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Global Sensitivity and Uncertainty Analysis of an Expanded Process-Based Ecosystem Model to Simulate the Soil Nitrogen Cycle of Winter Wheat-Summer Maize Rotation Systems in the North China Plain

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ABSTRACT

Accurately simulating the soil nitrogen cycle is crucial for assessing food security and resource utilization efficiency. The accuracy of model predictions relies heavily on model calibration. This study focused on the soil nitrogen cycle of winter wheat-summer maize rotation systems in the North China Plain (NCP). Firstly, the expanded Vegetation-atmosphere Interface Processes (VIP) model was calibrated to capture the dynamics of soil nitrogen cycle by using field measurements in three stations during 2000 to 2015. Secondly, the Morris and Sobol' algorithm were adopted to identify the sensitive parameters which greatly impact the soil nitrate concentration, denitrification and ammonia volatilization rates. Finally, the SCE-UA algorithm was used to optimize the selected sensitive parameters to improve the prediction accuracy. The results showed that: (1) the sensitive parameters related to soil nitrate concentration were the potential nitrification rate, Michaelis constant, microbial carbon-nitrogen ratio and slow humus carbon-nitrogen ratio; the sensitive parameters related to denitrification rate were the potential denitrification rate, Michaelis constant and N_2O production rate; the sensitive parameters related to ammonia volatilization rate were the coefficient of ammonia volatilization exchange and potential nitrification rate; (2) With the optimized parameters, prediction efficiency was increased noticeably assessed by the coefficient of determination, the average length (ARIL) at the 95 % confidence level for soil nitrate concentration, denitrification and ammonia volatilization rate were 11.92, 0.008 and 4.26, respectively, and the percent of coverage of the measured values in 95% confidence interval (P-95CI) were 68 %, 86 % and 92 %, respectively. By identifying sensitive parameters related to soil nitrogen supports explicit guidance, the expanded VIP model optimized by SCE-UA algorithm can effectively simulates the dynamics of the soil nitrate concentration, denitrification and ammonia volatilization rate in the NCP.

Key Words: ammonia volatilization, denitrification rate, global sensitivity analyses, SCE-UA algorithm, VIP model

INTRODUCTION

The increase in grain yield relies heavily on the large investment of nitrogen fertilizer in the North China Plain (NCP), which is a key region of grain production (Hartmann *et al.*, 2015; Wang *et al.*, 2017). The amount of average annual nitrogen fertilizer application is as high as 550-600 kg hm^{-2} in the winter wheat-summer maize rotation systems, which is much higher than the demand of crops in this region (Chen, 2003). Besides, the improper management practices, such as excessive irrigation, incorrect application rates and inadequate sowing rates, will restrict the improvement of nitrogen use efficiencies and cause a series of environmental problems (Zhu and Chen, 2002; Ju *et al*., 2006; Liu *et al*., 2006; Guo *et al*., 2010). Studying the mechanisms of nitrogen transformation in the winter wheat-summer maize rotation systems is essential to achieve high crop yield, to utilize efficiently the nitrogenous resources and to reduce the risk of environmental pollution (Zhou *et al*., 2006; Erisman *et al*., 2007; Padgett *et al*., 2008; Zhang *et al*., 2017; Zhang *et al*., 2018), which will be of great significance for making rational agricultural policies to ensure food security and environmental sustainability.

Due to the constraints of complex soils, crops and planting patterns, it is time-consuming and laborious to rely solely on field experiments to study the soil nitrogen transformation in agroecosystems (Smith *et al.*, 2008), while process-based models, as an important research tool, can economically assess the effects of interactions between soil, climate and agricultural management on soil nitrogen dynamics. So far, numerous models have been developed, such as EPIC (Williams, 1995), APSIM (McCown *et al*., 1996), DAISY (Abrahamsen and Hansen, 2000), RZWQM (Team *et al*., 1998), WNMM (Li *et al.*, 2007), DNDC (Li *et al.*, 1992) and WOFOST (Van Diepen *et al.*, 1989). These models were typically developed to achieve specific objectives and applied to multiple types of researches in NCP (Lu and Fan, 2013; Zhang *et al.*, 2017; Chen *et al.*, 2018). For instance, the WOFOST, which is a mechanistic model that forecasts crop production, biomass or water use efficiency on the basis of the biochemical processes (e.g., photosynthesis, respiration) influenced by environmental conditions, is widely used to quantify the potential crop yield in the NCP (Wu *et al.*, 2006; Lu and Fan, 2013). The DNDC, which is designed to simulate carbon and nitrogen biogeochemistry in agroecosystems, is used for predicting soil carbon dynamics (Zhang *et al.*, 2017; Chen *et al.*, 2018), nitrogen leaching (Li *et al.*, 2014) and emissions of trace gases (Li *et al.*, 2010). RZWQM coupled with the DSSAT crop models, is initially focused on assessing the productivity and water quality of various cropping systems for various soil, climate and field management (Team *et al*., 1998), and its applications mainly include nitrogen transport and utilization efficiency in the NCP (Yu *et al.*, 2006; Li *et al.*, 2015). Because of models having their functional focuses and limitations, previously developed models have advantages in assessing crop yield, soil carbon dynamics, water movement, nitrogen use efficiency and emissions of trace gases to a certain extent. To further describe accurately the processes of soil nitrogen cycle, it is necessary to develop a soil nitrogen cycle module which is suitable for climatic conditions and field management in the NCP.

Generally, the mechanistic models require many input parameters, which make it difficult to calibrate and lead an obvious uncertainty. It is necessary to identify parameters which have a significant impact on model performance through sensitivity analysis (SA) before calibration. Fixing non-influential parameters at reasonable values will greatly decrease the computational cost (Saltelli and Annoni, 2010). Most previous studies used local sensitivity analysis (LSA) methods to evaluates model responses by consecutively varying one parameter while keeping other parameters at a constant value (Heinen, 2006; Mo *et al.*, 2012; Liang *et al.*, 2016). For example, Liang *et al.* (2016) analyzed soil nitrate and ammonium concentration by varying ± 10 % of each input parameter in the WHCNS model, and found that soil ammonium content was sensitive to nitrogen conversion parameters, and the hydraulic parameters had little effect on it. However, local SA method cannot analyze the effect of interactions between the different parameters on model performance. As alternative, the global sensitivity analysis (GSA) methods, such as Morris (Morris, 1991), Sobol' (Sobol, 2001) and FAST algorithms (Cukier *et al.*, 1973), can be used to evaluate the response to model performance by simultaneously varying all parameters, which is helpful to fully understand the sensitivity of the model parameters (Lamboni *et al.*, 2009; Mo *et al.*, 2012; Liang *et al.*, 2017). Such as, Morris and Sobol' methods were used to evaluate the response of nitrate leaching to soil hydraulic and soil organic transformation parameters and found that soil saturated water content and field capacity were the most influential parameters (Liang *et al.*, 2017). Chen *et al.* (2018) used Sobol' method to screen out the influential parameters for nitrogen transportation and identified the most sensitive parameter is potential denitrification rate. However, there were few studies that adopted the GSA methods to identify completely the sensitive parameters of soil nitrogen cycle.

