity
DAY	1/12 of the day's hours of daylight
NM	Number of days in the month
T <sub>m</sub>	Mean monthly air temperature
a	ET parameter
I	ET parameter
DB	Daily increase in crop biomass (kg ha <sup>-1</sup> )
WUE	Water use efficiency (g water/g crop)
Wiltpt	Wilting point
k1, k2	Coefficients for discharge water flow
D	Soil depth (m)
Clay	Clay fraction of soil

## Appendix B. Major equations of soil N biogeochemistry routines in DNDC

Equations	Description
$dSOC[i] = a \times F_{tm} \times k[i] \times SOC[i]$	Decomposition rate of SOC pool I (kg C/ha/day)
$dNH_4 = \frac{dSOC[i]}{R_{cn}[i]}$	Mineralization rate (kg N/ha/day)
$dUREA = [urea]DOC \times F_t \times F_m$	Hydrolysis of urea (kg N/ha/day)
$[NH_3] = \frac{[NH_4][OH]}{K_a}$	NH <sub>3</sub> concentration in liquid phase (mol/l)
$K_a = (1.416 + 0.01357T) \times 10^{-5}$	NH <sub>4</sub> <sup>+</sup> /NH <sub>3</sub> equilibrium constant
$[OH] = \frac{K_w}{[H]}$	OH <sup>-</sup> concentration (mol/l)
$K_w = 10^{(0.08946 + 0.03605T)} \times 10^{-15}$	H <sup>+</sup> concentration (mol/l)
$NH_3(g) = [NH_3(l)] \left(\frac{T}{T_0}\right)^2$	Water dissociation constant
$Flux(NH_3) = NH_3(g) \times AFPS$	NH <sub>3</sub> concentration in soil gas phase (kg N ha <sup>-1</sup> )
$NH_{4(liq)}^+ = c \times NH_{4(ads)}^+$	NH <sub>3</sub> volatilization rate (kg N/ha/day)
$c = 0.0144 \times e^{0.0981CEC}$	Free NH <sub>4</sub> <sup>+</sup> /adsorbed NH <sub>4</sub> <sup>+</sup> equilibrium
$dG = 0.0166 \left( \frac{DOC}{1+DOC} + \frac{F_m}{1+F_m} \right)$	Soil adsorption coefficient
$dD = 0.008BIO_n \frac{1+F_m}{1+DOC}$	Relative growth rate of nitrifiers
$R_n = 0.005[NH_4^+] \times BIO_n \times pH$	Relative death rate of nitrifiers
$GR_{NO_x} = F_t \times GR_{max} \frac{C}{K_c + C} \frac{NO_x}{k_n + NO_x}$	Nitrification rate (kg N/ha/day)
$dDOC = \left( \frac{GR}{Y_C} + Mc \right) BIO_d$	DOC consumption rate by denitrifiers (kg C/h)
$dNO_x = \left( \frac{GR_{NO_x}}{Y_{NO_x}} + M_{NO_x} \frac{NO_x}{N} \right) BIO_d$	Consumption rates of N oxides (kg N/h)
SOC[i]	Soil organic carbon pool i
F <sub>tm</sub>	Factor of temperature and moisture on decomposition
k[i]	Specific decomposition rate of SOC pool I
R <sub>cn</sub> [i]	C/N ratio for SOC pool i
[NH <sub>4</sub> <sup>+</sup> ]	Ammonium concentration (kg N ha <sup>-1</sup> )
[urea]	Urea concentration (kg N ha <sup>-1</sup> )
DOC	Dissolved organic carbon concentration (kg C ha <sup>-1</sup> )
F <sub>t</sub>	Factor of temperature
F <sub>m</sub>	Factor of moisture
T	Soil temperature (°C)
pH	Soil pH
AFPS	Soil air-filled porosity
Clay	Soil clay content
NH <sub>4(liq)</sub> <sup>+</sup>	Ammonium in liquid phase (kg N ha <sup>-1</sup> )
NH <sub>4(ads)</sub> <sup>+</sup>	Adsorbed ammonium (kg N ha <sup>-1</sup> )
BIO <sub>n</sub>	Nitrifier biomass (kg C ha <sup>-1</sup> )
BIO <sub>d</sub>	Denitrifier biomass (kg C ha <sup>-1</sup> )
CEC	Cation exchange capacity (kg N ha <sup>-1</sup> )
a, b, c	Constant coefficients

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