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Calibration of DNDC model for nitrate leaching from an intensively cultivated region of Northern China

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ABSTRACT

Nitrogen (N) loss through nitrate leaching in arable cropping systems in China has been recognized as one of the most common agricultural sources of groundwater contamination. The Denitrification–Decomposition or DNDC model, equipped with detailed soil hydrological and biogeochemical processes, was adopted in the study to quantify nitrate leaching for an intensively cultivated region in northern China. Several key parameters embedded in DNDC were calibrated against leaching data measured at a typical field with winter wheat–corn rotation within the target domain region. Five more sites representing the predominant cropping systems in the study region were selected for validating the modified model. In comparison with the original version of DNDC, the revised version yielded better results in simulated soil water and N leaching losses. To upscale the model simulation to regional level, we linked the validated DNDC to a regional database containing meteorological data, soil properties, vegetation types, and management practices for the target domain. Results from the regional simulation indicated that the total potential nitrate leaching load from the simulated 16.31 million ha croplands (sown area) ranged from 1.5 to 2.15 Tg N per year, with an average of 1.8 Tg N, which was equivalent to 26.1% of the total amount of N fertilizer applied in the region in 2009. The modeled results showed clear spatial patterns of nitrate leaching rates across the region due to the spatially differentiated fertilizer application rates as well as the soil water regimes. Alternative water management practices were suggested to effectively reduce nitrate leaching losses from the agricultural region in northern China.

1. Introduction

Nitrogen (N) is an essential nutrient needed to increase and maintain worldwide agricultural production. However, the overuse of N fertilizer for intensive farming and cropping systems with low N use efficiency is usually responsible for nitrate leaching into groundwater (McLay et al., 2001; Norse, 2005; Tilman et al. 2001). Groundwater contamination by nitrate is a growing problem driven by the burgeoning global population and its demand for food supplies. To meet the demand of food production, the N fertilizer consumption in China has been remarkably increased over the past 20 years. N losses through nitrate leaching in intensive farming regions in China has been recognized as one of the most common agricultural sources of groundwater contamination(Liu and Wu, 2002; Sun et al., 2008; Zhu et al. 2006). For example, Lu et al. (1998) reported that over 21.5% of wells' nitrate concentrations exceeded national standard in their analysis of 93 agricultural wells in Shaanxi province. In a survey across 14 provinces including Beijing, Shandong, Hebei, etc., Zhang et al. (1996) found that N fertilizer application rates in most counties were over 500 kg N ha^{-1}, leading to heavy groundwater contamination. This is particularly a problem in the main crop production areas in the North China Plain that is responsible for 42.5% of the total national food production, receives adequate irrigation water and fertilizers, and followed by intensive management (Bureau of Statistics of China, 2011). In this region, 73% of the cropping systems possess well developed irrigation facilities, and the average fertilizer application rates for these cropping systems were as high as 600 kg N ha^{-1} (Liu et al., 2006; Zhong et al., 2006).

Therefore, quantifying the impacts of alternative management practices on the N losses from croplands is essential for mitigating the N loading. A large number of experiments have been conducted to derive management practices to mitigate such losses, and the results indicated that appropriate fertilizer, water and soil management can minimize nitrate leaching and increase crop yields (Berstrom and Johansson, 2001; Kuo and Jellum, 2000). However, N transport and turnover processes are complex and are influenced by a number of soil and environmental variables, interacting soil water and N processes, crop uptake and management practices (Ma et al., 2007; Thompson et al., 2007; Whitmore

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and Schrader, 2007). The spatial and temporal characteristics of nitrate leaching are difficult to determine with limited field experiments. Therefore, a comprehensive process-based model is required to simulate such a complex process and to derive management practices to mitigate nitrate leaching. A list of the most widespread models to simulate crop development and nutrient transport were as follows: APSIM (Keating et al., 2003), CropSyst (Stöckle et al., 2003), DSSAT (Jones et al., 2003), DAISY (Hansen et al., 1991), DNDC (Li et al., 1992a,b; Tonitto et al., 2007), LEACHM (Hutson, 2000), NCSOIL (Molina et al., 1983), etc. However, these models originally developed upon crop growth, hydrology or biogeochemistry have their advantages and disadvantages. The hydrologic models incorporate spatial distribution algorithms for simulating water movement but usually lack detailed nutrient biogeochemical processes, while the biogeochemical models or crop models have relatively detailed nutrient turnover processes but with marginal hydrological features (Deng et al., 2011; Qiu et al., 2011). For example, DNDC model usually has a relative advantage in describing biogeochemical processes such as C and N transformations which are crucial for simulating the losses of soil N, but it equips with a simple module for movement of soil water (Li et al., 2006). As water flow and N transformation jointly control N loading in soils, it would be ideal to integrate the hydrologic process and detailed nutrient biogeochemistry into a single model framework. Nowadays, the DNDC has been modified and improved by adding new features. The modified DNDC has been enhanced to capture the magnitudes and patterns of both water flow and N leaching for the different crop systems (Deng et al., 2011; Li et al., 2006). However, it is noted that the modeled N leaching for the target region remains largely unclear because of the limited observations for model validation (Li et al., 2009). In this paper: (1) the DNDC model was calibrated for simulating water dynamics and N leaching on site scale using monitored data from a winter wheat–summer corn rotation field; (2) five more sites representing the prevailing cropping systems across the study region in northern China were selected to further validate the behavior of the revised model; and (3) the enhanced model was linked to a GIS database to upscale the potential N leaching from the farming ecosystems at regional scale. We hope that the model can be accepted to serve as a regional N leaching prediction tool that can be used for farm management planning.

2. Material and methods

2.1. Study area

The study area is located in northern China, including the entire Beijing, Tianjin city administrative area and Hebei and Shandong provinces, covering about a total area of 369,000 km^2 (Fig. 1). This region lies at 45 m to 60 m above sea level. The climate is warm and moist with plenty of sunshine and a long growing season. Annual average rainfall is 500–700 mm, with a mean temperature of 8 to 15 °C. The frost-free period is over 200 days per year. The local soils are fertile and rich in soil organic matter. The flat topography, abundant precipitation and fertile soils have made the alluvial plain favorable for agricultural cultivation. The farming systems are managed with single-cropping and double-cropping systems (i.e., two crops are planted consecutively per year),with corn, wheat, green onion and vegetables as major crops. Relying on well-established irrigation systems as well as intensive management, the agriculture in the region has been prosperous for centuries.