Generally, the sources contributing to modeling uncertainty are incorrect input data, unreasonable model structure and uncertain parameters values (Refsgaard and Storm, 1996). Various methods have been developed to deal with parameter uncertainty, such as the generalized likelihood uncertainty estimation (GLUE) (Beven and Binley, 1992), Simulated Annealing algorithm (Kirkpatrick *et al.*, 1983), Genetic algorithm (Whitley, 1994) and SCE-UA algorithm (Duan *et al.*, 1994), have been developed. These algorithms were widely used in parameter calibration and uncertainty analysis (Vrugt *et al.*, 2003; Dai *et al.*, 2009; Zhang *et al.*, 2009). For example, six parameters of CN-SIM were carried out with a multi-objective genetic algorithm (NSGA-II), by minimizing the Relative Root Mean Squared Error between observations and simulations with data of respired C and soil inorganic N measured on three soils (Cavalli and Bechini, 2012). Rafique *et al.* (2015) used PEST software to optimize the parameters of N_2O emissions in the DayCent model and found that the simulated accuracy of the optimized N_2O flux was improved by 63%. Previous researches have individually optimized parameters related to the nitrogen cycle processes, such as soil organic matter decomposition or denitrification process (Cavalli and Bechini, 2012; Rafique *et al.*, 2015). Based on the prior SA results, it can greatly improve the efficiency of parameter calibration by selecting the appropriate calibration algorithm. However, there were few studies on optimizing the parameters related to the nitrogen cycle as a whole in an agroecosystem. In this study, based on SA results, the SCE-UA algorithm was used to calibrate the model and provide technical support for the promotion and application of the VIP (Vegetation-atmosphere Interface Processes) model.

The VIP model mainly accounts for soil organic matter decomposition processes, photosynthesis, soil hydrothermal processes, vegetation dynamics and energy partition (Mo and Liu, 2001; Mo *et al.*, 2012). After years of development and uncertainty study of model parameters, the VIP model has been successfully used to simulate winter wheat-summer maize yield, evapotranspiration and water use efficiency in the NCP (Mo *et al.*, 2012). This study tries to identify the sensitive parameters that affect the soil nitrogen cycle in a winter wheat-summer maize rotation system in the NCP and calculate the uncertainty interval of the simulation results caused by parameter uncertainty. The objectives of this study are: (1) to expand the nitrogen cycle module in VIP model based on the existing soil nitrogen cycle theory and method to improve its performance in soil nitrogen cycle; (2) to conduct a global sensitivity analysis by Morris and Sobol' algorithm to identify the sensitive parameters of nitrogen cycle process in the study area; (3) to perform parameters optimization by SCE-UA algorithm based on the previous SA results and calculate the uncertainty interval of the VIP performance.

MATERIAL AND METHODS

Description of the study area

The NCP, which is located in eastern China, lies between 31º 14' – 40º 25' N latitude and 112º 48' – 122º 45' E longitude (Fig. 1). Its area is about 330,000 km^2, 70 % of which is agricultural land. It belongs to the semi-arid monsoon climate zone with most rainfall occurring in summer (Hu, 2012). The annual average temperature varies from 10 °C to 15 °C and sunshine duration is about 2800 h in the central region. It is a key granary in China, in which the winter wheat-summer maize rotation system is the main planting pattern in this region (Hu, 2012). Therefore, this dominant planting pattern was selected for soil nitrogen cycle simulations. Data of field experiments in three ecological stations (Fengqiu, Yucheng and Luancheng) in NCP were selected (Fig. 1).

Fig. 1 Location map of the study area and the spatial distributions of agricultural ecology experimental stations.

Data

Data for simulation. The driving data consisted of daily meteorological records, soil data and field management data were employed. Among them, a considerable amount of daily meteorological variables was collected at three ecology stations (Fengqiu, Yucheng and Luancheng station) from China Ecosystem Research Network (CERN) (http://www.cnern.org.cn/data/). The time period was from 2007 to 2010 at Fengqiu Ecology Station, from 2000 to 2015 at Yucheng Ecology Station and from 2003 to 2010 at Luancheng Ecology Station (Table I).

TABLE I

Overview of site information collected for driving expanded VIP model

Data type	Description	Source
Meteorological data	The meteorological data maximum temperature, minimum temperature, average temperature, relative humidity, sunshine hours, precipitation and wind speed. The meteorological data are monitored according to the CERN specifications.	CERN
Soil data	Percentages of sand, silt, clay and soil organic matter as well as bulk density of the different soil layers at three ecology station. Hydraulic characteristics were estimated using the pedo-transfer function.	Huang *et al.*, 2015; Ma, 2004; Li, 2007
Field management	Nitrogen fertilizer is applied before precipitation or irrigation. About 50 % of total N fertilizer was applied into the surface soil before sowing and the rest was applied at heading stage for winter wheat. Half of N fertilizer was applied at jointing stages and the rest at tasseling stages for summer maize.	CERN; Fang, *et al.*,2006; Huang, 2011

Soil data includes soil physical, chemical, and hydraulic properties in different layers (Table II). The physical and chemical properties of the soil (particle fraction, soil bulk density, and organic matter) were collected from the literature (Huang *et al.*, 2015; Ma, 2004; Li, 2007). The Rosetta tripod transfer function was used to estimate the hydraulic characteristics of the soil from the bulk density and the percentages of sand, silt, and clay using the pedo-transfer function (Schaap *et al.*, 2001). The means of indirect estimating soil hydraulic parameters by pedo-transfer function has been widely used in agricultural hydrological simulation studies (Mishra *et al*., 2013; Jiang *et al*., 2015; Li and Ren, 2019).

