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Simulating agroecosystem soil inorganic nitrogen dynamics under long-term management with an improved SWAT-C model

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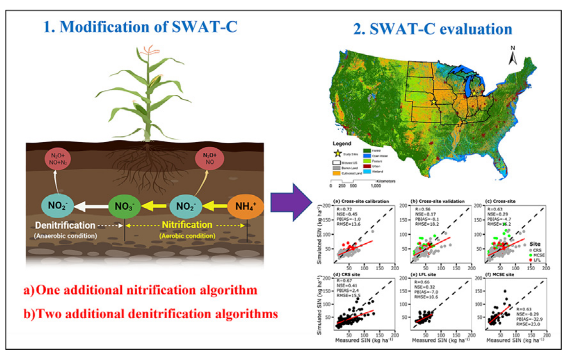
HIGHLIGHTS

- We incorporated new nitrification denitrification algorithms into the SWAT-C model.
- Newly added algorithms help achieve much improved performance for simulating soil inorganic nitrogen.
- The revised SWAT-C model captured the impact of fertilization, crop rotation, and tillage on soil inorganic nitrogen.
- The revised SWAT-C model will serve as a useful open-source tool to inform N management for agroecosystem sustainability.

GRAPHICAL ABSTRACT



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ABSTRACT

Despite the extensive application of the Soil and Water Assessment Tool (SWAT) for water quality modeling, its ability to simulate soil inorganic nitrogen (SIN) dynamics in agricultural landscapes has not been directly verified. Here, we improved and evaluated the SWAT–Carbon (SWAT-C) model for simulating long-term (1984–2020) dynamics of SIN for 40 cropping system treatments in the U.S. Midwest. We added one new nitrification and two new denitrification algorithms to the default SWAT version, resulting in six combinations of nitrification and denitrification options with varying performance in simulating SIN. The combination of the existing nitrification method in SWAT and the second newly added denitrification method performed the best, achieving *R*, *NSE*, *PBIAS*, and *RMSE* of 0.63, 0.29, −4.7 %, and 16.0 kg N ha^{-1}, respectively. This represents a significant improvement compared to the existing methods. In general, the revised SWAT-C model's performance was comparable to or better than other agroecosystem models tested in previous studies for assessing the availability of SIN for plant growth in different cropping systems. Sensitivity analysis showed that parameters controlling soil organic matter decomposition, nitrification, and denitrification were most sensitive for SIN simulation. Using SWAT-C for improved prediction of plant-available SIN is expected to better inform agroecosystem management decisions to ensure crop productivity while minimizing the negative environmental impacts caused by fertilizer application.

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1. Introduction

Globally, excess nitrogen (N) application in agroecosystems is a leading cause of worldwide environmental problems, such as surface and subsurface water quality degradation and trace N gas emissions (Hashemi et al., 2016; Hoben et al., 2011; Padilla et al., 2018). Numerous agricultural conservation management practices such as crop rotation, conservation tillage or no-till, reduced fertilizer, and cover crops have been applied to improve nutrient use efficiency (NUE) in corn (*Zea mays* L.) production systems in the U.S. Midwest (Hess et al., 2020; Robertson and Hamilton, 2015; Sanchez et al., 2004). In spite of the proven effectiveness of conservation management practices for optimizing crop NUE (Dinnes, 2004; Dunn et al., 2011; Pandey et al., 2018), the selection of appropriate site-specific practices to curtail nutrient loss remains challenging because of the variability in local climate, as well as site-specific settings such as soils, topography, management, and genetics (Hansen et al., 2017; Liang et al., 2020; Ouyang et al., 2013). Predicting the potential benefits of using multiple conservation management practices and their environmental impacts is complex and cannot be exhaustively tested via field experiments (Robertson et al., 2011). As such, modeling approaches have often been used by researchers and decision makers as a proxy for field-based evidence to support sustainable agricultural management for productivity, climatic, environmental, and social goals (Hood et al., 2019; Rabotyagov et al., 2014; Zhang et al., 2010; Zhang et al., 2015).

Soil inorganic nitrogen (SIN) in agroecosystems is highly dynamic because the cycling of SIN is affected by the interplay of management decisions with multiple complex biophysiochemical processes (e.g., mineralization/immobilization of soil organic matter (SOM), plant uptake, nitrification, denitrification, volatilization, and leaching) (Robertson and Groffman, 2023). Effective evaluation of the long-term interaction between land management and SIN dynamics under a wide range of climate, soil, and management conditions is crucial for improving N fertilization recommendations and reducing N loss risks from agricultural soils. Moreover, SIN estimates can be valuable for parameterizing other models that use SIN as input parameters. For example, Saha et al. (2021) fed SALUS (Basso and Ritchie, 2015) estimated daily SIN to a machine learning model to improve the performance of daily nitrous oxide (N_2O) fluxes simulation. However, the accurate estimation of SIN dynamics remains challenging due to the complex nature of N cycling in agricultural soils. The quantification of SIN relies on process-based models by extrapolating field experimental results to a wider range of management and climate scenarios, and larger scales (Banger et al., 2019; Franqueville et al., 2018; Robertson et al., 2007).

An extensive list of process-based models has been developed with the capabilities to study SIN dynamics in agricultural landscapes. These models offer the potential to quantify the contribution of an individual process to the entire system and help to understand how environmental conditions combined with land management practices interact with N cycling. The N cycling related algorithms in these models range from simple empirical relationships to complex mechanistic algorithms. For example, the field scale model LEACHM (Leaching Estimation and CHemistry Model) (Hutson and Wagenet, 1989) uses first-order reaction functions to estimate N mineralization, nitrification, and denitrification processes. Johnson et al. (1999) suggested that the LEACHM model severely underestimated or overestimated soil nitrate (NO_3^--N) and ammonium (NH_4^+-N) due to the unrealistic hydraulic properties and N mineralization rate constants determined through laboratory experiments. The DSSAT (Decision Support System for Agrotechnology Transfer) model (Jones et al., 2003), allows the simulation of N balance while the embedded CERES-Maize (Jones, 1986) model accounts for water and N availability effects on photosynthesis, leaf expansion, and other corn yield determinants. Even though the DSSAT model can predict corn yield reasonably well, it is still a challenging task for the model to simulate SIN under multi-site and multi-treatment conditions (Banger et al., 2018; Banger et al., 2019). The DNDC (DeNitrification DeComposition) model (Li et al., 1992) uses a microbial growth model to allow nitrification and denitrification to occur simultaneously in aerobic and anaerobic microsites (Li et al., 2000). The DNDC model was successfully applied to predict soil NO_3^--N in a single study site (Chirinda et al., 2010; Kim et al., 2014), but the model performance decreased substantially when multiple sites with diverse climatic, soil, and management conditions were involved (Molina-Herrera et al., 2016). In the APSIM (Agricultural Production System Simulator) (Keating et al., 2003) and SWAT (Soil and Water Assessment Tool) (Arnold et al., 1998) models, the processes of nitrification and denitrification are described via empirical reaction equations with the consideration of key environmental factors such as soil temperature and soil water. However, the lack of volatilization routines in APSIM can potentially lead to the overestimation of SIN (Archontoulis et al., 2014). Archontoulis et al. (2014) also point out that site-specific calibration strategies may be needed to accurately reproduce SIN dynamics, such as initializing the model with a warm-up period before the targeted study period to stabilize SOM pools. Despite the extensive modeling efforts in SIN estimation, quantifying SIN is still very challenging because of the large spatial and temporal variability of N cycling processes. Notably, it is even more challenging to accurately predict N fluxes in crop rotations than in monoculture (Yin et al., 2020) and in tilled soils than in no-tilled soils (Oorts et al., 2007).

The SWAT model has been widely applied to examine water quality problems across the globe (Wellen et al., 2015), particularly in agricultural watersheds to explore sustainable agricultural management practices to improve N utilization efficiency and mitigate N pollution. Despite the >4000 peer-reviewed journal articles (https://www.card.iastate.edu/swat_articles/) that have reported the SWAT model applications for water quality modeling and assessment (Cherry et al., 2008; Fu et al., 2019; Gassman et al., 2007; Hashemi et al., 2016; Ouyang et al., 2008), this model has not been directly verified for simulating dynamics of SIN (i.e., NO_3^--N and NH_4^+-N) stocks in agricultural soils. Given the wide use of SWAT in supporting sustainable agricultural and water quality management, including the U.S. Department of Agriculture's Conservation Effects Assessment Project (CEAP) (Richardson et al., 2008) and U.S. Environmental Protection Agency's Better Assessment Science Integrating Point and Non-Point Source (BASINS) program (EPA U, 2019), there is an urgent need to assess this model's capacity to simulate SIN under diverse cropping systems.

As one of the most intensive agricultural production regions in the world, the U.S. Midwest hosts >85 %, 80 %, and 50 % of total corn, soybean, and wheat production, respectively, in the U.S. (NASS, 2021). In addition, the U.S. Midwest is home to over 80 % of domestic biorefineries and likely will undergo further development to support bioenergy production (Zhang et al., 2021). A major persisting issue is the excess input of N fertilizer and its low utilization efficiency by crops, which has resulted in a substantial amount of N losses to the environment through leaching, runoff, and gaseous emissions (Robertson and Vitousek, 2009; Tilman et al., 2002; Tilman et al., 2001). For example, N loss from the Upper Mississippi River Basin (UMRB) has been identified to be the major contributor of N load to the Gulf of Mexico due to the intensive agricultural activities in the U.S. Midwest (David et al., 2010; McLellan et al., 2015). To mitigate the hypoxia in the Gulf of Mexico and reduce GHG emissions, efficient N management in agricultural production systems in the U.S. Midwest is urgently needed. Since soil is the largest source of active N, accurate prediction of SIN is essential for assessing measures for efficient N utilization, mitigating N loss, and developing effective agricultural management practices.