2.2. Model descriptions

The DNDC model adopted for the study was originally developed for predicting trace gas emissions, including the CH_4 and N_2O fluxes from upland agroecosystems (Li et al., 1992a, 1994). The core of DNDC was built up by integrating a group of biochemical and geochemical reactions commonly occurring in agroecosystems, which govern carbon (C) and N transport and transformation in the plant–soil systems. DNDC consists of six interacting sub-models for simulating soil climate, plant growth, decomposition, nitrification, denitrification and fermentation, respectively. The soil climate submodel simulates soil temperature and moisture profiles based on soil physical properties, weather, and plant water use. The plant growth submodel calculates water and N uptake by vegetation, root respiration and plant growth, and partitioning of biomass into grain, stalk, and roots. Biomass partitioning is determined by the physiological parameters stored in the crop library files. For the empirical module, the fractions of grain, leaf plus stem and root remain constant although the total biomass can vary. The decomposition submodel simulates decomposition and CO_2 production by

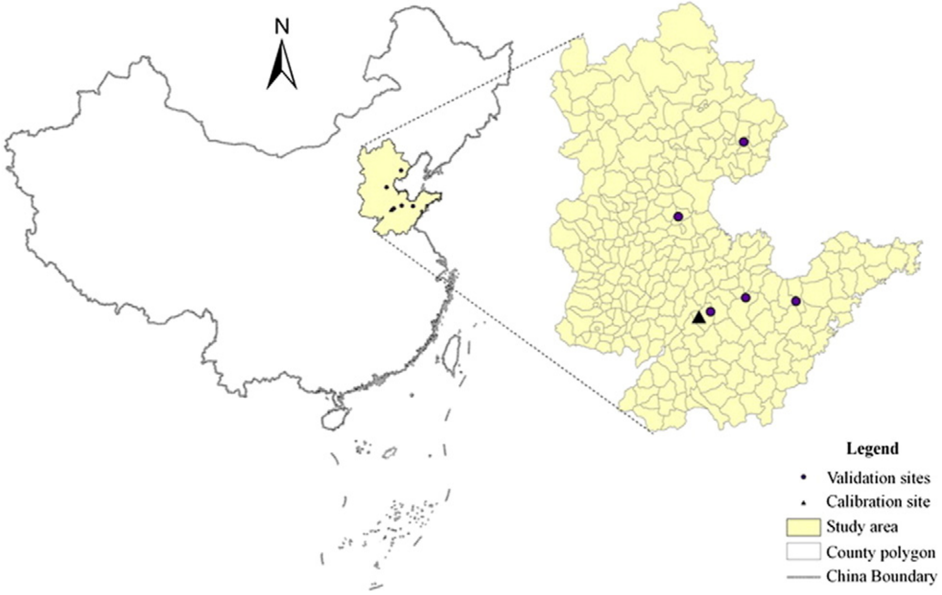

Fig. 1. Location of the study area in China and monitoring sites and counties in the study area.

soil microbes and NH_3 volatilization. The nitrification submodel tracks growth of nitrifiers and turnover of NH_4^+ to NO_3^-. The denitrification submodel simulates denitrification and the production of NO, N_2O, and N_2, whereas the fermentation submodel quantifies CH_4 production, oxidation, and transport. More details are described by Li et al. (1992a, 1994, 2006), Li (2000), Wang et al. (2008) and Qiu et al. (2009). These parameters supporting for the model running include daily climatic data (i.e., temperature and rainfall), soil property (i.e., soil density, texture, initial SOC and pH), land use (i.e., crop type and rotation system), and management practices (i.e., tillage, fertilizer, irrigation, crop residue returned rates and grass cutting).

2.3. Crop growth, water balance and N leaching in DNDC

Crop growth was estimated by using a generalized crop growth curve (Li et al., 1994). Thus the model tightly couples crop growth with soil biogeochemical and climatic components in terms of water and nitrogen uptake, water and nitrogen stress on crop growth. Crop water uptake depends on potential transpiration demand determined by LAI and climate conditions and uptake capacity determined by soil moisture, root length and its distribution in soil. Water stress factor is estimated based on the ratio of actual water uptake and potential transpiration demand. Crop N uptake depends on crop demand and uptake capacity simulated based on Godwin and Jones (1991). Crop demand is simulated based on the assumption that at any time plant has a critical N concentration below which plant growth will be reduced (Godwin and Jones, 1991). This principle is also used for estimating N stress. N uptake capacity depends on mineral N concentration in root zone and soil moisture, which are simulated by soil biogeochemical and hydrological components. Crop N pools are divided into shoot (leaf and stem), grain and root according to their input C/N ratio, biomass. Therefore, the input data include climate drivers, soil features, crop parameters and farming practices. The output includes soil C and N pools and fluxes, crop (leaf, stem, grain and root) biomass, etc. The primary time step of the simulation is 1 day.

As water moves through the soil it relocates nutrients, thus influencing the overall fertility of the soil, and when it finally leaves the root zone, nitrate and other nutrients can be leached out. Therefore, an accurate modeling of soil water dynamics is a prerequisite for accurately simulating N turnover in the soil–plant system. The soil water dynamics is calculated in the soil climate submodel of DNDC, which yields average hourly and daily soil temperature as well as moisture profiles (Li et al., 1992a; Zhang et al., 2002). The model simulates water balance by tracking all the factors that impact water movement, such as daily rainfall, irrigation, gravitational redistribution (as a downward flow), matric redistribution (an upward and a downward flow), plant interception and surface runoff, infiltration, transpiration, and evaporation. The water balance is calculated based on daily climatic input data. Throughfall is calculated depending on the interception capacity derived from vegetation biomass (leaf and wood) and Leaf Area Index (LAI). Intercepted water evaporates from the canopy according to evaporation demand. The latter is related to daily potential evaporation, which is derived by a modified Thornthwaite equation. Soil infiltration is limited by the infiltration capacity of the top soil layer (organic layer). The percolation of water within the soil profile is described by a cascading bucket model. Percolation between soil layers depends on layer specific physical properties, i.e. field capacity, wilting point, and saturated hydraulic conductivity, as well as the actual water content of two adjacent soil layers. The output of soil water content is given in per cent water filled pore space (WFPS) layer by layer (Li et al., 2006).

Soil N transformation is simulated in the decomposition, nitrification, and denitrification submodels, which contain a relatively complete suite of N transformation reactions in soils, including decomposition, nitrification, denitrification, urea hydrolysis, ammonium–ammonia equilibrium, ammonia volatilization, among others (Li, 2000; Li et al., 1992a,b). N is added as an input to the model through inorganic fertilizer and manure. The contribution of N due to atmospheric deposition is calculated from the data on daily rainfall and its N content. Similarly, the N contribution of irrigation water is calculated from the data on irrigation provided as an input to the model. Addition of N through biological fixation is empirically calculated by using a crop-dependent coefficient. As soon as NH_4^+ ions are introduced into a soil through fertilization, atmospheric deposition, irrigation or biological fixation, the ions will be readily fixed by either assimilation or adsorption. The fixed 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 NH_4^+ fixed on the adsorbents can be released through chemical equilibrium. The NH_4^+ released into the soil liquid phase can be quickly converted to NO_3^- by nitrifies. Although 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 NO_3^- to move to the leaching water flow. 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.). Both NH_4^+ and NO_3^- are subject to plant uptake and microbe assimilation. NO_3^- movement in soil solution is simulated as mass flow with water flux and diffusion driven by concentration gradient (Biggar and Nielsen, 1976). It is necessary to mention that NH_4^+ leaching is assumed to be negligible in DNDC due to the strong binding of NH_4^+ by clay minerals and organic matter.

The detailed descriptions about the hydrological equations and parameters have been reported in several former publications (e.g., Li et al., 1992a,b; Zhang et al., 2002). The major equations utilized for the water drainage and N leaching are summarized in Li et al. (2006).