TABLE II

Soil physicochemical properties and hydraulic parameters of the three experimental fields used for expanded VIP simulation

Location	Soil layer	Particle fraction sand	silt	clay	BD	SOM	θr	θs	α	n	Ks
	cm	%	%	%	g cm^{-3}	g kg^{-1}	cm^3 cm^{-3}	cm^3 cm^{-3}	cm^{-3}	–	cm day^{-1}
Fengqiu	0-20	72.75	17.53	9.72	1.52	11.12	0.0442	0.3821	0.0353	1.5274	56.33
	20-40	66.86	21.39	11.75	1.52	6.13	0.0451	0.3805	0.0307	1.4483	38.23
	40-60	46.95	34.58	18.47	1.49	6.98	0.0560	0.3836	0.0137	1.4563	13.23
	60-80	43.34	40.37	16.29	1.48	6.58	0.0524	0.3750	0.0112	1.4952	13.51
	80-100	30.94	55.43	13.63	1.43	2.65	0.0521	0.3760	0.0063	1.6219	20.13
	100-120	35.97	55.77	8.26	1.41	2.34	0.0416	0.3628	0.0074	1.5887	34.12
Yucheng	0-15	13.46	73.44	13.10	1.47	14.40	0.0883	0.4554	0.0039	1.7977	21.11
	15-70	8.06	79.12	12.82	1.56	5.50	0.0745	0.4249	0.0027	1.7420	14.16
	70-76	5.38	77.00	17.62	1.45	6.40	0.0985	0.4946	0.0020	1.9215	14.97
	76-113	15.46	78.52	6.02	1.38	3.80	0.0462	0.4678	0.0040	2.6303	52.21
	113-121	5.78	63.08	31.14	1.50	7.10	0.2902	0.6558	0.0033	1.3132	5.57
Luancheng	0-20	41.80	53.60	4.60	1.22	10.40	0.0379	0.3896	0.0071	1.5912	94.67
	20-40	35.70	58.00	6.30	1.44	3.90	0.0380	0.3531	0.0082	1.5667	36.26
	40-110	29.20	57.40	13.50	1.46	6.40	0.0518	0.3712	0.0063	1.6209	18.31
	110-150	21.90	64.10	14.00	1.56	6.70	0.0532	0.3631	0.0065	1.5987	12.36

Note: BD represents soil bulk density; SOM represents soil organic matter; θ_r represents residual water content; θ_s represents saturated water content; α and n represent shape factors; Ks represents saturated conductivity.

The planting system is winter wheat-summer maize rotation. The planting methods and field management recorded at three ecology stations were collected from the literature (Huang, 2011; Fang, *et al*.,2006) and from CERN. The details on planting date, harvesting date, nitrogen fertilizer and irrigation can be found in Table III. Urea was used as nitrogen fertilizer. Nitrogen was divided into base fertilizer and topdressing application. Irrigation treatment is performed immediately after the topdressing of wheat in the season, and after the topdressing of the maize season, according to weather conditions, if there is no precipitation process or the rainfall is low, the irrigation treatment is performed.

TABLE III

Overview of site information about planting methods and field management recorded at three ecology stations

variable	site	crop type	planting date	harvesting date	Nitrogen fertilizer	irrigation
					Kg ha^{-1}	mm
Soil nitrate concentration	Fengqiu	wheat	2007/10/17	2008/6/6	207	125
		maize	2008/6/10	2008/9/20	207	100
		wheat	2008/10/17	2009/6/7	207	125
		maize	2009/6/9	2009/9/24	207	100

	Yucheng	wheat	2000/10/10	2001/6/8	300	248
		maize	2001/6/12	2001/9/25	300	202
		wheat	2001/10/5	2002/6/5	300	347
		maize	2002/6/8	2002/9/28	300	324
	Luancheng	wheat	2003/10/7	2004/6/3	150	150
		maize	2004/6/8	2004/9/28	173	—
		wheat	2004/10/7	2005/6/6	253	190
		maize	2005/6/9	2005/9/26	276	270
Denitrification rate	Fengqiu	wheat	2008/10/11	2009/6/3	230	163
		maize	2009/6/10	2009/9/23	230	67
		wheat	2009/10/14	2010/6/11	230	213
		maize	2010/6/13	2010/9/19	230	103
	Yucheng	wheat	2013/10/15	2014/6/10	212	338
		maize	2014/6/15	2014/10/5	240	—
	Luancheng	wheat	2008/10/11	2009/6/11	200	80
		maize	2009/6/14	2009/9/23	200	65
		wheat	2009/10/9	2010/6/7	200	60
		maize	2010/6/10	2010/9/27	200	70
Ammonia volatilization rate	Fengqiu	wheat	2008/10/11	2009/6/3	230	163
		maize	2009/6/10	2009/9/23	230	67
		wheat	2009/10/14	2010/6/11	230	213
		maize	2010/6/13	2010/9/19	230	103
	Yucheng	wheat	2014/10/24	2015/6/11	225	240
		maize	2015/6/18	2015/10/2	225	135
	Luancheng	wheat	2003/10/7	2004/6/3	104	210
		maize	2004/6/5	2004/9/28	173	60
		wheat	2009/10/9	2010/6/7	180	80
		maize	2010/6/10	2010/9/27	150	65

Note: "—" means no irrigation.

Data for calibration and validation. The observed data were measured at three ecology stations (Table IV). Field measurements of soil nitrate concentrations were obtained from the China Ecosystem Research Network (CERN). To determine the soil nitrate content, 10 g of each soil sample was extracted with 50 mL of 2 mol L^{-1} KCL. The soil nitrate concentration of the extract was measured directly at 220 and 275 nm (Norman *et al.*, 1985). The Nitrous oxide (N_2O) flux was conducted by a closed static system. During the measurement, a gas sample is taken from a sampling port at the top of the box, and 20 ml is taken each time. At the same time, the temperature in the box, the soil temperature of 10 cm and the air temperature are measured. Then the samples were measured with a HP-5890 (manufactured by Hewlett-Packard) gas chromatography / electron capture detector (GC / ECD). The measurement conditions: the front column and the analysis column were stainless steel packed columns, and the inner diameter was 2 mm × 1 mm; column temperature was 55 ℃, ECD detector temperature was 330 ℃; and high purity nitrogen (30 ml min^{-1}) was used as the carrier gas. The NH_3 volatility flux was measured using a semi-open static system described by Liu *et al.* (2003). After fertilization, the ammonia capture system was placed in each plot. A vacuum pump was used to make the ammonia (NH_3) volatilized from the soil entering the scrubber with the air stream, and then absorbed by 2 % boric acid. Absorbed ammonia was determined by indophenol blue colorimetry at 625 nm (UV1800, Shimadzu) (Denmead *et al.*, 1976).

TABLE IV

Overview of observation information collected to calibrate and validate the expanded VIP model simulation

Variable	station	period	source	Sampling method
soil nitrate concentration	Fengqiu	2007 – 2009	CERN	Soil samples were collected in layers at a distance of 20 cm and each plot was randomly taken at two points in layers.
	Yucheng	2000 – 2002	Fang *et al.*, 2006	During wheat-maize growing period, soil nitrate nitrogen was taken in 20 cm intervals at monthly intervals during each growing season.
	Luancheng	2003 – 2005	CERN	Soil samples were collected in layers at a distance of 20 cm after harvest.
Denitrification rate	Fengqiu	2008 – 2010	Huang, 2011; Huang *et al.*, 2015	The samples were collected at one weekly intervals during the wheat and maize growing period.
	Yucheng	2013 – 2014	Xu *et al.*, 2015	The wheat wintering period (mid-December to early March of the following year) was collected only once, and the sampling for other growth periods were one weekly interval.
	Luancheng	2008 – 2010	Wang *et al.*, 2011	The observation frequency was once a week during the wheat and maize growing period, and each treatment was repeated 3 times.
Ammonia volatilization rate	Fengqiu	2008 – 2010	Huang, 2011	The measurement was started on the day after fertilization. samples were taken at 8:00 the next morning. Each measurement lasted 18 – 20 days.
	Yucheng	2014 – 2015	Wen, 2016	Sampling is performed daily after fertilization. After one week, samples were taken every 1 – 3 days according to the degree of ammonia volatilization, and then the interval was extended to 7 days until no ammonia volatilization can be monitored.