The major objective of this study is to improve and evaluate the performance of the SWAT-Carbon (SWAT-C; https://sites.google.com/view/swat-carbon) model under prevailing cropping systems in the U.S. Midwest, which is a globally significant breadbasket and the major contributor to water degradation in the Mississippi River Basin and the Gulf of Mexico (David et al., 2010; McLellan et al., 2015). Specifically, we aim to: (1) extend the capability of the SWAT-C model in simulating the turnover of SIN with new nitrification and denitrification algorithms; (2) examine the sensitivity of SIN simulations to the existing and newly available methods representing nitrification and denitrification processes; and (3) evaluate the overall performance of the SWAT-C model in simulating long-term SIN dynamics in agricultural soils in the U.S. Midwest.

2. Materials and methods

2.1. Existing and new nitrogen cycling algorithms in SWAT-C model

The SWAT-C model divides a watershed into subbasins then subdivides subbasins into hydrologic response units (HRUs), representing unique combinations of homogenous soil, slope, and land use. The SWAT-C model simulates N cycling in the soil profile through processes such as mineralization, immobilization, plant uptake, leaching, nitrification, and denitrification in each HRU. It also determines the amount of N loading to the main channel through processes such as surface runoff, lateral flow, leaching, and groundwater transport in each subbasin. The N cycle in the land phase is a dynamic process that involves the interaction of soil, water, plant, and the atmosphere (Neitsch et al., 2011).

Recent developments in the SWAT-C model further linked the soil organic matter (SOM) module of the CENTURY model (Parton et al., 1994) with SWAT (Zhang, 2018; Zhang et al., 2013b) and have been successfully verified for simulating watershed scale carbon cycling as well as the effects of crop management practices on SOM (Liang et al., 2022; Qi et al., 2020b). Those changes also led to strong improvement in water quality modeling in the UMRB (Du et al., 2019; Liang et al., 2022; Qi et al., 2020a; Qi et al., 2020c; Wang et al., 2021). Despite the extensive testing for simulating soil C cycles (Zhang et al., 2013b; Zhang, 2018; Liang et al., 2022) in the SWAT-C model, it has not been assessed for simulating SIN.

In the SWAT-C model, N is partitioned into two major pools, organic and inorganic. The organic N pool is further divided into five pools, namely the slow humus, passive humus, metabolic litter, structural litter, and microbial biomass (Izaurralde et al., 2006; Zhang, 2018; Zhang et al., 2013b). Organic C and N flow among these pools through multiple pathways as controlled by biotic and abiotic factors. The decomposition of SOM can either immobilize or mineralize SIN, including NO_3^--N and NH_4^+-N. Soil inorganic N is mainly sourced from direct inputs of synthetic N fertilizers and atmospheric deposition, or indirect inputs derived from nitrogen fixation, compost and manure, and plant residues. Nitrogen can be transformed/removed from the soil through multiple biogeochemical processes such as plant uptake, leaching, volatilization, nitrification, denitrification, and erosion (Neitsch et al., 2011). Building on the SWAT-C model, we added new algorithms for nitrification and denitrification to further enhance its performance in predicting SIN dynamics (Table 1). The main equations of different algorithms are described below with more details provided in the SI.

2.1.1. Nitrification methods

Nitrification is a two-step process in which bacteria convert ammonia N to nitrite and then to NO_3^-. The SWAT-C model provides two options for representing the nitrification process (Table 1). The first option is the original SWAT method (Nit1) (Neitsch et al., 2011), wherein nitrification is estimated as a function of soil ammonia content, soil water factor, and soil temperature factor. NO_3^- production (N_{nit}, kg N ha^{-1}) through nitrification was calculated as:

$$N_{nit} = sol_{NH4} * \left(1 - e^{(-TMPF1*SWF1)}\right) \tag{1}$$

Table 1
Summary of different methods used to represent nitrification and denitrification processes in SWAT-C. Nit1 and Denit1 are referring to the original nitrification and denitrification methods in the SWAT model. Nit2, Denit2, and Denit3 are the newly added methods in the SWAT-C model.

Name	Equation no.	References
Nit1	Eq. 1	Neitsch et al. (2011)
Nit2	Eq. 2	Parton et al. (2001), Yang et al. (2017)
Denit1	Eq. 3	Neitsch et al. (2011)
Denit2	Eq. 4	Parton et al. (2001), Yang et al. (2017), Del Grosso et al. (2000)
Denit3	Eq. 5	Parton et al. (1996), Wagena et al. (2017)

where sol_{NH4} is the amount of NH_4^+ (kg N ha^{-1}) in the soil profile, and TMPF1 and SWF represent a soil temperature factor and soil water factor, respectively.

The second new option (Nit2) estimates nitrification following Yang et al. (2017) and Parton et al. (2001), which considers the effects of soil pH. Nitrification is regulated by the soil water factor, soil temperature, and soil pH factor:

$$N_{nit} = SWF2 * TMPF2 * pHF1 * N_{max} + N_{base} \tag{2}$$

where $TMPF2$ and $SWF2$ represent the impacts of soil temperature and soil water on nitrification. $pHF1$ is the soil pH factor. N_{max} is the maximum nitrification rate, $N_{max} = 0.4\, g*m^{-2}d^{-1}$. N_{base} is the minimum nitrification rate, $N_{base} = 10^{-5} g*m^{-2}d^{-1}$.

2.1.2. Denitrification methods

Denitrification is the process through which bacteria remove NO_3^--N from soil under anaerobic conditions by the stepwise reduction of nitrogen oxides. We added two new options for the representation of denitrification in the SWAT-C model on top of the original algorithm (Table 1). The original approach in the SWAT model (Denit1) (Neitsch et al., 2011) estimates denitrification (N_{denit}) as a function of soil water content, soil temperature, and soil carbon content:

$$N_{denit} = sol_{no3} * \left(1 - e^{(-cdn*cdg*vof*sol_{cbn})}\right) \tag{3}$$

where sol_{no3} is the amount of NO_3^- (kg N ha^{-1}) available in the soil profile. cdn represents the rate coefficient for denitrification, cdg represents soil temperature control, vof is the soil voidness factor, and sol_{cbn} is the initial organic carbon content in the soil layer (%).

The first of the two added options (Denit2) estimates denitrification using algorithms described by Yang et al. (2017), Parton et al. (2001), and Del Grosso et al. (2000). The amount of NO_3^- loss through denitrification N_{denit} (kg N ha^{-1}) was estimated as:

$$N_{denit} = 10 * DN_{flux} * DN_{\beta} \tag{4}$$

where DN_{flux} is the denitrified NO_3^- (ppm N d^{-1}), DN_{β} represents the effect of the water filled pore space on denitrification, and:

The second of the two added options (Denit3) estimates denitrification following Wagena et al. (2017), which obtained the methods for denitrification flux estimation from Parton et al. (1996) and Mosier et al. (2002).

$$N_{denit} = \min(DN_{no3\ max}, DN_{Cmax}) * SWF3 * TMPF3 * pHF2 * 10^{-3} \tag{5}$$

where N_{denit3} is the denitrification rate per unit area per day (kg N ha^{-1} d^{-1}), $DN_{no3\ max}$ is the maximum rate of total N gas flux for a given soil NO_3^- level under optimal condition (g N ha^{-1} d^{-1}), DN_{cmax} is the maximum rate of total N gas flux for a given soil C level under optimal conditions (g N ha^{-1} d^{-1}), $SWF3$, $TMPF3$, and $pHF2$ represent the effects of soil moisture, soil temperature, and pH on denitrification, respectively. Site and experiment description and model setup.

2.2. Model evaluation

Performance of the SWAT-C model was evaluated against time series observations from the 40 treatments (Table 2). Seven indices used in previous studies (Archontoulis et al., 2014; Banger et al., 2019; Yin et al., 2020) that assessed agroecosystem models for simulating SIN were calculated in this study, including the Pearson correlation coefficient R, the Nash-Sutcliffe Efficiency (NSE) (Nash and Sutcliffe, 1970), root mean square error ($RMSE$), mean biased error (MBE), mean absolute percentage error ($MAPE$), index of agreement (IA), and percent bias ($PBIAS$). R, ranging

Table 2
Key management practices of the 40 treatments used to test the SWAT-C model.

Site	Trt ID	Fertilizer	Crop rotation[a]	Tillage[b]
MCSE	1	High N	Corn-Soybean-Wheat	Con Till
MCSE	2	High N	Corn-Soybean-Wheat	No-till
LFL	1–2	High N	Corn-Soybean- Others	Con Till
LFL	3	High N	Corn	Con Till
LFL	4–5	High N	Corn-Soybean- Others	Con Till
LFL	6	High N	Corn	Con Till
LFL	7–8	High N	Corn-Soybean- Others	Con Till
LFL	9	High N	Corn	Con Till
LFL	10–11	High N	Corn-Soybean-Others	Con Till
LFL	12	High N	Corn	Con Till
LFL	13–14	High N	Corn-Soybean-Others	Con Till
LFL	15	High N	Corn	Con Till
CRS	1	0 N	Corn	Con Till
CRS	2	Low N	Corn	Con Till
CRS	3	High N	Corn	Con Till
CRS	4–5	0 N	Corn-Soybean	Con Till
CRS	6–7	Low N	Corn- Soybean	Con Till
CRS	8–9	High N	Corn- Soybean	Con Till
CRS	10–11, 20–23	0 N	Corn-Soybean- Others	Con Till
CRS	12–15	Low N	Corn-Soybean- Others	Con Till
CRS	16–19	High N	Corn-Soybean- Others	Con Till

[a] Others include crops such as wheat, sorghum, or oats.
[b] Con Till represents conventional tillage.

from −1 to 1, measures to what extent the observed data are explained by the model. R was calculated as:

$$R = \frac{\sum_{i=1}^{N} (S_i - \overline{S})(O_i - \overline{O})}{\sqrt{\sum_{i=1}^{N} (S_i - \overline{S})^2 \sum_{i=1}^{N} ((O_i - \overline{O})^2}} \quad (6)$$

where N is the number of observations, S_i represents the ith simulated value, O_i represents the ith observed value.