2.4. Data source for model calibration

In the DNDC manual (available via the website http://www.dndc.sr.unh.edu), it suggested that for the model calibration it was necessary to firstly adjust the crop growth parameters, and then several independent parameters which did not affect other processes according to the study item. As our main interest was the water and N losses in croplands, the calibration should mainly focus on crop growth, soil physical parameters which directly affected the movement of water, and then soil chemical parameters which affected N turnover depending on the measurements. In agroecosystems, crop growth plays a key role in determining the soil water and nutrient status. Correctly simulating the crop growth is a precondition for modeling soil biogeochemical processes. Generally, the calibration of crop growth is not necessary to make any adjustments to the internal parameters or processes in the model and may be achieved by optimizing several combinations of parameters, such as the crop heat/water/N demands, growth curve, biomass partitioning, or yield. In this study, settings of dDVD, DF and FSF described in Table 1 were the key parameters adjusted to improve capability of DNDC (Ver.9.3) in simulating water movement and N turnover. Changes to dDVD determined water loss from the soil pores space within each soil layer. Estimation of N leaching required the modification of the parameter DF to calculate N leaching from upper to lower soil layers, or, of the parameter FSF to account for NH_3 volatilization ultimately determining the total amount of N leaching out of the system. A 2-year (October 2007–October 2008) field measurement was conducted at a winter wheat–summer cornfield, located in Tangwang town, Jinan city, Shandong province (36.52 N, 117.14 E) within the study area for model calibration (Fig. 1). The site was 40 m above the mean sea level with a typical semi-arid climate (yearly mean temperature 13.2 °C, annual precipitation 700.3 mm). About 80% of the precipitation occurred during the period from June to September. The experimental site was dominated by a loam soil with bulk density 1.48 g cm^{-3}, pH 7.97, total N 0.91 g kg^{-1} and initial soil organic matter (SOM) content 22.4 g kg^{-1} for the top 20 cm soil profile.

Table 1
Water and NO_3^--N leaching parameters emphasized in calibration of the DNDC model codes.

Parameters	Descriptions	Default	Tested range
DF	Desorption coefficient, directly determining the fraction of the nitrate leached rate	15	2–30
dDVD	Power function coefficient describing the amount of water that is lost from the soil pore space	0.0001	0.0001–0.002
FSF	Power function coefficient, which determines the fraction of NH_3 volatilization that ultimately affected nitrate leached from the system	0.01	0.001–0.01

The ground water table depth was 3–8 m. Two crops, corn and winter wheat, were planted in rotation within a 1-year cycle. For the purpose of model validation on crop growth, the crop field data included root, stem, leaf and grain biomass of wheat and corn at main crop growth periods. The crop samples were air dried and taken into a laboratory to test the C/N ratio and N uptake of grain, stem and root. Daily and annual measured leached water and N fluxes were used to compare with the model predictions. Lysimeter technique was used to measure leached water flows which permanently installed in three replicate of 8 by 4 m plots. In October, before planting wheat, a lysimeter was set up in each plot to collect leaching water samples once or twice per month (Fig. 2). The method is described in detail by Li et al. (2009). During the rainy season, a water sample was collected every 10 days whenever drainage occurred. The NO_3^--N and NH_4^+-N concentration in the soil solution was analyzed with a colorimetric analysis conducted by an automated flow injection analysis. Since the NH_4^+-N concentrations were negligible, the N leaching was obtained by multiplying leached water volume by the measured NO_3^--N concentrations with the water bottle located at 0.9 m depth. While water sampling, the soil samples were also collected from each plot with a 0.2 m increments, to a depth of 1 m, using a hand auger. The information of the local weather data (rainfall, daily minimum and maximum air temperatures), crop yields and farming management practices were also collected during the experimental period.

2.5. Site selection for model validation

Five more experimental sites representing the predominant cropping systems in the study area for validating the revised model were selected at Zhangqiu, Huantai, Shouguang, Luanxianand Qingxian, respectively (Fig. 1). These sites had different soil types, cropping systems and were exposed to different climatic conditions (Tables 2 and 3). The cropping systems, fertilization, and other farming management practices at the lysimeter plots were consistent with those conventionally in the area. Several crop properties required by the DNDC model were adjusted to conform to local standards, in particular actual yield, temperature degree-day (TDD), grain:stem:root ratio and the C/N ratio of grain, stem and root (Table 4). The measured items and sampling method in each site was the same as that in Tangwang site. Statistical tools such as the coefficient of model efficiency (*EF*) and the coefficient of determination (R^2) were adopted to assess the "goodness of fit" of model predictions (see details in Smith et al., 1997). The two "goodness of fit" measures were calculated separately as below:

$$EF = 1-\frac{\sum_{i=1}^{n}(Pi-Oi)^2}{\sum_{i=1}^{n}\left(Oi-\overline{O}\right)^2};\ \ R^2=\left(\frac{\sum_{i=1}^{n}\left(Oi-\overline{O}\right)\left(Pi-\overline{P}\right)}{\sqrt{\sum_{i=1}^{n}\left(Oi-\overline{O}\right)^2\sum_{i=1}^{n}\left(Pi-\overline{P}\right)^2}}\right)^2$$

Where *Oi* were the observed (measured) values, *Pi* were the predicted values, $\overline{O}$ and $\overline{P}$ were their averages and *n* was the number of paired values. A positive *EF* value indicated that the model prediction was better than the mean of observations, and the best model performance had *EF* value equal to1. The coefficient of determination (R^2) examined the correlation between model predictions and field observations.

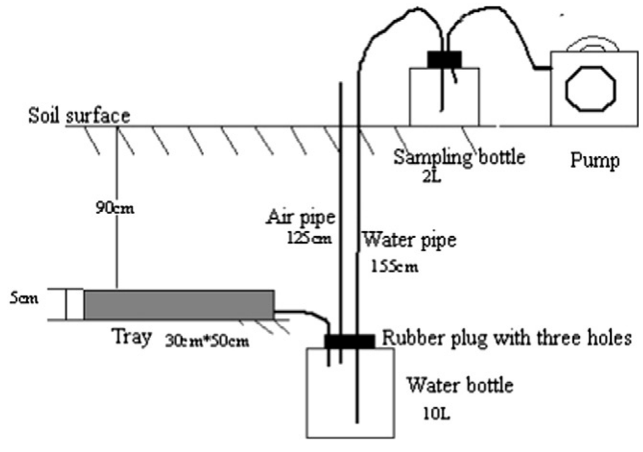

Fig. 2. The sketchmap of field lysimeters.

2.6. Sensitivity analysis of DNDC on input parameters

A sensitivity test was conducted within DNDC to find out the most sensitive input parameters for N leaching in regional simulation. DNDC was run with a 1-year baseline scenario that was based on the actual climate, soil and management conditions in Tangwang site aiming at the major cropping system (i.e., winter wheat–summer corn rotation) in the study area. The sensitivity tests were conducted by varying a single input factor in a range which was commonly observed in the local farmland practices within the county scope, while keeping all other input parameters constant as in the baseline scenario. DNDC was run with each of the scenarios to produce an annual flux of nitrate leaching for the tested site. The sensitivity order of the drivers was determined by comparing the annual nitrate leaching fluxes induced by varying each of the drivers. In order to bring the comparison into a quantitative manner, a relative sensitivity index was calculated for quantifying the impacts of the input factors on the output items based on Li et al. (2006):

$$S=\frac{(O_2-O_1)\big/O_{12}}{(I_2-I_1)\big/I_{12}}$$

Where S is the relative sensitivity index, I_1, I_2 the minimum and maximum input values tested for a given parameter, I_{12} 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_{12} is the average of O_1 and O_2. A higher S absolute value indicated that the input factors had greater impacts on the output items.