Luancheng	2003 – 2004; 2009 – 2010	Dong *et al.*, 2011, 2013	After fertilization, the daily measurement was performed. The measurement time were 6 – 9 days after application of wheat base fertilizer, wheat topdressing, and maize topdressing.

Model description

The VIP model is a process-based ecosystem model independently developed by the Mo Xingguo Research Group of the Chinese Academy of Sciences. The model includes the photosynthesis, vegetation growth dynamics, the soil hydrothermal movement process, the soil carbon cycle, and the energy balance. Soil heat transfer and soil water movement are calculated using the thermal diffusion equation and the Richards equation, respectively. The detailed description of the VIP model can be found in the literature (Mo and Liu, 2001; Mo *et al.*, 2012). In the original VIP model, soil nitrogen cycle module accounts for the turnover and mineralization process between the soil organic nitrogen pools and neglects the conversion between inorganic nitrogen pools. On this basis, the processes of the nitrogen cycle module including nitrification, volatilization, denitrification and immobilization were completed in this study (Fig. 2).

Fig. 2 Carbon and nitrogen pools and fluxes in expanded VIP model.

Soil organic matter mineralization. The soil organic matter mineralization module is adopted from the CENTURY model (Parton *et al.*, 1993). Soil organic C and N are divided into five pools: structural litter pool, metabolic litter pool, microbial biomass pool, slow humus pool and passive humus pool. In addition to the magnitude difference, the turnover rates of five pools are also different from a few weeks to hundreds of years. Different organic C pools are controlled by the first-order kinetic equations and the decomposition rate is proportional to the size of the pools (Parton *et al.*, 1993):

$$\frac{dC_i}{dt} = -k_i \cdot C_i \tag{1}$$

Where C_i is the carbon content of the pool i, k_i is the decomposition rate of the pool i; it is influenced by soil moisture and temperature, wherein the decomposition rate is:

$$k_i = k_i^* \cdot f(t) \cdot f(w) \tag{2}$$

where, k_i^* is the decomposition rate of organic matters under optimal moisture and temperature conditions, d^{-1}; t is the soil temperature, °C; w is the soil water content, g kg^{-1}; $f(t)$ and $f(w)$ represent temperature and moisture correction function, respectively. The decomposition rates of different organic N pools are:

$$\frac{dN_i}{dt} = \frac{C_i/dt}{(C/N)_i} \tag{3}$$

Where N_i is the soil nitrate concentration of the pool i, and $(C/N)_i$ is the carbon-nitrogen ratio of the pool i.

*Nitrification rate***.** The substrate (NH_4^+、O_2、CO_2) content, soil temperature and water content are considered to be the abiotic factors which have the effect of nitrification rate. In the case of relatively high soil moisture (1.5 < pF < 2.5), pH value of 4-8 and temperature above 5 °C, soil microbial metabolic activity is limited by soil organic carbon content. In the absence of oxygen stress, most ammonium nitrogen (NH_4^+) is rapidly oxidized into nitrate (NO_3^-), and the nitrification rate in expanded VIP model is described by the Michaelis-Menten equation (Abrahamsen and Hansen, 2000):

$$\delta_{nit} = \frac{V_{nit}^* \cdot f_{nit}^t(t) \cdot f_{nit}^h(h) \cdot C_{am}}{K_{nit} + C_{am}} \tag{4}$$

$$f_{nit}^t(t) = \begin{cases} 0 & T \leq 2\,°C \\ 0.15(T-2) & 2\,°C < T \leq 6°C \\ 0.10T & 6\,°C < T \leq 20\,°C \\ exp\left(0.47 - 0.027T + 0.00193T^2\right) & T > 20\,°C \end{cases} \tag{5}$$

$$f_{nit}^h(h) = \begin{cases} 0 & h \geq -10^{-2} \\ \dfrac{lg(-100h)}{1.5} & 1-10^{-2} > h \geq -10^{-0.5} \\ 1 & -10^{-0.5} > h \geq -10^{0.5} \\ 1 - \dfrac{lg(-100h)}{2.5} & -10^{0.5} > h \geq -10^{-2} \\ 0 & -10^{-2} > h \end{cases} \tag{6}$$

Where: δ_{nit} is the nitrification rate, μg cm^{-3} day^{-1}; V_{nit}^* is the nitrification rate constant under optimal temperature and moisture content, μg cm^{-3} day^{-1}; C_{am} is the ammonium concentration, μg cm^{-3}; K_{nit} is the semi-saturation constant, μg cm^{-3}; $f_{nit}^t(t)$ and $f_{nit}^h(h)$ are soil temperature functions and pressure potential function, respectively.

Denitrification rate. Denitrification rates are multiplicative functions of soil potential denitrification rate and dimensionless functions that explicate nitrate concentrations, soil temperature and moisture effects (Johnsson *et al.*, 1991). Henault *et al.* (2000) proposed a NEMIS denitrification rate prediction model based on the measured values of denitrification rate of undisturbed soil, nitrate concentration and water-filled pore space. Denitrification rate is expressed as (Henault *et al.*, 2000):

$$\xi_{den} = \frac{V^*_{den} \cdot f^t_{den}(t) \cdot f^{wf}_{den}(wf) \cdot C_{nt}}{K_{den} + C_{nt}} \quad (7)$$

$$f^{wf}_{den}(wf) = \begin{cases} 0 & WFPS < 0.62 \\ \left(\frac{WFPS - 0.62}{0.38}\right)^{1.74} & WFPS \geq 0.62 \end{cases} \quad (8)$$

$$f^t_{den}(t) = \begin{cases} exp\left(\frac{(t-11)\, ln\,(89) - 9 \cdot ln\,(2.1)}{10}\right) & t < 11\ ℃ \\ exp\left(\frac{(t-20) \cdot ln\,(2.1)}{10}\right) & t \geq 11\ ℃ \end{cases} \quad (9)$$

Where: ξ_{den} is the denitrification rate, μg cm^{-3} day^{-1}; V^*_{den} is the nitrification rate constant under the optimal temperature and moisture content, μg cm^{-3} day^{-1}; K_{den} is the semi-saturation constant, μg cm^{-3}; $f^t_{den}(t)$ is the soil temperature function; $f^{wf}_{den}(wf)$ is the water-filled pore space function; C_{nt} is the soil nitrate content, μg·cm^{-3}.