The NSE value ranges from -∞ to 1, with the value of 1 indicates a perfect match between simulation and observation. The NSE was expressed as:

$$NSE = \frac{\sum_{i=1}^{N} (O_i - S_i)^2}{\sum_{i=1}^{N} (O_i - \overline{O})^2} \quad (7)$$

The *RMSE*, *MBE*, and *MAPE* are indicators of data concentration around the best fit. The closer these indicators are to zero, the lower the prediction error of the model. *RMSE, MBE*, and *MAPE* are expressed as the following equations:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N} (S_i - O_i)^2}{N}} \quad (8)$$

$$MBE = \frac{\sum_{i=1}^{N} (S_i - O_i)^2}{\mathrm{N}} \quad (9)$$

$$MAPE = \frac{\sum_{i=1}^{N} | S_i - O_i |}{\sum_{i=1}^{N} O_i} \quad (10)$$

The *IA* is a dimensionless metric and has been widely used for measuring the degree of model prediction error (Willmott, 1981). It ranges from 0 to 1, where 1 indicates a perfect match between simulation and observation. It was calculated by the following equation:

$$IA = 1 - \frac{\sum_{i=1}^{N} (S_i - O_i)^2}{\sum_{i=1}^{N} (|S_i - \overline{O}| + |O_i - \overline{O}|)^2} \quad (11)$$

The *PBIAS* provides a measure of the average tendency of the simulations to be larger or smaller than observations. Positive *PBIAS* values indicate model underestimation and negative values indicate model overestimation (Gupta et al., 1999). The *PBIAS* was expressed as:

$$PBIAS = 100 * \frac{\sum_{i=1}^{N} (O_i - S_i)_i}{\sum_{i=1}^{N} O_i} \quad (12)$$

To evaluate the performance of the SWAT-C model, we identified three corn production experimental sites with long-term SIN measurements and detailed management records available in the U.S. Midwest (Fig. 1; Table S1). They were the Main Cropping System Experiment (MCSE) and the Living Field Lab Experiment (LFL) sites at the Kellogg Biological Station (KBS) in Michigan, and the Crop Rotation System (CRS) experiment near Ithaca, Nebraska.

The LFL and MCSE sites (42°25′N, 85°22′W) were part of the KBS Long-term Ecological Research (LTER) Network and Long-term Agroecosystem Research (LTAR) Network that aim to address the impacts of agricultural management on ecosystem services. They involve multiple agricultural treatments defined by crop rotation, tillage, fertilizer, and cover crops. We selected the conventional chisel plow (T1) and no-till (T2) corn production systems from the MCSE experiment. The T1 treatment received conventional tillage practices (chisel plow) and chemical inputs (fertilizers and pesticides). The T2 treatment received conventional inputs but was not tilled. Both T1 and T2 treatments started with a two-year corn-soybean rotation in 1989 and later changed to a three-year corn-soybean-winter wheat rotation (Hess et al., 2020; Robertson and Hamilton, 2015). Data collected during 1989–2020 was in this study.

The LFL experiment was established in 1993 to extend the basic findings of the MCSE experiment (Robertson and Hamilton, 2015). The LFL experiment treatments considered variability in fertilizer and crop rotation. The three fertilization treatments included Integrated Compost, Integrated Fertilizers, and Conventional Fertilizers. For the Integrated Compost treatment, composted dairy manure was applied to all crops at a rate of 79–-160 kg N ha^{-1} (4 Mg ha^{-1} dry weight basis; 19–29 g N kg^{-1}, 250–380 g C kg^{-1}) before tillage except for soybean (Culman et al., 2013; Fortuna et al., 2003). The Integrated Fertilizer treatment followed low-input practices, with targeted applications of herbicide (herbicides applied only within rows for an application rate one-third that of commercial practice), reduced tillage, and detailed accounting of N inputs to minimize N fertilizer requirements. The Conventional treatment represented typical farmer practices in the region with regard to soil management, fertilizer rates and application practices, and herbicide applications (Culman et al., 2013). Several treatments include four-year crop rotations with two years of corn plus soybean and winter wheat. In these treatments, some had the first-year corn started in 1993, while other treatments had the second-year corn started in 1993 (Sanchez et al., 2004). As a result, 15 treatments that include crop rotation and fertilizer treatments were identified from the LFL experiment. Our study period for LFL was 1993–1997 for which SIN measurements are available.

Based on the experimental records of the CRS experiment near Ithaca, Nebraska (31°10′N, 96°25′W), we identified 23 experimental treatments related to corn production. These treatments included different crop rotations and N fertilizer levels between 1984 and 2002. Crop rotations included continuous corn, two-year soybean-corn or corn-soybean, and four-year rotations (i.e., corn–soybean–grain sorghum (*Sorghum bicolor* L. Moench] – oats (*Avena sativa* L.)/clover (80 % *Melilotus officinalis* Lam. + 20 % *Trifolium pretense* L.) mixture rotation and corn–oat/clover–grain sorghum–soybean rotation). In the two-year and four-year treatments, there were treatments with the same crops, but the sequences of crops were different. Conventional tillage practices were applied to all treatments during the experimental period. Corn was typically planted in the first week of May and soybean was generally planted in mid-May. Herbicide application often varied between years for different crops and at least one application of glyphosate occurred for corn and soybean each season. N Fertilizer treatments started in 1984, including zero N, low N, and high N levels, which correspond to 0, 90, and 180 kg N ha^{-1} for corn and 0, 34, and 69 kg N ha^{-1} for soybean, grain sorghum, and oat/clover, respectively (Sindelar et al., 2016).

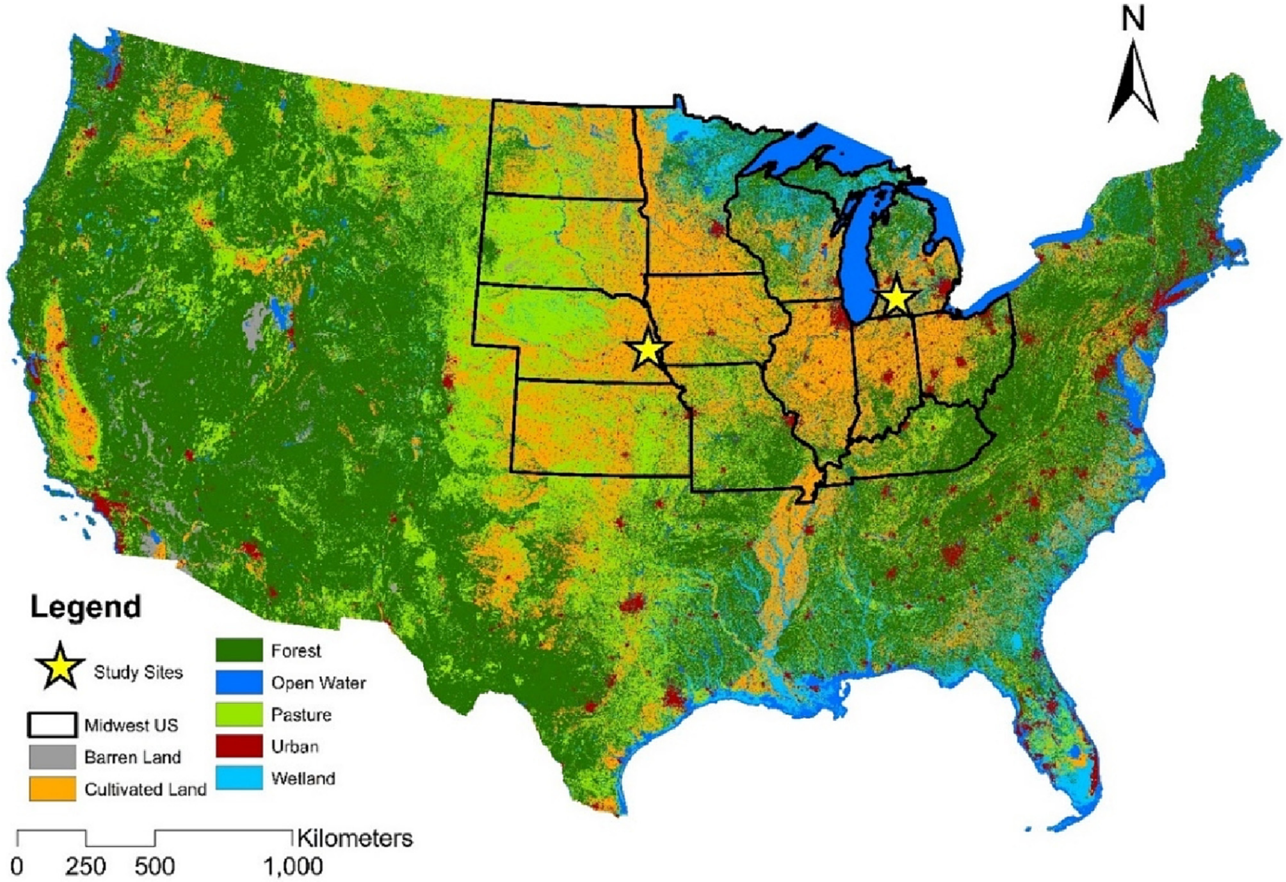

Fig. 1. Location of the study sites and 2011 land use in the Conterminous U.S.