2.7. Input data for DNDC regional simulations

A major challenge in applying an ecosystem model at regional scale is assembling adequate data sets needed to initialize and run the model. Most of the Chinese agricultural statistical data were county-based so that county should be chosen as the basic geographic unit of the database to maintain the maximum accuracy of the original data sets. The datasets consisted of several sub-datasets including (1) a climate dataset, including daily weather data for 2009 (precipitation, maximum and minimum air temperature) which were acquired from 12 weather stations within the region, each county being assigned to the nearest weather station; (2) a soil properties dataset, including bulk density, clay content, initial SOC content and pH, obtained from the 1:1,000,000 Scale Soil Map of the People's Republic of China (The Office

Table 2
Climate and soil parameters [a] from the 6 selected sites for DNDC model running.

Sites	Latitude (N)	Average temp. (°C)	Annual rainfall (mm)	Soil texture	Bulk density (g/cm^3)	Soil pH	Field capacity	Wilting point	Clay fraction	Hydro-conductivity	Soil organic carbon (g kg^{-1})
Tangwang	36.52°	13.2	680	Clay loam	1.48	7.96	0.57	0.27	0.41	0.015	22.4
Zhangqiu	36.6°	12.81	600	Silty clay loam	1.68	8.33	0.55	0.26	0.34	0.016	21.9
Huantai	37°	12.5	587	Silt loam	1.42	8.58	0.7	0.5	0.14	0.0259	23.7
Shouguang	37.2°	12.7	593	Loam	1.48	7.63	0.49	0.22	0.19	0.025	18.95
Qingxian	38.6°	12.1	618	Clay loam	1.39	8.58	0.57	0.27	0.26	0.0088	23.66
Luanxian	41.1°	10.5	680.4	Sandy clay loam	1.4	7.5	0.52	0.24	0.27	0.0226	18.04

[a] Measured at 0–20 cm soil depth.

for the Second National Soil Survey of China, 1995); (3) a dataset of crop types, including physiological data of typical crops and cropping data (planting date and harvest date), maximum yield, etc.; (4) management practices dataset, including cropland acreages, sown acreages per crop, the rate and date of nitrogen fertilizer application, tilling date, crop area and fraction of above-ground residue returned into soil. All county-based agricultural census data and agricultural management practices were prepared from two sources: (a) the Agricultural Statistics Yearbook; and (b) field investigations of typical cropping areas. During the model running, DNDC performed simulation for each unit four times with the maximum and minimum values of the soil properties, full irrigation and zero irrigation, respectively. The 4 simulations produced two pairs of N leaching for each unit, which formed a range that was later used for quantifying the uncertainty generated by upscaling the simulation (please refer Li et al., 2004a,b for details of the Most Sensitive Factor method).

3. Results

3.1. Calibration of the model

3.1.1. Modeling results in Tangwang site using default parameters

Fig. 3 showed the patterns and magnitudes of the modeled and observed crop growth dynamics. DNDC model with the default parameters can generally simulate the actual fluctuations of measured root, stem, and leaf. The measured and modeled grain yields were comparable (Table 5), even though the modeled corn yield was slightly higher than the observed one. These results suggested that the default DNDC was capable of simulating crop N and water uptake in the tested field.

The comparisons of simulated and observed soil water leaching flux were shown in Fig. 4a, from which it can be seen that the DNDC model was in the correct range, and tracked the fluctuations driven by heavy rainy or irrigation event ($R^2 = 0.72$). However, simulations with the default model settings did not yield satisfying results, in that, the DNDC underestimated the amount of water losses through leaching ($EF = 0.31$), especially when the rainfall period (June to September) had about 80% of the annual precipitation. That is, the model underestimated the high water losses caused by high precipitation. Furthermore, the observed and modeled soil water contents (i.e. water filled pore space, WFPS) had large deviations (Table 5). The negative EF of −0.83 (0–20 cm soil layer) and −0.66 (20–40 cm soil layer) indicated that the default model described the WFPS data less well than the mean of the data. The model generally underestimated the soil water content in both soil layers throughout the year.

As for the N leaching, the model captured the actual peak value of measured nitrate leaching driven by application of fertilizer during the period of seedling establishment for winter wheat and jointing stage for summer corn ($R^2 = 0.62$). However, as for water loss, the model tended to underestimate the N loss ($EF = 0.18$), especially in December due to an irrigation event which was usually called the winter irrigation in China (Fig. 4b). The model failed to reflect the large N leaching loss by the irrigation event and led to a difference bigger than 16 kg N ha^{-1} (57% of the measured data, Table 5) between the observed and modeled annual data. The main reason was the strong overestimation of the N loss through NH_3 volatilization (occupying nearly half of total N fertilizer input), which resulted in few available N for leaching. Overall, the performance was poor (low EF but high R^2, Table 5), indicating that the default parameters given by DNDC may not always be suitable though the key dynamic change trends of N turnover and water processes are consistent.

3.1.2. Modeling results using modified parameters

A stepwise testing and calibration procedure on Tangwang site was applied, focusing firstly on leached water fluxes, secondly on N leaching, and finally on comparison between simulated and measured soil water content in the soil profile. Through testing the overall range of possible parameter combinations for the three parameters emphasized in our calibration (Table 1), we determined the best parameters for

Table 3
Common farming management practices for selected 6 sites in study area.

Sites	Years observed	Cropping system	Planting date (day/month)	Harvest date (day/month)	Tillage date (day/month)	Anual N fertilizer rate[a] (kg N ha^{-1})	Irrigation (mm)[b]	Manure application (kg C ha^{-1})
Tangwang	2007–2008	Wheat–corn	7/10, 12/6	10/6, 6/10	6/10	590	250	0
Zhangqiu	2008–2009	Wheat–onion	7/10, 28/6	10/6, 19/11	6/10	600	500	900
Huantai	2008–2009	Wheat–corn	9/10, 12/6	8/6, 7/10	6/10	600	250	0
Shouguang	2009	Vegetables	31/1	4/7	10/7	1450	900	6000
Qingxian	2008–2009	Wheat–corn	17/10, 16/6	14/6, 15/10	15/6	270	200	0
Luanxian	2009	Spring corn	9/5	17/9	9/5	270	0	0

Sites	N fertilizer rate per time (kg N ha^{-1})	N fertilizer application date (day/month)	Amount of irrigation (mm)	Irrigation date (day/month)
Tangwang	85, 345,70, 90	3/7, 26/7, 28/3, 6/10	50, 50, 50, 50, 50	15/6, 5/7, 28/7, 28/3, 25/11
Zhangqiu	59, 30, 100, 100, 110, 70, 96	27/6, 12/8, 28/8, 10/9, 23/9, 28/3, 16/10	50, 80, 100, 100, 100, 70	28/3, 25/8, 7/9, 1/10, 25/10, 25/11
Huantai	80, 350, 80, 90	1/7, 27/7, 1/4, 9/10	50, 50, 50, 50, 50	15/6, 5/7, 28/7, 28/3, 25/11
Shouguang	600, 85, 85, 85, 85, 85, 85, 85, 85, 85, 85,	25/1, 29/2, 27/3, 7/4, 15/4, 20/5, 8/9, 28/9, 7/10, 14/10, 20/11	90, 90, 90, 90, 90, 90, 90, 90, 90, 90, 90	25/1, 29/2, 27/3, 7/4, 15/4, 20/5, 8/9, 28/9, 7/10, 2/11, 20/11,
Qingxian	85, 50, 85, 50	16/6, 17/7, 27/3, 16/10	50, 50, 50, 50	16/6, 17/7, 27/3, 16/10
Luanxian	170,100	8/5, 9/7	0	–

[ab] The timing and amount of irrigation and N applications.