Ammonia volatilization rate. The rate of ammonia volatilization is affected by soil ammonium concentration, soil temperature and soil pH (Sherlock and Goh, 1984). It is expressed as:

$$\varphi_{vol} = \frac{k_{soil2air} \cdot NH_x}{k_{aq2soil}\left(1 + 10^{\left(0.09018 + \frac{2729.92}{T+237.15} - pH\right)}\right)} \quad (10)$$

Where: φ_{vol} is ammonia volatilization rate, kg hm^{-2} day^{-1}; NH_x is total amount of NH_4 and NH_3 in the soil, kg hm^{-2}; T is soil temperature, °C; pH is soil pH value; $k_{soil2air}$ is the exchange coefficient of ammonia in soil and air; $k_{aq2soil}$ is the exchange coefficient of ammonia in soil liquid water and soil.

Urea hydrolysis rate. Most of the nitrogen fertilizer applied is urea in the NCP. In the case of higher temperature and soil moisture, urea hydrolysis finishes in a few days, while it will take a longer time under lower temperature and dry conditions (Li *et al.*, 2007). The models, such as NLEAP, GLEAMS and EPIC, assume that urea hydrolysis occurs immediately, and urea is directly treated as ammonium nitrogen (Liang *et al.*, 2016). The urea hydrolysis process is described as (Li *et al.*, 2007):

$$R_{hys} = N_{urea} \cdot (1 - \exp(-0.5 \cdot WFPS \cdot K_{urea})) \quad (11)$$

Where: N_{urea} is the urea content in the soil, kg·hm^{-2}; *WFPS* is water-filled pore space.

Model initialization and parameters

Daily meteorological data measured at three ecology stations, which include maximum temperature, minimum temperature, average temperature, relative humidity, sunshine hours, precipitation and wind speed, was used to drive the expanded VIP model. The initial values of vegetation characteristics, such as initial crop height, maximum rooting depth, soil temperature and soil water content were specified from field observations or general site knowledge (Mo *et al*., 2001, 2012; Huang *et al*., 2015; Ma, 2004; Li, 2007; CERN). Soil organic turnover and mineralization parameters in the expanded VIP model mainly include different organic matter decomposition rates, carbon-nitrogen ratios, ammonia volatilization rates and denitrification rate (Table V), which were collected from the literatures (Parton *et al*., 1993; Abrahamsen and Hansen, 2000; Henault *et al*., 2000; Sherlock and Goh, 1984; Li *et al*., 2007; Williams *et al*., 1989). The model was spun-up for 300 years, using randomly selected forcing from five years of observation data at Yucheng stations. The model's carbon and nitrogen pools stabilized after about 200 years. After the spin up, the model was continually run forward from Oct. 1st, 2007 to Sep. 30th, 2010 at Fengqiu Ecology Station, from Oct. 1st, 2000 to Sep. 30th, 2015 at Yucheng Ecology Station and from Oct. 1st, 2003 to Sep. 30th, 2010 at Luancheng Ecology Station, using the observed forcing. Output obtained from these simulations was compared with corresponding observations.

TABLE V

Soil and crop nitrogen parameters in the expanded VIP model

Parameter	Description	maize	wheat	Unit
k_{sl}	Structural litter decomposition rate	0.0437	0.0437	day^{-1}
k_{ml}	Metabolic litter decomposition rate	0.0507	0.0507	day^{-1}
k_{mb}	Microbial decomposition rate	0.02	0.02	day^{-1}
$\boldsymbol{k_{sh}}$	Slow humus decomposition rate	0.0004	0.0004	day^{-1}
$\boldsymbol{k_{ph}}$	Inert humus decomposition rate	0.000008	0.000008	day^{-1}
$\boldsymbol{k_{ur}}$	Urea hydrolysis rate	10.0	10.0	kg hm^{-2} day^{-1}
$\boldsymbol{cn_{mb}}$	Microbial nitrogen to carbon ratio	0.125	0.125	
$\boldsymbol{cn_{sh}}$	Slow humus nitrogen to carbon ratio	0.165	0.165	
$\boldsymbol{cn_{ph}}$	Inert humus nitrogen to carbon ratio	0.145	0.145	
$\boldsymbol{V_{s2a}}$	exchange coefficient (between soil and air)	0.3624	0.3624	day^{-1}
$\boldsymbol{V_{w2s}}$	exchange coefficient (between soil and soil water)	0.03	0.03	
$\boldsymbol{\xi_{nit}}$	Potential nitrification rate	8.0	8.0	g m^{-3} day^{-1}
$\boldsymbol{\xi_{den}}$	Potential denitrification rate	20.0	20.0	g m^{-3}
$\boldsymbol{k_{den}}$	Michaelis constant (denitrification)	22.0	22.0	kg hm^{-2} day^{-1}
$\boldsymbol{k_{nit}}$	Michaelis constant (nitrification)	55.0	55.0	
$\boldsymbol{\varphi_{den}}$	Generate N_2O rate	0.25	0.25	mg kg^{-1}
$\boldsymbol{T_b}$	Base temperature	8.0	0.0	℃

T_c	Accumulated temperature	1800.0	3200.0	℃
bn_1	Seedling nitrogen concentration	0.064	0.060	
bn_2	Intermediate nitrogen concentration	0.0164	0.0231	
bn_3	Nitrogen concentration during maturity	0.0148	0.0134	

Sensitivity analysis and optimization

For complex agroecosystems models, parameter optimization requires a high computational cost. Through SA, the parameters, which have considerable effect on model performance, can be identified. Then, non-influential parameters are fixed at reasonable values, which will decrease the computational cost without reducing the model accuracy (Campolongo, 2007). In this study, the Morris method (Morris, 1991) is used firstly to screen the influential parameters related to soil nitrate concentration, denitrification and ammonia volatilization rate in the expanded VIP model. Then the first-order, second-order and total sensitivity indices of the identified parameters are further quantitatively analyzed by Sobol' method (Sobol, 2001). Finally, the SCE-UA algorithm (Duan *et al.*, 1994) automatically optimizes the selected parameters within the range of values, so that it can achieve the best agreement between simulated values and corresponding measured values of soil nitrate concentration, denitrification and ammonia volatilization rate. Software PSUADE (Problem Solving environment for Uncertainty Analysis and Design Exploration) is used for SA and optimization (Tong, 2016). It provides several global SA methods, which include the Morris, Sobol' method and SCE-UA optimization methods involved in this study. See the appendix for more details of Morris, Sobol' and SCE-UA algorithm.