In total, there were 11,272 measurements (including replications) of SIN at the top 25 or 30 cm for the 40 experimental treatments across the three study sites between 1984 and 2020. Experimental data and further model result analysis was performed using R version 4.1.2. To facilitate the evaluation of model performance under different fertilization levels and crop rotations, we further categorized the 40 experimental treatments into three fertilizer treatments based on N input amount for corn [zero N, low N (0–100 kg N ha^{-1}) and high N (>100 kg N ha^{-1})] and three crop rotation treatments (continuous corn, corn- soybean, and corn-soybean-other crops). More information on the three sites and 40 treatments are shown in Table 2. Among the 23 treatments at CRS, there were nine treatments with zero N, seven treatments with low N, and seven treatments with high N input (Table 2). Based on the number of crops involved in a crop rotation, we categorized the crop rotations into three groups, continuous corn (three treatments), corn-soybean rotation (six treatments), and corn-soybean and others (e.g., sorghum and oats) (14 treatments) (Table 2). The 15 treatments at LFL included different fertilization and crop rotations. There were six treatments with composted dairy manure, six treatments with reduced fertilizer and three treatments with conventional fertilizer. Based on the amount of N applied through these treatments, all 15 treatments were grouped as high N treatments (> 100 kg N ha^{-1}). In terms of crop rotation, there were five treatments of continuous corn, and the remaining 10 treatments were four-year rotations involving two-year corn, one-year soybean, and one-year wheat, with the crop sequences varying across treatments (Table 2).

2.3. Model setup and calibration

We prepared inputs for the SWAT-C model for each study site/treatment using the ArcSWAT 2012 interface (Winchell et al., 2013), including topography, soil, climate, and land management. Digital elevation model (DEM) data were obtained from the NASA (National Aeronautics and Space Administration) Shuttle Radar Topography Mission (SRTM) (Farr et al., 2007), and soil data were derived from the SSURGO (Soil Survey Geographic Database) (Soil Survey Staff, Natural Resources Conservation Service, United States Department of Agriculture, 2022) database by the National Cooperative Soil Survey. Climate data from the nearest station to each study site that used to drive the SWAT-C model for the period of 1980–2020 were retrieved from the National Oceanic and Atmospheric Administration (NOAA). To accurately capture the long-term dynamics of SIN, detailed records of management are required as input. We obtained the field records for the period of 1988–2020 and 1993–2002 for the MCSE and LFL experiments from the KBS data catalog (https://lter.kbs.msu.edu/datatables), respectively. Field records for the CRS site were obtained from the AgCROS (Agricultural Collaborative Research Outcomes System) database (https://agcros-usdaars.opendata.arcgis.com/) established by USDA-ARS (United States Department of Agriculture, Agricultural Research Service).

Calibration and evaluation of daily SIN content were performed using the SPE (SWAT Parameter Estimator) program in the SWAT-CUP (SWAT Calibration and Uncertainty Procedure) 2019 Premium software package (Abbaspour, 2022; Abbaspour et al., 2015). A four-year warm-up period (1980–1983) was used to initialize the model.

2.4. Sensitivity analysis

Sensitivity analysis was performed to determine the most influential parameters for the prediction of SIN. The Global Sensitivity Analysis procedure in the SPE program was used (Abbaspour et al., 2004). This method estimates the change in the objective function (i.e., PBIAS in the present study) resulting from changes in each parameter while all other parameters are changing, given as:

$$g = \alpha + \Sigma_{i=1}^{m} \beta_i \cdot b_i \quad (13)$$

where g is the objective function value, α and β_i are regression coefficients, b_i is the calibration parameter for the i^{th} parameter, and m is the number of parameters considered. This method provides a measure of relative sensitivity. The sensitivity of each parameter was evaluated by two statistics: the t-stat index and the p value. The t-stat index indicates the magnitude of the sensitivity of parameters; the larger the absolute value of t-stat the higher the probability that the parameter is sensitive. A p-value <0.05 indicated a sensitive parameter (Abbaspour et al., 2004; Brighenti et al., 2019).

We identified a list of parameters for sensitivity analysis by reviewing previous studies that calibrated soil N cycling related processes using the SWAT or SWAT-C model (Cai et al., 2016; Moriasi et al., 2013; Yuan and Chiang, 2014). As a result, 15 parameters were identified (Table 3) for sensitivity analysis. These parameters control N related cycling processes such as organic matter decomposition, immobilization, plant uptake, and nitrification/denitrification. Those sensitive parameters were subsequently calibrated. Note that parameters that control SOM decomposition in the SWAT-C model, such as OX_aa_para, OX_bb_para, PRMT_45_para, PRMT_51_para, Tf_nit, and DF, were only used for the newly added algorithms and were not used in the SWAT 2012 model.

3. Results and discussion

3.1. The overall performance of different configurations of nitrification and denitrification algorithms for simulating SIN

As shown in Table 2, treatments at the CRS and LFL sites include different fertilization levels and crop rotations. At the CRS site, measured SIN ranged from 10.3 kg N ha^{-1} to as high as 216.0 kg N ha^{-1} with an average of 39.9 kg N ha^{-1}. Across the 23 treatments at CRS, measured average SIN ranged from 32.4 kg N ha^{-1} for the corn-soybean-sorghum-oat rotation with low N input to 64.6 kg N ha^{-1} for continuous corn treatment with high N input. Measured SIN at the LFL site ranged from 5.3 kg N ha^{-1} to 142.9 kg N ha^{-1} with an average of 42.1 kg N ha^{-1}. The two treatments at the MCSE site were conventional-till and no-till treatments under corn-soybean rotation. Measured SIN at MCSE ranged from 5.1 kg N ha^{-1} to as high as 355.3 kg N ha^{-1}. The average measured SIN was 34.5 kg N ha^{-1} and 33.0 kg N ha^{-1} for the conventional-till and no-till treatments, respectively. The variation in SIN was mainly explained by key N cycling processes such as fertilizer application (Table 2), crop uptake during the growing season, tillage, cover crop, and mineralization of soil organic matter. Cropping systems with N fertilizer application or cover crop utilized much more N than those with zero N application (Dharmakeerthi et al., 2006; Liang et al., 2019; Zebarth et al., 2004), and tillage practices (conventional tillage) could substantially improve plant N uptake during the early growing season based on an experimental study in southern Ontario (Dharmakeerthi et al., 2006). Net N mineralization in clover-amended soils could be as much as five times higher than that in soils amended with compost or manure (Masunga et al., 2016). We then compared the simulated annual SIN with measurements for all treatments (including 276, 75, and 64 annual SIN observations for the CRS, LFL, and MCSE sites, respectively) (Fig. 2).

The two nitrification methods and three denitrification methods (Table 1) resulted in a total of six combinations. For each combination, we ran the model 2000 times using the Latin hypercube sampling (LHS) algorithm and chose the best performing parameter set. The LHS algorithm partitions the parameter space into equal probability segments based on the indicated number of simulations, then a single parameter value is sampled from each segment in a way that ensures a thorough and efficient exploration of the entire parameter range (Abbaspour, 2013). The six combinations of nitrification and denitrification methods exhibited a wide range of performance (Table 4). R ranged from 0.45 to 0.63, NSE from −0.31 to 0.29, $PBIAS$ from −4.7 % to −17.3 %, and $RMSE$ from 16.0 to 22.0 kg N ha^{-1}. Among the six combinations, scenario S5 (N1-D3), which represents the combination of the default nitrification method in SWAT with the second newly added denitrification method, generally outperformed the other combinations and achieved R, NSE, $PBIAS$, and $RMSE$ of 0.63, 0.29, −4.7 %, and 16.0 kg N ha^{-1}, respectively. The overall results suggest that nitrification method N1 performed slightly better in simulating SIN dynamics. Among the three denitrification methods (D1, D2, and D3), the results show that the newly added denitrification method D3 consistently outperformed the other two methods.

Hereafter, we focus on the analysis of the SIN simulations with the best performing scenario S5 (N1-D3) configuration within the SWAT-C model. The measured average annual SIN at the CRS site was 39.9 kg N ha^{-1} versus 38.6 kg N ha^{-1} for simulation. Overall, the SWAT-C model captured the dynamics of SIN well across different sites. The cross-sites correlation coefficient R, NSE, $PBIAS$, and $RMSE$ were 0.63, 0.29, −4.7 %, and 16.2 kg N ha^{-1}, respectively. The performance of SWAT-C varied across the three individual sites. With R, NSE, $PBIAS$, and $RMSE$ ranging from 0.63 to 0.67, −0.29 to 0.41, −32.9 % to 2.4 %, and 10.6 to 23.0 kg N ha^{-1}, respectively (Fig. 2).

Our SWAT-C model performance was comparable to or even better than other modeling studies on SIN dynamics (Archontoulis et al., 2014; Banger et al., 2019). For example, Archontoulis et al. (2014) applied the APSIM model to predict SIN as affected by manure application in the 20 cm topsoil at two corn production sites in the U.S. Midwest, and achieved a $RMSE$ of 7.7–17.6 kg N ha^{-1}. A "fair" performance was obtained by the DSSAT model in predicting SIN during the growing season of corn production systems in the U.S. Midwest (Banger et al., 2019).

Table 3
List of calibrated parameters and ranges.