Table 4
Summary of input data of crop properties for the DNDC model from the 6 sites.

Crops	Grain yield (kg C ha^{-1})	Grain: stem: root (%)	C:N grain	C:N stem	C:N root	TDD (°C)
Winter wheat	3200	50: 45: 5	20	82	75	1900
Summer corn	4200	45: 50: 5	50	120	200	2000
Green onion	3600	1: 97: 3	10	30	27	2200
Tomatoes	6000	70: 29: 1	20	15	15	2000
Spring corn	4200	45: 45: 10	50	80	80	2200

dDVD = 0.002, FSF = 0.008, DF = 15 that improved the simulated water and N leaching rate, while did not affect the crop growth dynamics. The DNDC model performed much better within the new parameters than that with the default ones for both N leaching and water losses. The model results using the modified parameters yielded a satisfying *EF* value = 0.72 for nitrate leaching and 0.78 for water losses. After calibration,theR^2 values for total nitrate leaching and water flow losses improved to 0.93 (n = 12) and 0.91 (n = 12), respectively. The optimization of the FSF value generally decreased simulated NH_3 volatilization, and thus increased the estimation of N content remaining in the soil. Therefore, the calibration to DNDC reduced the maximum difference between modeled and measured value from about 16 to 4 kg N ha^{-1} for nitrate leaching, and results of seasonal water losses were in a much better agreement between simulations and measurements. Furthermore, optimized DNDC default parameters increased the modeled soil water content, which showed a good agreement with the measurements in different soil layers: the values of EF increasing to 0.56 (0–20 cm soil layer) and 0.84 (20–40 cm soil layer), and R^2 to 0.67 and 0.85, respectively. These results generally indicated that the revised model improved applicability to reproduce the variation of water losses and N leaching rates in the tested fields compared with the original DNDC model.

3.2. Validation of the model from other 5 sites

Table 6 compared the crop yield, annual N leaching and water losses predicted by the revised DNDC model with field observations for 29 samples from the tested 5 sites. The modeled yields of wheat and corn were in agreement with observations for all the sites, with deviation ranging from 4% to 12%. This indicated that the calibration DNDC was still capable of simulating crop N and water uptake in the tested fields. For the N leaching rates, the highest N losses were observed at two fields (i.e., Shouguang and Zhangqiu) with the highest N fertilizer application rates, implying that N fertilizer was an important factor for N leaching. In most cases, the revised DNDC model showed an acceptable agreement with the observed losses, because it explicitly calculated the amount of water that was lost from the soil pore space (Table 6). Conversely, the predictions of the original model deviated from the observed losses by up to 200% (data not shown). Similarly, the revised model showed significantly higher correlation with observation than did the original model. The model performance measures of R^2 and EF were improved with values ranging from 0.45 to 0.91 (Fig. 5a–h). The simulations could explain more than 50% of the variation of the measurements of water and N leaching for the 5 sites. However, for the vegetables field of Shouguang site, simulations tended to slightly underestimate N leaching losses (13%), but could explain about 60% of their variation (Fig. 5f). The simulations of N leaching for other sites mostly matched the measurements despite the underestimation. Overall, the revised DNDC had improved applicability of simulating N leaching from different cropping agricultural fields compared with the original DNDC model.

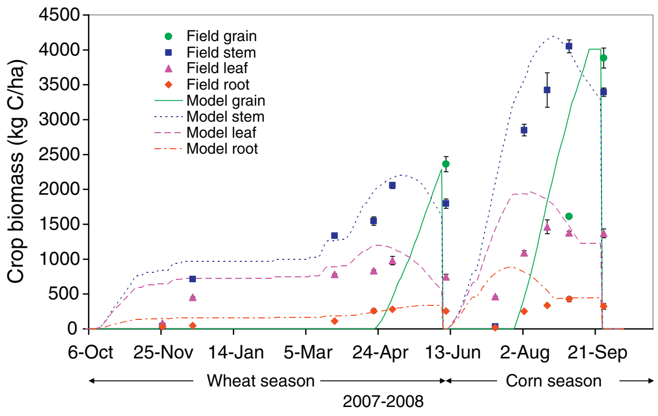

Fig. 3. The patterns and magnitudes of the modeled and observed (means and standard errors, n = 3) crop growth dynamics, including the root, stem, leaf and grain dynamics, during one whole winter wheat and summer maize rotation period.

3.3. Sensitivity tests

Table 7 presented the calculated sensitivity indices for the impacts of the main environmental factors (i.e. precipitation, SOC content, fertilizer rate, and so on) on N leaching. The results in Table 7 indicated that the fertilizer rate had the greatest impact on soil N leaching. N fertilizer application elevated N storage in the adsorption pool and hence increased the potential of N leaching. This model result was highly consistent with field studies performed in the same region by Sun et al. (2008) and Li et al. (2004a,b). Moreover, the soil N leaching rate was most sensitive to soil porosity, irrigation and precipitation by increasing the volume of draining water and favoring water drain to the soil layer below. The results were also in agreement with observations reported by other researchers (Struthers et al., 2007, Wang et al., 2001, 2005; Yan et al., 2006). The sensitivity test may provide crucial information for regional simulations as we know which input parameters could most sensitively affect the modeled results and hence should be paid with the greatest considerations.

Table 5
Measured (means and standard errors, n = 3) and modeled yields of winter wheat and summer corn and cumulative N leaching in Tangwang site. Statistics on the measured and modeled soil water dynamics and N leaching are also given. Modeled data include default and calibration results.

	Measured	Model-default	Model-calibration
Yields			
Winter wheat grain (kg C ha^{-1})	2361.1(107.9)	2288.76	2301.84
Summer corn grain (kg C ha^{-1})	3882.1(143.24)	4007.62	3901.25
Water losses			
Leached water (mm)	176.49(29.9)	116	170
EF (Water)	–	0.31	0.78
R^2 (Water)	–	0.72	0.91
N leaching rates			
Cumulative N leaching (kg N ha^{-1}/year)	38.76(6.35)	22.1	42.3
EF (N leaching)	–	0.31	0.72
R^2 (N leaching)	–	0.62	0.93
Soil water			
Mean WFPS(%) for 0–20 cm layer	52.37	41.46	49.3
EF (WFPS)	–	−0.83	0.56
R^2 (WFPS)	–	0.55	0.67
Mean WFPS (%)for 20–40 cm layer	51.59	42.23	51.53
EF (WFPS)	–	−0.66	0.84
R^2 (WFPS)	–	0.76	0.85