Objective function. During the optimization process, the core of SCE-UA algorithm (Duan *et al.*, 1994) is to solve the minimum value of the objective function, which is used to evaluate the consistency between the observation and simulation value. Different objective functions are used to evaluate the different characteristics of the model. Gupta *et al.* (1998) summarized several objective functions for parameter optimization. In this study, root mean squared error is used to define the objective function. Depending on the type of observations, the observations are grouped and weighted accordingly. The objective function is divided into three groups: soil nitrate concentration, ammonia volatilization rate, and denitrification rate. The specific form of the objective function is as follows:

$$\varphi = \sqrt{\frac{1}{n}\sum_{i=1}^{n_n}(O_{ni}-S_{ni})^2\cdot\alpha_{ni}} + \sqrt{\frac{1}{n}\sum_{i=1}^{n_{an}}(O_{ani}-S_{ni})^2\cdot\alpha_{ani}} + \sqrt{\frac{1}{n}\sum_{i=1}^{n_{den}}(O_{deni}-S_{deni})^2\cdot\alpha_{deni}} \qquad (12)$$

Where: φ is the objective function, n_n、 n_{an} and n_{an} are the observed values of soil nitrate concentration, ammonia volatilization and denitrification rate, respectively. O_{*i} and S_{*i} represent measured and simulated values, respectively. α_{ni}、 α_{ani} and α_{deni} are the weighting coefficients of soil nitrate concentration, ammonia volatilization and denitrification rate, respectively, and their value is 1/3 in this study.

Evaluating indicators of model performance. The single indicator is difficult to evaluate comprehensively the model performance. It is necessary to describe the simulation accuracy by different indicators. In this study, three statistical indicators are used to assess the agreement between measured values and corresponding simulated values. The indicators are the root mean square error (RMSE) (Willmott, 1982), the Nash-Sutcliffe efficiency coefficient (NSE) (Nash and Sutcliffe, 1970), and the decision coefficient (R^2) (Nagelkerke, 1991). In addition to the statistical indicators (RMSE, NSE and R^2) mentioned above, this study uses two other statistical indicators, which are the average relative interval length (ARIL), and the percent of measured values coverage (P-95CI) at the 95 % confidence level, proposed by Li *et al.* (2010) to evaluate the uncertainty of the model performance. The equations were expressed as follows:

$$\mathrm{ARIL} = \frac{1}{N}\sum_{i=1}^{N}(S_{97.5\%}(i) - S_{2.5\%}(i))/O(i) \quad (13)$$

$$\mathrm{P-95CI} = \frac{NO_{in}}{N}\cdot 100\% \quad (14)$$

Where: $S_{97.5\,\%}$ and $S_{2.5\,\%}$ are the quantile value at the 97.5 % and 2.5 % of the simulated value set after 10,000 samples by Monte Carlo; NO_{in} is the number of measured values within the 95 % confidence interval. Smaller ARIL values indicate that the uncertainty interval is very narrow and a larger value of P-95CI indicates that the uncertainty interval is very reliable (Li *et al.*, 2010).

RESULTS

Sensitivity analysis

Screening the sensitive parameters by the Morris method. The Morris method is adopted to distinguish qualitatively sensitive parameters related to soil nitrate concentration, denitrification and ammonia volatilization rate. It needs to define the number of levels p (Yang, 2011), and the value of p is 8 in this study. Besides, this study assumes that all inputs are evenly distributed within the parameter range.

The results are shown by a plot with modified mean values μ^* (Fig. 3), respectively. The relatively larger magnitude of deviation from the origin of coordinates for a parameter indicates its importance. It is shown that the sensitive parameters related to soil nitrate concentration are potential nitrification rate, urea decomposition rate, semi-saturation constant, the decomposition rate of structural litter, the decomposition rate of metabolic litter, microbial decomposition rate, microbial nitrogen to carbon ratio and slow humus nitrogen to carbon ratio. The sensitive parameters related to denitrification rate are potential denitrification rate, potential nitrification rate, the decomposition rate of structural litter, the decomposition rate of metabolic litter, microbial nitrogen-carbon ratio, slow humus nitrogen-carbon ratio and the Michaelis constant of nitrification. The sensitive parameters related to ammonia volatilization rate are ammonia volatilization exchange coefficient, maximum nitrification rate and urea decomposition rate.

Fig.3 Sensitivity analyzing results of Morris for soil nitrate concentration, denitrification rate and ammonia volatilization rate at Fengqiu, Yucheng and Luancheng ecology stations. Sample size, which is calculated by $N = (n + 1) \times r$, is 440 in this study (n number parameter and replication times r is 20).

Quantitative analysis of the sensitive parameters by Sobol' method. Due to the Morris method is difficult to obtain the quantitative sensitivity of specific parameters, the Sobol' method is used to estimate the first-order sensitivity index, second-order sensitivity index and total sensitivity indices of expanded VIP parameters. The first-order sensitivity index and total sensitivity indices of soil nitrate concentration, denitrification and ammonia volatilization rate at Fengqiu, Yucheng and Luancheng Ecology Stations are shown in Figure 4.

At three stations, the ranking of the parameters for soil nitrate concentration obtained from the results of first-order sensitivity indices is consistent with that obtained from the total sensitivity indices. In detail, the potential nitrification rate is the most sensitive parameter at three the stations (Fig. 4A), and its first-order indices are 0.202, 0.246 and 0.189, respectively, at three ecology stations. This result can be explained by the Michaelis-Menten equation (Eq. 4) (Abrahamsen and Hansen, 2000), and the potential nitrification rate directly determines the nitrification process. From the results of total sensitivity indices (Fig. 4B), the soil nitrate concentration is highly affected by the potential nitrification rate, urea decomposition rate, semi-saturation constant and metabolic litter decomposition rate, which on average accounts for 29 %, 16 %, 14 %, and 11 % of soil nitrate concentration variability, respectively.

According to the results of first-order indices, the denitrification rate is the most sensitive to potential denitrification rate and potential nitrification rate at three the stations (Fig. 4C). The first-order indices are 0.19, 0.25 and 0.19 for potential denitrification rate and 0.18, 0.24 and 0.17 for potential nitrification rate at Fengqiu, Yucheng and Luancheng Ecology Stations, respectively. From the total sensitivity index (Fig. 4D), the denitrification rate is sensitive to potential denitrification rate, potential nitrification rate and urea decomposition rate, which on average accounts for 31 %, 23 % and 30 % of denitrification rate variability, respectively.

From the results of first-order sensitivity indices, ammonia volatilization exchange coefficient is the most sensitive parameter for ammonia volatilization rate at all three ecology stations (Fig. 4E), and its first-order indices are 0.17, 0.20 and 0.17, respectively. The sensitive parameter from the results of total sensitivity indices is similar to that from the results of first-order sensitivity indices, with a little different: exchange coefficient (v_{w2s}) rather than exchange coefficient (v_{s2a}) is the most sensitive parameter for ammonia volatilization rate at Fengqiu and Yucheng ecology stations (Fig. 4F). In general, the ammonia volatilization rate is sensitive to ammonia volatilization exchange coefficients (v_{s2a} and v_{w2s}), potential nitrification rate and urea decomposition rate, which on average accounts for 23 %, 28 %, 17 % and 12 % of ammonia volatilization rate variability, respectively.