ID	Parameter	File	Definition	Relative/Replace[a]	Max	Min	Fitted value	Sensitivity ranking
1	ANION_EXCL	sol	Fraction of porosity from which anions are excluded	v	0	1	0.047	6
2	BIOMIX	mgt	Biological mixing efficient	r	−0.2	0.2	−0.175	14
3	DF	hru	Decomposition coefficient	v	0	1.5	1.122	5
4	ERORGN	hru	Organic N enrichment ratio	v	0	5	1.667	8
5	N_UPDIS	bsn	Nitrogen uptake distribution parameter	r	−0.5	0.5	−0.862	10
6	NPERCO	bsn	Nitrogen percolation coefficient	r	−0.5	0.5	0.124	13
7	OX_aa_para	tes	Soil oxygen coefficient	v	0	20	4.753	4
8	OX_bb_para	tes	Soil oxygen coefficient	v	0.001	0.05	0.005	3
9	PRMT_45_para	tes	Coefficient adjusts microbial activity	r	−0.4	0.4	0.17	11
10	PRMT_51_para	tes	Coefficient adjusts microbial activity	r	−0.4	0.4	−0.076	12
11	RSDIN	hru	Initial residue cover (kg/ha)	v	0	10,000	2794.5	9
12	SDNCO	bsn	Denitrification threshold water content	r	−0.5	0.5	−0.294	7
13	SOL_CBN	sol	Initial organic carbon content in the soil layer (%)	v	0	5	2.35	1
14	SOL_NO3	chm	Initial NO_3^--N concentration in the soil layer (mg/kg)	v	5	40	30.21	15
15	TF_nit	bsn	Temperature factor in controlling nitrification	v	0	0.5	0.155	2

[a] v indicates relative change of a parameter; r indicates replace of a parameter.

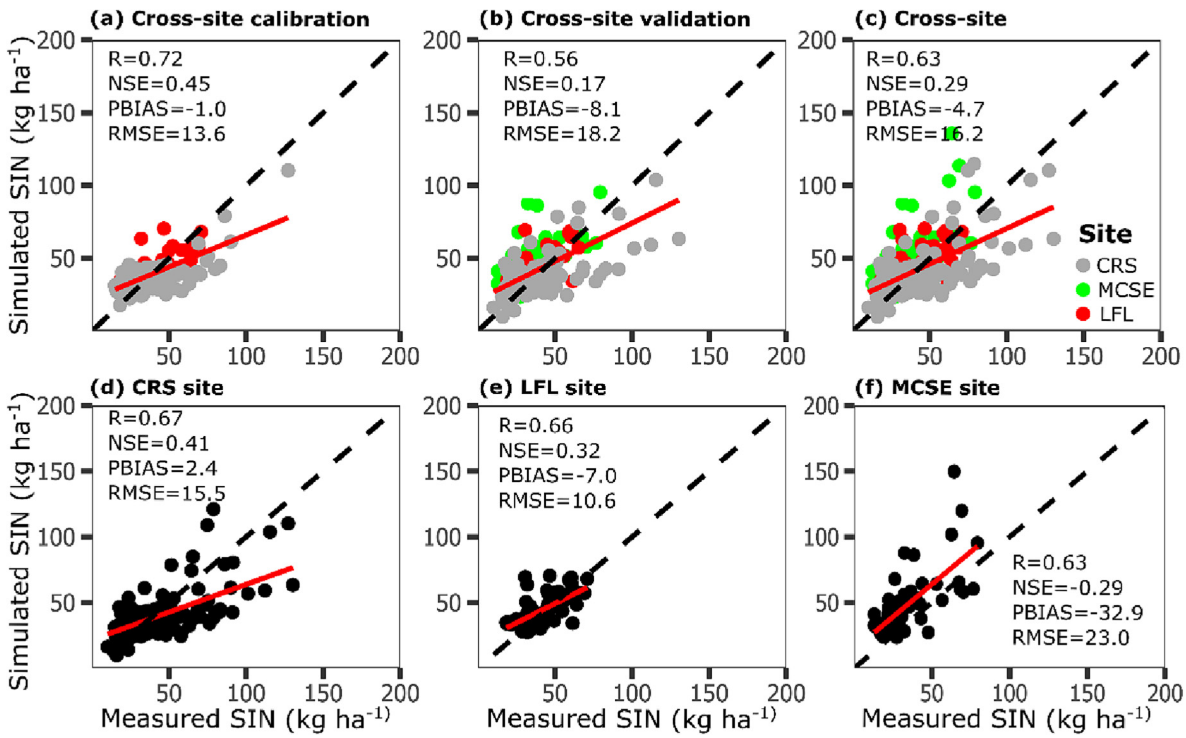

Fig. 2. Simulated and observed average annual SIN for all sites (a), (b), (c) and at each individual site. The dashed black line indicates the 1:1 identity line and the solid red line represents the linear regression line.

3.2. Model performance against time series data

We examined model performance in predicting SIN dynamics for different treatments across the three sites (Figs. 3–6). At the CRS site, the SWAT-C model achieved the least error among the three sites, with *R, NSE, PBIAS, RMSE, MAE, MAPE,* and *IA* of 0.56, 0.22, 3.2 %, 17.5 kg N ha^{-1}, −1.3, 0.33, and 0.73, respectively. At the MCSE site, the SWAT-C model performed slightly poorer than at the other two sites. The model captured well the temporal dynamics of SIN (R = 0.62, NSE = 0.20, & IA = 0.75), but was subject to large bias ($PBIAS$ = -36.6 %, $RMSE$ = 34.3, MBE = 12.4, & $MAPE$ = 1.2). This was likely due to the long-term and higher temporal resolution datasets used for model evaluation at the MCSE site compared to the other two sites, which makes it more challenging to simulate. Overall, as illustrated in Figs. 4–6, the model can capture the temporal and spatial variation of SIN reasonably well for most of the treatments. The large spread between the two ends of the error bars (i.e., the range of observed values from multiple replicates) suggests large uncertainties associated with measured SIN. The peaks of SIN often followed fertilizer or manure application or the mineralization of returned crop residues. Fertilizers were normally applied within a month after the sowing of corn in early May or late April. The peaks in the fall were likely due to enhanced mineralization due to the return of crop residues or manure application to the soil.

Table 4
Performance of different combinations of nitrification and denitrification methods in simulating SIN. Bold values represent the optimal combination of methods.

Scenarios	Nitrification method	Denitrification method	*R*	*NSE*	*PBIAS* (%)	*RMSE* (kg N ha^{-1})
S1	N2	D1	0.56	−0.18	−16.4	20.84
S2	N1	D1	0.57	−0.09	−11.6	20.05
S3	N1	D2	0.45	0.07	5.5	18.49
S4	N2	D2	0.57	−0.29	−16.6	21.81
S5	**N1**	**D3**	**0.63**	**0.29**	**−4.7**	**16.20**
S6	N2	D3	0.62	−0.31	−17.3	22.00

As shown in Figs. 4–6, the model simulations generally reflected the interannual and intral-annual changes of SIN caused by key N cycling processes such as N application and crop growth. Continuous corn treatments (CRS T1–3 and LFL T3, T6, T9, T12, T15) had the highest amount of SIN, with the simulated and observed average SIN values of 48.7 kg N ha^{-1} and 44.5 kg N ha^{-1}, respectively. This is understandable since corn generally receives higher N applications compared to other rotational crops such as soybean, winter wheat, and oats. Large overestimation was found for treatment 3, which was a high N treatment under continuous corn. Simulated SIN showed a larger variation under the high N treatment as compared to measurements under zero and low N treatments. This was likely because most of the measurements (81.2 %) were taken during the non-growing season at the CRS site. The relatively small fraction of dataset from the growing season for model calibration could cause uncertainties in SIN simulation because the rapid change of SIN normally occurs during the growing season shortly after the application of N fertilizer.

Compared to the LFL and CRS sites, long term and more frequent data were available at the MCSE site (Fig. 6). The correlation coefficient for the two treatments at the MCSE site were 0.58 and 0.66, which was slightly better than the results in Cai et al. (2016), who reported correlation coefficients of 0.58 and 0.56 for soil NO_3^- simulation at the MCSE site between 1989 and 2011 using the built-in soil N cycling modules of the SWAT model. In our study, the simulated SIN at the MCSE site was calibrated simultaneously with the other two sites. This calibration helps with model generalization and application at broader scales.

To further compare our model with the results reported in Cai et al. (2016), we calibrated the SWAT-C model against experimental data from the MCSE site. The performance of SWAT-C further improved, with the overall *R, NSE, PBIAS,* and *RMSE* values of 0.63, 0.32, −8.0 %, and 31.7 kg N ha^{-1}, respectively. The correlation coefficient *R* for treatment 1 (T1) and treatment 2 (T2) were 0.61 and 0.66, respectively. The findings indicate that the new algorithms added to the SWAT-C model outperformed the algorithms used in the SWAT2012 model. Meanwhile, we also note that