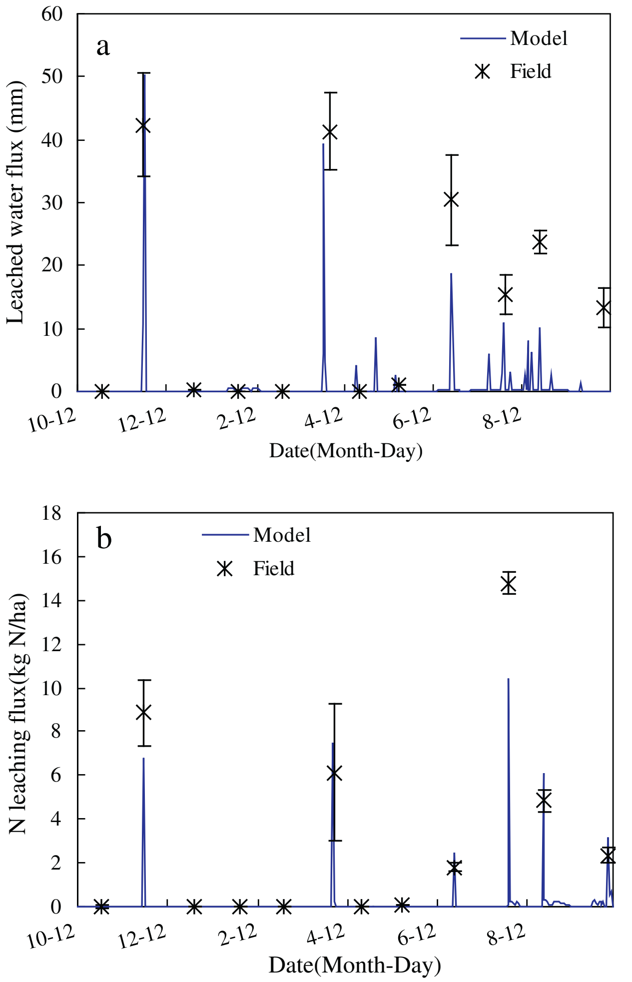

Fig. 4. Comparisons of modeled and measured soil leached water flux (a) and N leaching (b) with default DNDC parameters. The fluctuations of the amount of leached water and N leaching were driven by heavy rainy or irrigation event. Measured values are the mean values of three replicates. The vertical bars represent standard errors.

3.4. Upscaling of N leaching from northern China plain regions

The results from the model using the maximum and minimum soil properties indicated that the total nitrate leaching from the simulated 16.31 million ha croplands (sown area) ranged from 2.08 to 2.15 Tg N under full irrigation conditions, at a range from 127.66 to 132.12 kg N ha^{-1}(Table 8). Shifting the abundant irrigation to the zero irrigation conditions reduced the regional N leaching to 1.5–1.55 Tg N (91.97–94.88 kg N ha^{-1}) per year, implying that the water management change in northern China drastically reduced nitrate leaching loss in the year 2009 (Table 8). These 4 simulations from different conditions hence formed a range from 1.5 to 2.15 Tg N, with an average of 1.8 Tg N, equating to approximately 26.1% of total amount of N fertilizer input (including chemical and organic fertilizer).

In addition, simulated N leaching rates per hectare in the year 2009 varied between 0 and 1585 kg N ha^{-1}, with a mean value of 111.6 kg N ha^{-1} (Table 8). Spatial patterns of N leaching showed a sharp discrepancy among these countries. The variability could be explained mostly by N fertilizer application rates (Fig. 6). High N leaching rates of up to >300 kg N ha^{-1} were simulated mainly for regions with greenhouse vegetable croplands in the city suburb, which were all characterized by high N fertilizer application (with average fertilizer application of 902 kg ha^{-1}) and high water irrigation. The low N leaching of <50 kg N ha^{-1} was identified in the north areas where the low chemical N fertilizer input (with average fertilizer application of 202 kg ha^{-1}), insufficient irrigation facilities and the poor soils limited the crop yields and biomass production, and hence resulted in the decrease of the amount of organic N returned to the fields by the straw amendments. For all other areas, leaching rates mostly ranged 50–150 kg N ha^{-1}. In these counties where agricultural production was intensive (with an over N input and high N surplus), double-cropping systems (such as winter wheat/summer corn rotation system) obtained more N fertilizer input (with annual average fertilizer application of 600 kg ha^{-1}) to sustain the relatively high crop yields. Besides, irrigation facilities were well-equipped because of the relatively developed economy that could provide sufficient irrigation water for the prevailing cropping systems. Based on the condition of abundant irrigation and fertilizer application, the N leaching in most of the east counties reached or exceeded the whole regional average level. Therefore, it required to assess the effects of N fertilizer rates and irrigation on N leaching losses and find suitable policies and measures for those important regions in China to minimize potential impacts on groundwater.

4. Discussion

4.1. Validation and calibration

The calibration in this study may have been required because of uncertainties in the new systems or environments. For instance, different

Table 6
Measured (means and standard errors, n = 3) and modeled yields, N leaching rates and water leached losses in five other sites. Statistics on the measured and modeled soil water dynamics and N leaching are also given. Modeled data refer to the calibration results.

Sites	Zhangqiu		Huantai		Shouguang		Qingxian		Luanxian	
	Measured	Model	Measured	Model	Measured	Model	Measured	Model	Measured	Model
Yields										
Winter wheat (kg C ha^{-1})	2513.56 (27.32)	2408.21	2094.33 (39.51)	2288.76	3064.73 (40.66)	2641.72	2012.54 (40.36)	2198.98	4136.89 (235.7)	3825.3
Green onion[a] (kg C ha^{-1})	2498.7 (106.78)	2199.4	3735.43 (163.05)	3847.2			3554.32 (163.05)	3341.2		
N leaching										
N leached rates (kg N ha^{-1}/year)	34.67 (4.22)	34.02	1.50(0.46)	1.538	214.04 (29.5)	190.18	1.39 (0.29)	1.29	0.63(0.04)	0.58
EF(N leached)	–	0.62	–	0.46	–	0.44	–	–	–	–
R^2 (N leached)	–	0.63	–	0.49	–	0.58	–	0.7	–	–
Water leached										
Water (mm)	259.18 (47.26)	256.26	45.93 (12.9)	40.51	332.42 (51.37)	304.16	25.74 (6.31)	27.645	4.25(1.08)	2.88
EF (water)	–	0.55	–	0.73	–	0.52	–	–	–	–
R^2 (water)	–	0.59	–	0.77	–	0.57	–	0.91	–	–

[a] Noted that the Yields refer to Green onion yield at Zhangqiu, Summer corn yield at Huantai, Vegetable(Tomato) yield at Shouguang, Summer corn yield at Qingxian, Spring corn yield at Luanxian.