Fig. 4 Sensitivity analysis results of Sobol' first-order and total index for soil nitrate concentration (A and B), denitrification rate (C and D) and ammonia volatilization rate (E and F) at Fengqiu, Yucheng and Luancheng ecology stations. Samples size of Sobol' can be estimated by $N = (n + 2) \times r$ (n represents number parameter and r represents replication times)

The second-order index represents the influence of the interaction between two parameters on the objective function. Fig 5 shows the second-order index between different parameters related to soil nitrate concentration, denitrification rate and ammonia volatilization rate at Fengqiu, Yucheng and Luancheng ecology stations. For soil nitrate concentration, the second-order index between potential nitrification and urea decomposition rate index shows the most interaction. And the second-order indices are 0.0046, 0.0026 and 0.0035, respectively, at Fengqiu, Yucheng and Luancheng Ecology Stations. For denitrification rate, the interaction between potential denitrification and urea decomposition rate is the most sensitive. And the second-order indices are 0.0145, 0.0116 and 0.0.0159, respectively. For ammonia volatilization rate, the interaction between two ammonia volatilization exchange coefficients (v_{s2a} and v_{w2s}) is the most sensitive. And the second-order indices are 0.0089, 0.0086 and 0.0084, respectively. Besides, when the first-order index of a parameter on the objective function is significant, the second-order interaction is also significant.

Fig. 5 Sensitivity analysis results of Sobol' second-order for soil nitrate concentration, denitrification rate and ammonia volatilization rate at Fengqiu, Yucheng and Luancheng ecology station.

Model calibration by SCE-UA optimization algorithm

According to the period and source of the observed data collected at the three experimental (Fengqiu, Yucheng and Luancheng) stations, this study calibrates the soil nitrate, denitrification rate and ammonia volatilization rate to validate performance of expanded VIP model in soil nitrogen cycle. Besides, to improve the calibration efficiency and accuracy, the SCE-UA algorithm is adopted to optimize the selected parameters based on the prior SA results, so that it achieves a good fit between measured and corresponding simulated values of soil nitrate, denitrification rate and ammonia volatilization rate. Evaluation indicators of soil nitrate concentration, denitrification and ammonia volatilization rate between reference value and SCE-UA optimization algorithm (Table VI). Specific parameter selection and the range of values of each parameter at three ecology stations are shown in Table VII.

TABLE VI

Evaluation indicators of soil nitrate concentration, denitrification and ammonia volatilization rate between reference value and SCE-UA optimization algorithm

Item	Reference value			SCE-UA optimization algorithm		
	RMSE	NSE	R^2	RMSE	NSE	R^2
Nitrate concentration	12.5	0.53	0.50	9.33	0.67	0.69
Denitrification rate	0.06	0.52	0.67	0.04	0.73	0.78
Ammonia volatilization rate	1.58	0.50	0.53	0.81	0.61	0.65

TABLE VII

Model related parameters after optimized by SCE-UA

Parameter	Description	Reference value	Range of values	SCE-UA optimization value			Unit
				Fengqiu	Luancheng	Yucheng	
k_{sl}	Structural litter decomposition rate	0.0437	(0.03496,0.05244)	0.0395	0.0474	0.0391	day^{-1}
k_{ml}	Metabolic litter decomposition rate	0.0507	(0.04056,0.06084)	0.0583	0.0711	0.0525	day^{-1}
k_{mb}	Microbial decomposition rate	0.02	(0.016,0.024)	0.024	0.0238	0.0216	day^{-1}
k_{ur}	Fertilizer decomposition rate	10	(8.0,12.0)	11.8	10.16	11.62	Kg hm^{-2} day^{-1}
cn_{mb}	Microbial nitrogen to carbon ratio	0.125	(0.1,0.15)	0.1	0.141	0.13	
cn_{sh}	Slow humus nitrogen to carbon ratio	0.165	(0.132,0.198)	0.132	0.1584	0.128	
V_{s2a}	exchange coefficient (between soil and air)	0.3624	(0.28992,0.43488)	0.325	0.391	0.414	day^{-1}
V_{w2s}	exchange coefficient (between soil and soil water)	0.03	(0.024,0.036)	0.0259	0.033	0.35	
ξ_{nit}	Maximum nitrification rate	8	(6.4,9.6)	9.5	8.4	0.855	g m^{-3} day^{-1}
ξ_{den}	Maximum denitrification rate	3	(2.4,3.6)	2.46	2.952	2.214	kg hm^{-2} day^{-1}
k_{den}	Michaelis constant (Denitrification)	22	(17.6,26.4)	22.3	25.76	20.07	mg kg^{-1}
k_{nit}	Michaelis constant (Nitrification)	55	(44,66)	45	51	40.5	
φ_{den}	Generate N2O rate	0.25	(0.2,0.3)	0.237	0.284	0.213	mg kg^{-1}

Dynamics of soil nitrate concentration during winter wheat-summer maize rotation system. Accurate simulation of soil nitrate concentration is helpful in further assessing the dynamics of soil organic turnover and mineralization. In this study, the simulated soil nitrate concentrations are evaluated with field observed values in soil surface (0 – 20 cm) and bottom layer (20 – 120 cm) during the growth periods of wheat and maize. The datasets of soil nitrate concentration from 2007 to 2008 at Fengqiu station and from 2000 to 2001 at Yucheng station were used to calibrate the expanded VIP model and the datasets from2008 to 2009 at Fengqiu station and from 2001 to 2002 at Yucheng station were used to validate the model (Fig 6). The statistical results show that, based on SCE-UA algorithm, the simulated soil nitrate concentration is close to the observed values in soil surface layer (0 – 20 cm) (Fig. 6A-1, 2), but it is overrated compared to measured values in soil bottom layer (20 – 120 cm) (Fig. 6A-3, 4) at Fengqiu station. In detail, the values of the RMSE, NSE and R^2 are 9.54 kg hm^{-2}, 0.59 and 0.61, respectively. The validation also obtains reasonable statistical results (RMSE = 11.52 kg hm^{-2}, NSE = 0.43, and R^2 = 0.49). The results also show that, at Yucheng station, the soil nitrate concentration values are not significantly overestimated or underestimated in both the calibration (Fig. 6B-1 and Fig. 6B-3) and validation (Fig. 6B-2 and Fig. 6B-4) periods. The simulation of soil nitrate concentration achieves good results with an RMSE of 8.36 kg hm^{-2}, NSE of 0.68 and R^2 of 0.62 in the calibration. The validation also shows good results (RMSE = 10.76 kg hm^{-2}, NSE = 0.59, and R^2 = 0.53). After calibration by SCE-UA algorithm, the RSME of soil nitrate concentrations are reduced by 34.2 % and 31.6 %, and the R^2 values are increased by 41.2 % and 39.1 %, respectively, at Fengqiu and Yucheng Station.