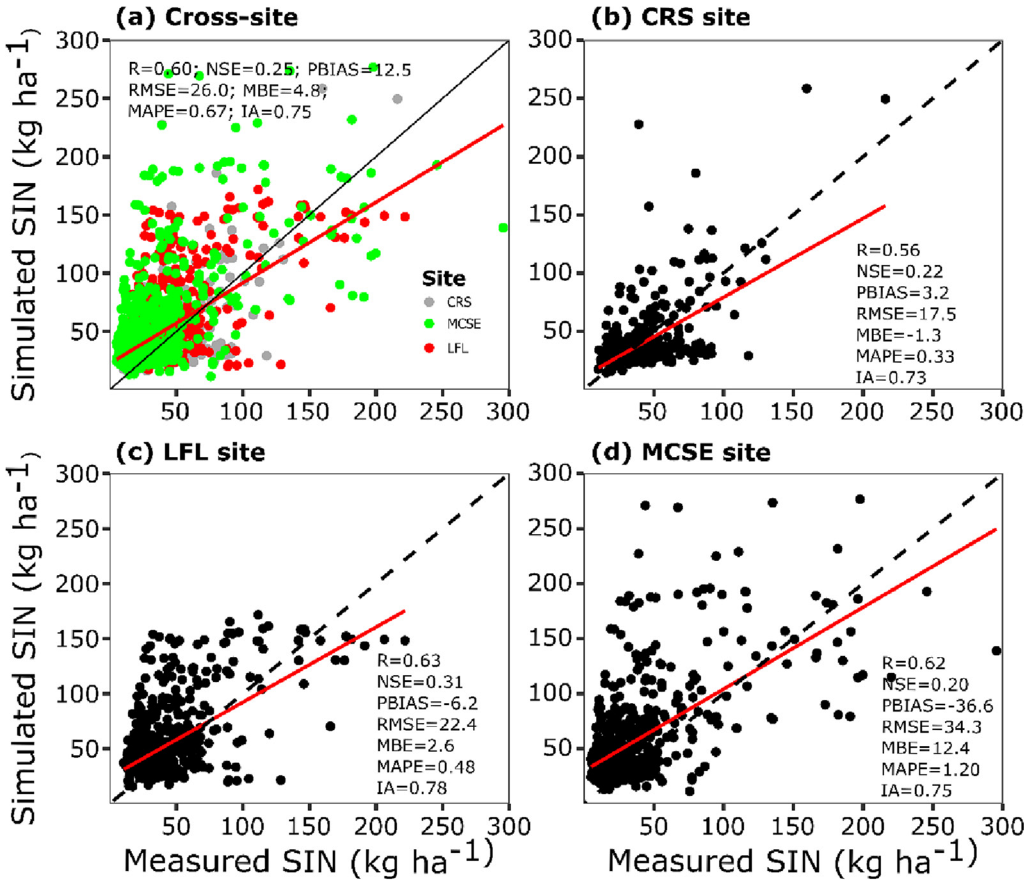

Fig. 3. Cross-site comparison of simulated and measured daily SIN in the U.S. Midwest. The dashed black line indicates the 1:1 identity line and solid red line represents the linear regression line.

there is further need of improving the algorithms to capture the temporal dynamics of SIN more accurately, particularly at a finer temporal resolution (e.g., daily time steps).

3.3. Comparison of the SWAT-C model with other models reported in previous studies

Multiple previous studies have evaluated process-based models in predicting SIN (Table 6) (Archontoulis et al., 2014; Banger et al., 2019; Yin et al., 2020), most of which were carried out at a single site or did not have long-term data to reflect the variation of soil and climate conditions. In contrast, our study used long-term experimental datasets from 40 experimental treatments across three sites for model evaluation. It is difficult to directly compare the performance of the SWAT-C model with those reported in previous studies, due to the use of different cropping systems, model simulation length, and number of observations. For example, Archontoulis et al. (2014) and Banger et al. (2019), respectively, evaluated APSIM and DSSAT for corn using <300 observations for periods $\leq$3 years. In contrast, Yin et al. (2020) evaluated six different process-based models for complex crop rotations against data over a 12-year period, but with only ca. 144 observations. Four out of the six models (APSIM, DAISY, FASSET and HERMES) underestimated SIN (observed = 60.3 kg N ha^{-1} vs simulated = 25.8 kg N ha^{-1}), the CROPSYST model overestimated SIN (observed = 59 kg N ha^{-1} vs simulated = 107 kg N ha^{-1}), and the STICS model simulated SIN relatively well with RMSE = 27, MBE = -1, MAPE = 2, and IA = 0.67. Also, it is worth noting that the same model could perform very differently in different studies. For instance, the APSIM model achieved RMSE of 12.6 as reported by Archontoulis et al. (2014), which is much lower than the value of 48 reported by Yin et al. (2020). In terms of complexity of cropping system and duration of assessment, the study of Yin et al.'s (2020) is more feasible for use to compare the performance of SWAT-C. Overall, the performance of the SWAT-C model in simulating SIN is comparable or even better than those process-based models reported in Table 5. It is worth noting that, the models reported in previous studies may exhibit different performance when evaluated using the datasets used to evaluate the SWAT-C model. Therefore, a more robust comparison between different models is deserved in the future with collaboration between experts on different models and usage of the same experimental datasets.

3.4. Model performance by treatments

Nitrogen fertilization and crop rotation were the two major practices examined at the 40 treatments in this study. Model simulations generally reflect the changes across treatments (Table 6 & Fig. 7). Fig. 7 shows that the model reproduced well the effect of crop rotation and fertilizer treatments on SIN across different sites. For the CRS site, the average measured and predicted daily SIN during the study period (mean ± std) under continuous corn, corn-soybean rotation, and corn-soybean-other crops rotation were 46.7 ± 27.6 vs 48.2 ± 34.6 kg N ha^{-1}, 39.5 ± 17.4 vs 40.4 ± 9.4 kg N ha^{-1}, and 38.6 ± 19.3 vs 36.3 ± 13.2 kg N ha^{-1}, respectively. At the LFL site, the average measured and predicted SIN under continuous corn and corn-soybean-other crops rotation were 41.2 ± 13.2 vs 49.4 ± 12.3 kg N ha^{-1}, 40.4 ± 12.9 vs 40.9 ± 10.2 kg N ha^{-1}, respectively. The model underperformed with the high N treatment, especially at the MCSE site, where the average simulated SIN was 35.9 % higher than the measurement (46.6 ± 24.1 vs 34.3 ± 20.4 kg N ha^{-1}). This is likely due to the lumped calibration strategy applied in this study, in which SIN was

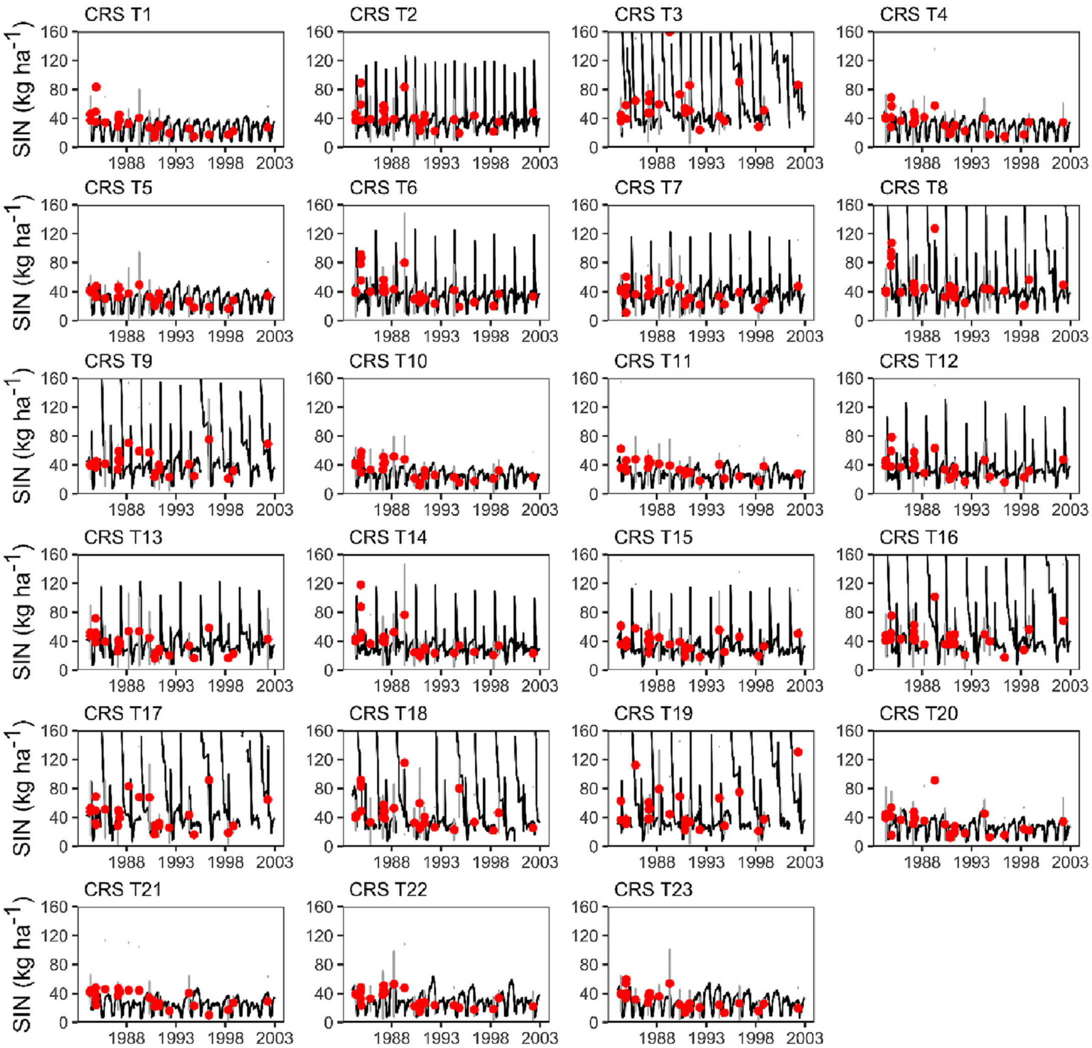

Fig. 4. Observed and SWAT-C model simulated daily SIN (kg N ha^{-1}) for treatment 1–23 between 1984 and 2002 for the long-term CRS experimental site in Ithaca, Nebraska.

calibrated simultaneously for all treatments across all sites without specifically considering local settings of the MCSE site. It has been reported (Archontoulis et al., 2014) that model performance could be reduced when conducting multi-site and multi-treatment calibration compared to single-site and treatment calibration.

3.5. Parameter sensitivity

As shown in Table 3 and Fig. 8, the 15 parameters demonstrated varied sensitivity for SIN simulation. The smaller the *p*-value and the larger the t-stats, the more sensitive the parameter. The top six sensitive parameters were SOL_CBN, TF_nit, OX_aa_para, OX_bb_para, DF, and ANION_EXCL (as indicated by the *p* values and t stats). The SOL_CBN defines the initial soil carbon content; TF_nit represents the temperature control on nitrification; both OX_aa_para and OX_bb_para control oxygen effects on decomposition; DF controls the SOM decomposition rate; and the ANION_EXCL is the fraction of porosity (void space) from which anions are excluded. Among those parameters, four of them can directly affect the amount of SOC and SOC decomposition. Our result is consistent with previous findings that SIN is highly sensitive to the cycling of SOM (Mitchell et al., 2000; Osterholz et al., 2016), as SOM is generally the dominant source of mineralizable N and predicting C and N mineralization of crop residues in soil is important for forecasting subsequent soil N availability during crop growth cycles (De Notaris et al., 2018; Liang et al., 2019).