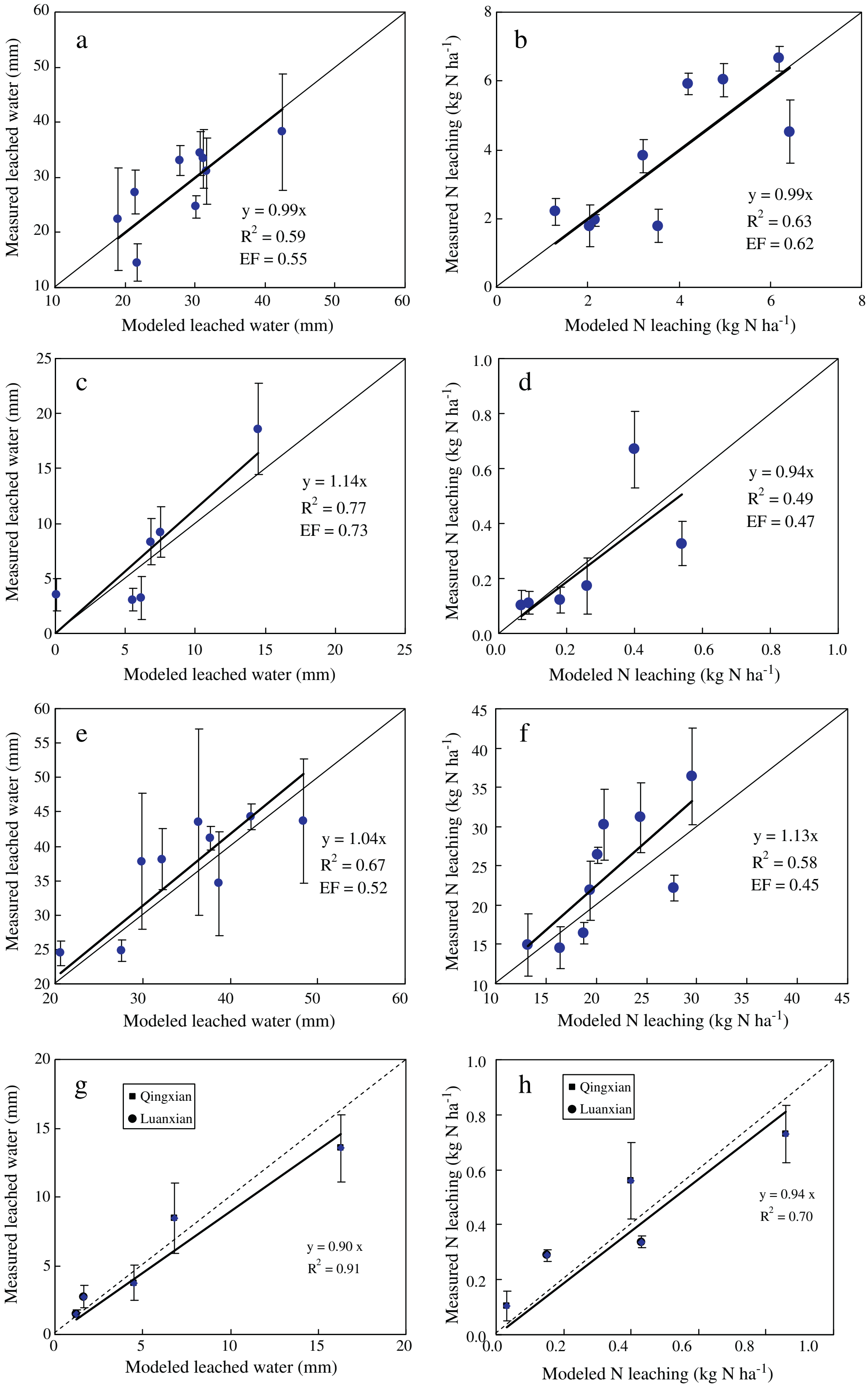

Fig. 5. Simulated and measured leached water and N leaching in 5 different cropping systems at 5 representative sites in the study region (a, b: Zhangqiu; c, d: Huantai; e, f: Shouguang; g or h Qinxian and Luanxian) for the years 2008–2009, including results of a linear regression of the measured (y) versus modeled (x) leached water and N leaching, and the coefficient of determination (R^2) as well as model efficiency (EF). Measured values are the mean values of three replicates. The vertical bars represent standard errors.

Table 7
Sensitivity indices (*S*) of different input parameters.

Parameters	Baseline	Range tested	Sensitivity index (*S*)
Precipitation (mm/year)	672	538–806	1.06
SOC content (kg C/kg)	0.013	0.003–0.052	0.93
Field capacity (wfps)	0.57	0.47–0.67	0.81
Hydro-conductivity (m/h)	0.01	0.005–0.02	0.48
Wilting point	0.27	0.17–0.37	0.27
Soil porosity	0.476	0.376–0.576	1.60
Fertilizer rate(kg N ha^{-1})	596	298–596	2.22
Irrigation (mm)	250	150–350	1.20

crop systems may largely affect soil N uptake and water dynamics, and thus lead the inaccuracy estimation of N leaching rates by the model. Many researchers suggested that the DNDC model should be calibrated and validated for predicting these key biogeochemical processes such as the long-term change in soil organic carbon (SOC), water dynamics, and nitrate leaching. Smith et al. (1997) reported poor modeling efficiency for SOC dynamics for a broad range of models applied to agricultural data sets. Kröbel et al. (2010) found that the simulated results of water dynamics were not satisfied using default parameters. Tonitto et al. (2007) applied the DNDC model to a typical corn–soybean rotation system in east-central Illinois, and reported that accurate simulation of nitrate leaching and drainage dynamics required significant changes to key soil physical and chemical parameters relative to their default values. They further reported that calibration of DNDC resulted in a good statistical fit between simulated and measured crop yield, nitrate leaching, and drainage. In this study, the initial discrepancies led to two major parameters modifications namely dDVD and DF, and the overestimation of NH$_3$volatilizationby the model led to parameter FSF modification. The modified model successfully predicted downward water flow and was able to simulate the daily dynamics of N losses via drain flow in different cropping systems in the study area. Whereas we were encouraged by the recent improvement to DNDC for nitrate leaching estimation, there were still limitations for widespread application of this tool. Firstly, model validation on regional scale was always problematic data scarcity on regional scales. Secondly, soil heterogeneity would be the major obstacle for applying the model across sites. For example, we optimized the default parameters related to key soil physical and chemical processes for the selected region, but the values may not be applicable to other regions with different soil and climate conditions. If the simulations were not satisfied in a new site, the tests to verify or modify the parameters were still needed to be carried out. Since the codes for the DNDC model were not open, the calibration of the model by modifying the default values in the codes may be impossible. To eliminate this inconvenience in the future, we will continue testing the model against more observations across climate zones, soil types, and management regimes. The key parameters very likely could be expressed as functions of soil texture or other soil physical properties. Thirdly, the modified model, however, still slightly underestimated soil water content in topsoil probably due to an overestimation of the water loss by evaporation and/or more likely uncertainties in model process with respect to the potential evapotranspiration. Kröbel et al.(2010) also found inaccuracies in the calculation of the flow of soil water and concluded that the evapotranspiration model approach used by the DNDC model was unsuitable, but unfortunately we did not have evaporation measurements available. Therefore, the model performance still had a large space to be improved according to the measures of R^2 and *EF*. Fourthly, the sensitivity tests were designed only for observing several basic behaviors of the modified model but not for thoroughly evaluating impacts of all environmental or management factors on soil N leaching. For example, soil N leaching rate could be affected by tillage management and cropping system (Ma et al. 2007; Thompson et al. 2007). Therefore, more alternative scenarios including the change of soil texture, pH, and management practices, and so on, should be applied to test the model's performance in future study. We hope that the tests reported in this paper have taken an initial step for model further application.

Table 8
Annual N leaching from study area fields under full irrigation and zero irrigation practices.

Parameter	Full irrigation		Zero irrigation	
	[a]Maximum	[b]Minimum	Maximum	Minimum
Total N leaching (Tg N)	2.08	2.15	1.5	1.55
Per unit area N leaching (kg N ha^{-1})	127.66	132.12	91.97	94.88

[a] Scenarios for maximum soil properties: maximum of SOC, pH and bulk density and clay content of soil.