3.6. Limitations and uncertainties

Previous studies indicated that SIN simulation is difficult due to the complexity of N cycling (Archontoulis et al., 2014; Banger et al., 2019; Franqueville et al., 2018; Moriasi et al., 2013). This study involved several major sources of uncertainties that could explain the discrepancy between the simulations and measurements, including model input and evaluation data, model structure, and model parameters.

3.6.1. Uncertainties associated with model input and evaluation data

In addition to the uncertainties associated with climate data (Qi et al., 2019; Sexton et al., 2010), accurate estimation of SIN requires reliable and detailed characterization of field managements such as the timing, type, and rate of fertilizer application, timing and type of tillage practices, crop types/varieties, and dates of planting and harvesting. The inaccuracy or mismatch in these management records could lead to misrepresentation of the N cycle in the model, and consequently cause model biases. In this study, detailed information such as the dates and types of the management practices applied for some of the treatments were not available, which could be a source of uncertainties in model simulations.

Also, initial soil conditions need to be prescribed for the model. For example, bulk density and soil organic carbon content are critical model inputs. In the SWAT-C model, soil bulk density was fixed for each soil layer in each hydrologic response unit (HRU) and used for the

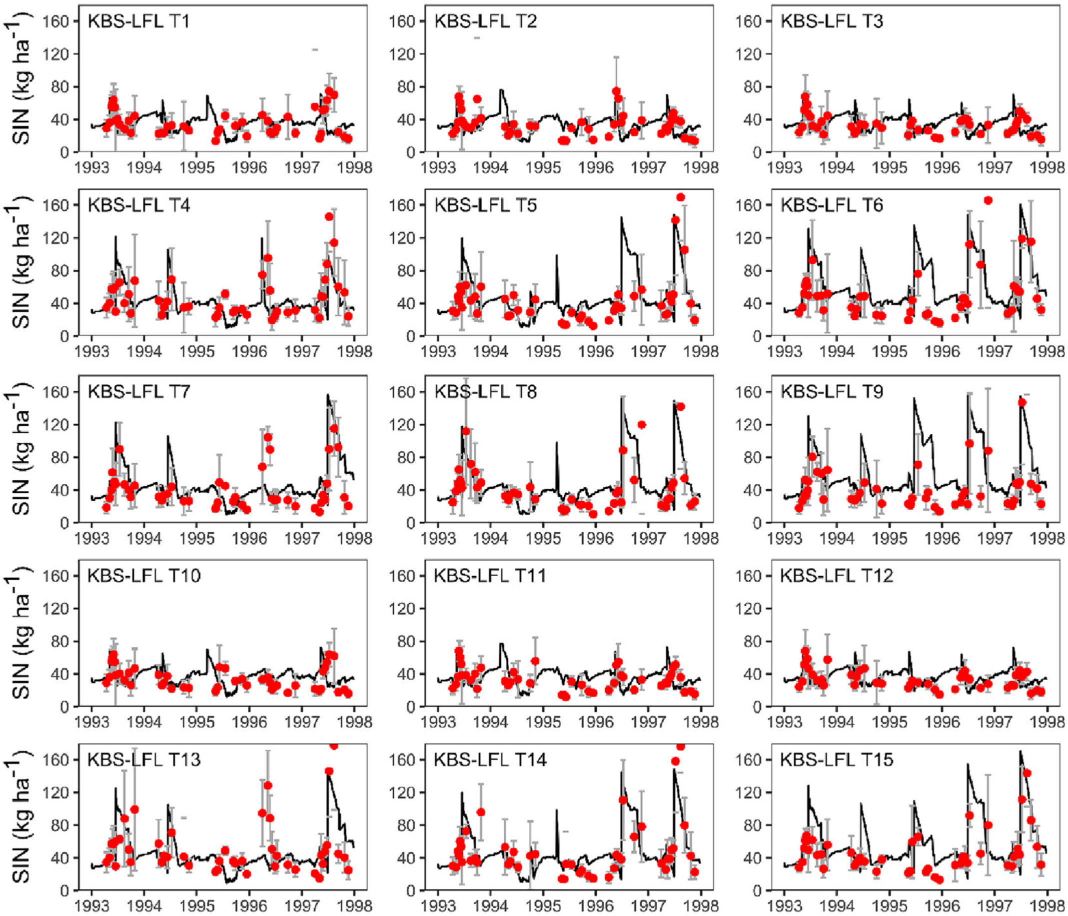

Fig. 5. Observed and SWAT-C model simulated daily SIN (kg N ha^{-1}) for treatment 1–15 between 1993 and 1998 at the LFL site at the KBS, Michigan.

calculation of soil nutrient and chemical content during the entire simulation period, therefore could not reflect the dynamics of soil bulk density as affected by factors such as tillage, soil compaction, and root development of plants. In addition, changes in temperature/moisture changes could affect soil bulk density (e.g., freeze-thaw, soil cracking, etc.). Measuring soil chemical content involves sampling soils from

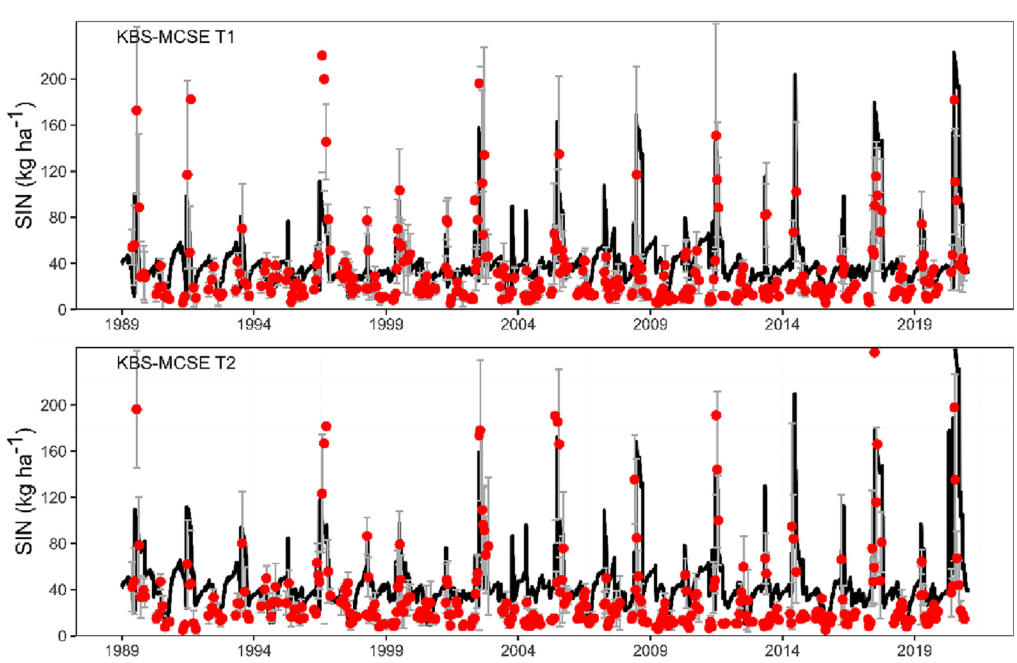

Fig. 6. Observed and SWAT-C model simulated daily SIN (kg N ha^{-1}) for T1 and T2 treatments between 1989 and 2020 for the KBS MCSE site, Michigan.

Table 5
Studies of SIN simulation by typical process-based models.

ID	Model	Reference	Region	Cross-site calibration	Metrics	N sites[a]	N Trts[b]	N Obs[c]	Growing and non-growing seasons	Crop	Trt[d]	Period
1	APSIM	Archontoulis et al. (2014)	U.S.	No	$RMSE$ = 12.6, R^2 = 0.60	4	2	48	Growing	Corn	Manure & N fertilizer	2000–2001
2	DSSAT	Banger et al. (2019)	U.S.	Yes	$PBIAS$ = −3.6, IA = 0.88	6	28	257	Growing	Corn	N fertilizer	2015–2017
3	APSIM	Yin et al. (2020)	France	No	$RMSE$ = 48, MBE = -30, $MAPE$ = 50, IA = 0.31	1	12	~144	Growing	Winter wheat, sugar beets, & pea' catch crop: radish	Crop rotation, N fertilizer & Cover crop	1991–2003
4	CROPSYST				$RMSE$ = 96, MBE = 48, $MAPE$ = 81, IA = 0.04				Growing			
5	DAISY				$RMSE$ = 40, MBE = -23, $MAPE$ = 38, IA = 0.49				Growing			
6	FASSET				$RMSE$ = 54, MBE = -47, $MAPE$ = 79, IA = 0.43				Growing			
7	HERMES				$RMSE$ = 45, MBE = -37, $MAPE$ = 62, IA = 0.49				Growing			
8	STICS				$RMSE$ = 27, MBE = −1, $MAPE$ = 2, IA = 0.67				Growing			
9	SWAT-C	Present study	U.S.	Yes	R = 0.60, $PBIAS$ = -12.5, $RMSE$ = 26.0, MBE = 4.8, $MAPE$ = 0.67, IA = 0.75	3	40	1994	Growing & non-growing	Corn, Soybean & Others	Crop rotation & N fertilizer	1984–2015

[a] Number of sites.
[b] Number of treatments.
[c] Number of measurements.
[d] Treatment types.

multiple locations at different depths in an experimental plot and/or multiple replication plots. The conversion of mass (i.e., mg/kg) to area (i.e., kg/ha) assumed that the samples can accurately represent the spatial variability of chemical content in a larger area. Notably, the coefficient of variation (CV = ratio of the standard deviation to the mean) for measured SIN between replications can range from 2.0 % to 186 % with an average of 29.1 % at the KBS MCSE site. The large range of CVs among experimental replications indicated large uncertainties in SIN measurements. Therefore, the SIN measurement errors in representing spatial variability and accuracy also contributed to the uncertainties in SIN calibration and assessment.

3.6.2. Uncertainties associated with model structure and parameters

Numerical models are simplified representations of the real world, therefore and hence subject to structural uncertainties (Beven, 1993). Previous studies have demonstrated that the SWAT-C model simulations are subject to structural uncertainties (Yen et al., 2014; Zhang et al., 2013a). Although the SWAT-C model is a comprehensive model that encompasses a large number of processes, there is still room to further improve its representation of additional processes related to the N cycling. For example, the nitrification and denitrification algorithms are approximations of the nitrification and denitrification processes occurring under natural conditions. Further improvements regarding multiple biogeochemical processes that are driven by different microbial communities hold promise to benefit the simulation of SIN (Daims et al., 2016; Kuenen and Robertson, 1994; Liang and Robertson, 2021).

Parameters in the SWAT-C model are often not directly available from field observations, therefore they are frequently adjusted to match model simulations and observed variables of interest. Despite the fact that model parameters vary by location (i.e., different sites have different parameter values), here we did not perform parameter calibration for each individual site. Instead, we simultaneously calibrated parameters across all three sites using a batch calibration approach. Whereas this strategy provided an objective and robust assessment of model performance for more general application across locations, the batch calibration likely did not represent the best results achievable by site-specific calibration. For example, the site-specific calibration for MCSE improved model performance compared to the batch calibration over all three sites (Fig. 6). It is reasonable to assume that a site-specific calibration strategy may be needed to reflect site conditions to accurately reproduce SIN dynamics (Archontoulis et al., 2014). We acknowledge that these limitations could be sources of uncertainties in SIN simulation.

Table 6
Evaluation metrics of SIN by N fertilizer treatment and crop rotation treatment.

Major treatments	Sub-treatments	$PBIAS$ (%)	R	NSE	$RMSE$ (kg N ha^{-1})
N Fertilizer	0 N	−19.9	0.32	−0.01	12.0
	Low N	−5.4	0.25	0.00	14.0
	High N	−18,8	0.66	0.31	18.5
Crop Rotation	Continuous Corn	−18.3	0.78	0.40	17.6
	Corn- Soybean	−33.2	0.59	0.08	17.6
	Corn-Soybean- Others	−6.1	0.61	0.37	14.3

4. Conclusions

We sought to improve the SWAT-C model in predicting the dynamics of SIN under typical cropping systems in the U.S. Midwest. We added new nitrification and denitrification algorithms into the SWAT-C model and evaluated the model performance for simulating SIN against experimental data compiled from three sites with a total of 40 treatments. The different algorithms for simulating nitrification and denitrification demonstrated varied performance for SIN simulation, which allowed us to identify the optimal combination for the study sites. The improved SWAT-C model captured both the magnitude and temporal variation of SIN. Sensitivity analyses showed that SIN dynamics was most sensitive to the parameters that control SOM decomposition and nitrification. The performance of the SWAT-C model in simulating SIN was comparable or even better than previously reported evaluation of process-based models. We expect the model developed and tested here will help to advance the capability of agroecosystem models in N simulation and facilitate improved understanding and quantification of N dynamics in complex agricultural landscapes.

Author contributions statement

KL compiled and analyzed the data, modified the code, conducted simulations, and prepared the draft. XZ supervise the study, modified the code, revised the manuscript. VJ, GB, MRS, and GPR provided the experimental data and contributed to writing. XL, GWM, and GEM commented on the methodology and contributed to writing.

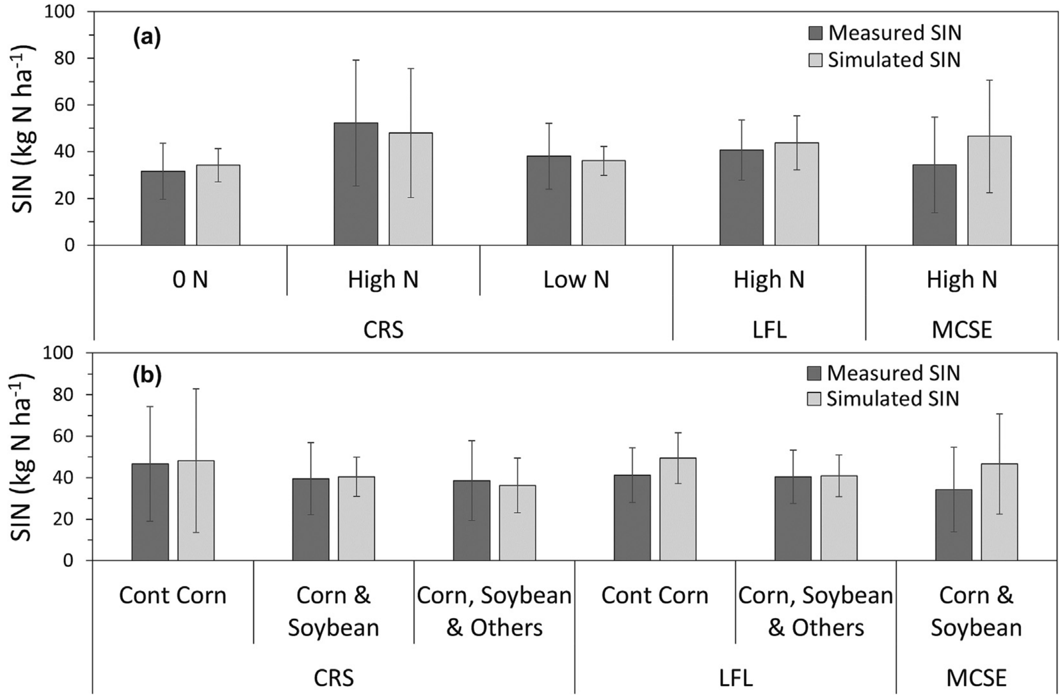

Fig. 7. Comparison of simulated and measured daily SIN during the study period under different fertilizer treatments (a) and crop rotation treatments (b) at the three study sites.

Data availability

Data will be made available on request.

Declaration of competing interest

The authors declare no conflict of interest.

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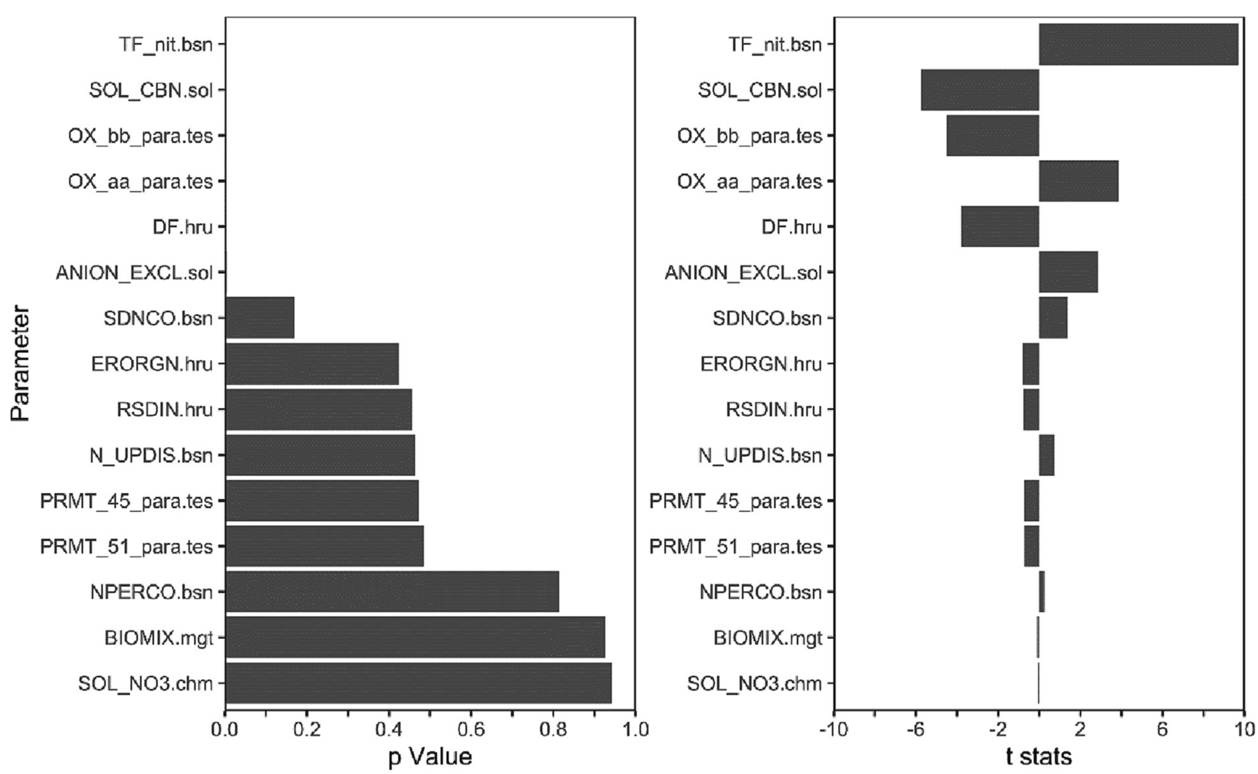

Fig. 8. Sensitivity of SWAT-C model parameters for simulating SIN.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.scitotenv.2023.162906.

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