[b] Scenarios for minimum soil properties: minimum of SOC, pH and bulk density and clay content of soil.

4.2. Uncertainties of regional results

While we were encouraged by the improvement to DNDC for nitrate leaching estimation, we realized that there were still limitations for upscaling application of this tool. Uncertainties mainly associated both with the quality of the available input data and the hydro-biogeochemical processes in the model.

Firstly, the variance in the input parameters could introduce high potential uncertainties just as shown by the sensitivity analysis. For instance, the initial soil properties database derived from the Second National Soil Survey, may not exactly represent the current soil status, especially for the soil porosity which was one of the most sensitive factors influencing water dynamics. However, the datasets at county level used in this study were the best ones currently available. In addition, the input parameters required by the DNDC model such as the sowing areas, fertilizer rates and farm management practices were derived from the statistical data reported by the Ministry of Agriculture, China, but unfortunately the data did not have practical irrigation rates and time, especially the sowing areas, fertilizer application rates and the amount of irrigation for greenhouse vegetables systems. The data from common vegetable systems substituted for greenhouse vegetable systems and irrigation index in database substituted for irrigation rates and areas inevitably differed from the practical situation, which could cause uncertainties for the county-scale simulations.

Secondly, the limitations of modeling approaches are likely sources of uncertainties. Firstly, the regional results are obtained on the basis of the presetting that all of the attributes in each model grid cell (country) are uniform, whereas it is actually impossible. For instance, soil properties (e.g., texture, SOC content, pH) and crop management practices are highly variable in space. Averaging the variations of the soil properties may not resolve the complexity as the correlation between water dynamics and any of the soil properties is nonlinear. Li et al. (1992a,b, 1994, 2004a,b) developed the most sensitive factor (MSF) method for solving the problem in regional applications of DNDC. According to the sensitivity tests in this study, the MSF were the soil porosity and irrigation. On the basis of this method, we constructed the soil databases with the range values (i.e., maximum and minimum porosity) and the irrigation practice with two values (i.e., full and zero irrigation) for each county. Therefore, when modeling N leaching in the full irrigation condition for a county, DNDC will automatically select the minimum porosity (with maximum SOC content, maximum pH, and maximum clay fraction) to form a scenario, which is assumed to produce a low value of N leaching rates, and then select the maximum porosity (with minimum SOC content, minimum pH, and minimum clay fraction) to form another scenario, which is assumed to produce a high value of N leaching rates for the county. Thus DNDC will run twice with the two scenarios for each county to produce two N leaching rates in the condition of full irrigation, and again produce other two N leaching rates in the condition of zero irrigation. The four simulations producing two pairs of N leaching rates will form a range, which is assumed to be wide enough to cover the “real” rates with a high

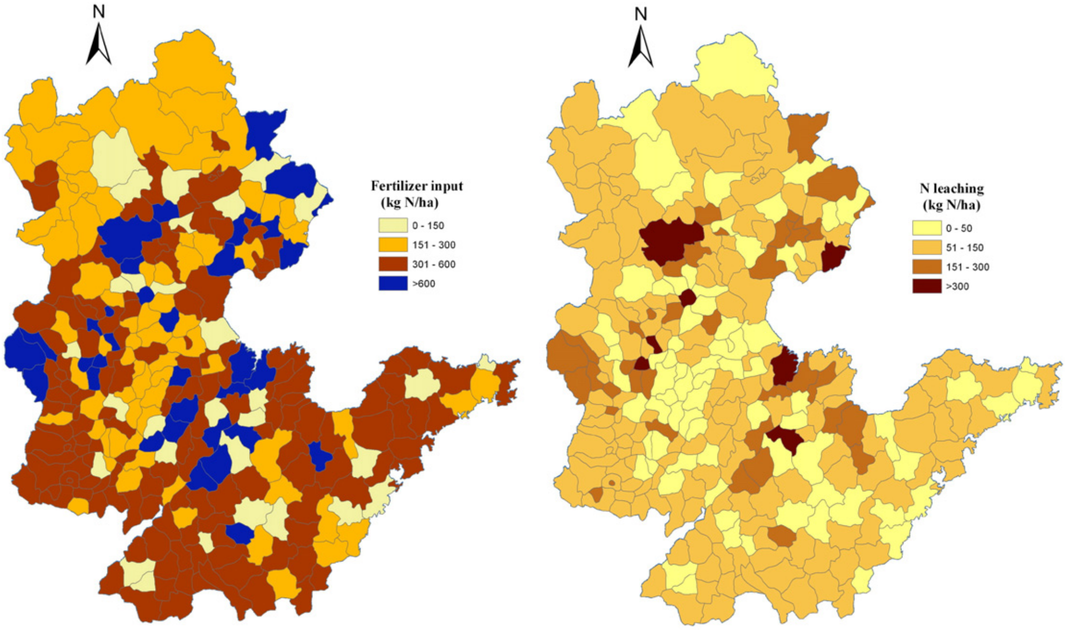

Fig. 6. Regional pattern of county-based total N fertilizer input and average N leaching rates (kg N ha^{-1}) from an intensively cultivated region in north China for the year 2009.

probability. Secondly, currently DNDC does not allow for a crop to seed in the last year. For this reason, we were unable to seed winter wheat in the previous year, which was a practice commonly used by farmers. The inability to accurately simulate these practices is a potential source of yield reductions, as there is little time for wheat to grow following corn harvest, and hence probably lead the overestimation of water losses and its consequent N leaching rates. Therefore, refining crop database is required.

Thirdly, this study only simulated water and nitrate movements in the vertical dimension, but did not consider horizontal water surface runoff since the study area was flat. This likely led to an increase in the leached water. In the DNDC calculation, working with more leached water would probably lead to an overestimation of the total N leaching.

4.3. Controlling policies

With the consumption of N fertilizer in China increasing substantially in recent decades, the environmental significance of N loss by leaching has attracted more attention. Through the modeling predictions in this study, N leaching losses from croplands may lead to great potential negative impacts on groundwater in northern China plain. The results implied that there was a great potential to reduce the N leaching from agricultural fields. The spatial distribution analysis of N leaching showed a sharp discrepancy between different counties due to the differences in climatic conditions, soil properties, and farm management practices (e.g., fertilization, irrigation, manure application, crop rotation). Therefore, we suggested that the future policies for optimizing agricultural management need to account for the local climate–soil conditions in a more precise way. Considering the pollution controlling cost, applying management alternatives, such as proper fertilizer application and water management, could be more efficient for decreasing N leaching rates. In addition, China needs a long-term policy based on scientific analysis to protect its soil resources to maintain soil fertility, sustainable yield, and environment safety. This requires more efforts in the future. We hope this paper will fuel more interest in this research area.

5. Conclusions

Our validation of the revised DNDC model using field-scale data demonstrated that the revised model predicted N leaching from croplands in northern China more accurately than the original model. The modified model had maturity description in N leaching because it successfully predicted downward water flow and was able to simulate the daily dynamics of N losses via drain flow in different cropping systems. At present, however, there were still limitations for widespread application of this tool in other region because of the uncertainties from spatial variations (e.g., precipitation and irrigation). For regional application of the model, further studies will be needed to lessen the uncertainties in input parameters for soil properties and field management (e.g., water regime). These studies will make the revised model an increasingly useful tool for predicting N leaching and evaluating practical mitigation options for croplands in China.

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