As shown in Fig. 6, the applied urea rapidly decomposes and converts into nitrate nitrogen, which leads to rapidly increase of soil nitrate concentration. The soil nitrate concentration decreases slowly during the seeding to reviving stage and then decreases rapidly after winter wheat reviving. The main reason is that the ammonia volatilization and denitrification process intensify with the temperature increased, and the crops nitrogen uptake increased rapidly after reviving stage. The results indicate that the expanded VIP model after calibrated by SCE-UA algorithm can simulate the soil nitrate concentration well. Given the complexity of nitrogen transformation, the ranges of these indices appear to be acceptable. These results indicated that the model performed well in simulating soil nitrate transport in this region. Liang *et al.* (2016) reported that the NSE values of soil nitrate concentrations simulation in different soil layers ranged from 0.29 – 0.63 for the four sites. Kersebaum *et al*. (2007) compared the simulation results of 13 soil crop models and found that the NSE of mineral N usually have negative values. In this study, these statistical indices are all within these reported acceptable ranges. Considering the high variability measured values of soil nitrate concentrations, the model prediction is accurate enough to provide guidance for decision making.

Fig. 6 Simulated and observed values for soil nitrate concentration (δ_{nit}) in soil surface ($0-20$ cm) and bottom layer ($20-120$ cm) during the growth periods of wheat and maize at Fengqiu and Yucheng ecology station during the calibration (A-1, A-3, B-1 and B-3) and validation (A-2, A-4, B-2 and B-4). Red arrow represents fertilization practice.

Denitrification rate. The datasets of denitrification rate during the growth periods of wheat and maize from 2008 to 2009 at Fengqiu and Luancheng station were used to calibrate the expanded VIP model and the datasets from 2009 to 2010 were used to validate the model in this study (Fig. 7). Based on SCE-UA algorithm, the statistical results of denitrification rate show that the expanded VIP model can effectively simulate the denitrification process in general during calibration (Fig. 7A-1 and Fig. 7B-1) and validation (Fig. 7A-2 and Fig. 7B-2) periods. The RMSE, NSE and R^2 are 0.04 kg hm^{-2}, 0.71, and 0.66, respectively, in calibration process at Fengqiu station. The corresponding values are 0.03 kg hm^{-2}, 0.77, and 0.72, respectively, at Luancheng station. The validation also shows fair statistical results based on the RMSE (0.06 kg $hm^{-2}$and 0.04 kg hm^{-2}, respectively), NSE (0.62 and 0.64, respectively), and R^2 (0.53 and 0.68, respectively). After calibration by SCE-UA algorithm, the results show that the RSME of denitrification rate are reduced by 29.8 % and 21.5 %, and the R^2 values are increased by 33.2 % and 35.6 % at Fengqiu and Luancheng Station. Besides, the 1:1 line of the fitting diagram also shows that the simulation of denitrification rate is acceptable.

The probability and intensity of denitrification progress during the maize growing season is greater than that in wheat growing season, as shown in Fig. 7. The low water content becomes the main limiting factor of the denitrification process during the wheat growing period. Furthermore, although the denitrification intensity has increased, there is no peak of denitrification in 2008 at Fengqiu station (Fig. 7A-1), because of the concentration of nitrate is already at a low level. The basic pattern of denitrification intensity in the maize period of 2009 (Fig. 7A-2) is similar to that at Luancheng station (Fig. 7B-1 and Fig. 7B-2), because the substrate (soil nitrate concentration) has maintained a relatively high level and is conducive to the microbial denitrification. In this study, the R^2 value of the denitrification rate was from 0.53 to 0.71, which is similar to the previous research conclusions (Li *et al*. 2007; Gu *et al* 2016). The DNDC model was used to simulate N_2O emissions during the winter wheat-summer maize growing season and the correlation coefficient ranged from 0.79 to 0.9. Gu *et al.* (2016) evaluated nitrous oxide emissions from a winter wheat-summer corn rotation during a 25-year fertilization trial in northwestern China. In addition, the expanded VIP model has a higher denitrification rate in the maize season than in the winter wheat season, which is consistent with previous results.

Fig. 7 Simulated and observed values for denitrification rate (ξ_{den}) during the calibration (A-1, and B-1) and validation (A-2, and B-2) at Fengqiu and Luancheng ecology station.

Ammonia volatilization rate. Ammonia volatilization is one of the main ways of nitrogen fertilizer loss in agroecosystems. The datasets of ammonia volatilization rate during the growth periods from 2008 to 2009 at Fengqiu station and from 2003 to 2004 at Luancheng station were used to calibrate the expanded VIP model and the datasets from 2009 to 2010 at Fengqiu station and Luancheng station were used to validate the model. Figure 8 presents the simulated and measured values of ammonia volatilization rate under fertilization treatments based on the SCE-UA algorithm and the reference values at Fengqiu and Luancheng station. The statistical results show that, based on SCE-UA algorithm, the simulated ammonia volatilization rate approximates the measured values in model calibration, with an RMSE of 0.91 kg hm^{-2} (Fig. 8A-1), but it is overestimated compared to measured values during model validation process, with an RMSE of 1.77 kg hm^{-2} (Fig. 8A-2) at Fengqiu station. The NSE values are 0.59 and 0.43 during model calibration and validation, respectively. The R^2 values are 0.64 and 0.55 in model calibration and validation process, respectively, at Fengqiu station. The results also show that, at Luancheng station, the prediction ammonia volatilization rates are close to the observed in both calibration (Fig. 8B-1) and validation (Fig. 8B-2). A good simulation of the ammonia volatilization rate is achieved with an RMSE of 0.86 kg hm^{-2}, NSE of 0.68 and R^2 of 0.79 during the model calibration process. The validation also shows good results (RMSE = 0.98 kg hm^{-2}, NSE = 0.59, and R^2 = 0.73). And the RSME of ammonia volatilization rates are reduced by 31.5 % and 30.2 %, and the R^2 values are increased by 35.3 % and 36.2 %, respectively, after optimized by SCE-UA algorithm at Fengqiu and Luancheng Station.

The results show that the ammonia volatilization rate was reduced to the lowest in mid-January and reached the highest in early August during the wheat and maize growing season. Since the relatively high temperature and humidity is beneficial to urea hydrolyzation, the volatilization rate gradually decreases and it tends to be stable in several days after the applied nitrogen fertilization. Besides, nitrogen fertilizer is generally applied to the soil surface, making it to be easily volatilized. Modeled NH_3 fluxes are highly sensitive to fertilizer practices. As indicated in Fig. 8, fertilizer application has virtually impact on NH_3 fluxes. Cui *et al*. (2014) modeled trace gas fluxes after fertilizer application, and the results indicate that application of fertilizers enhances NH_3 fluxes. The influence of change in fertilizer application date could be linked to two factors; change in temperature with time and the lag between fertilizer application and planting date. Applying fertilizers ahead of planting increases NH_3 fluxes since the time for nitrification and loss to the atmosphere before crop uptake is increased.

Fig. 8 Simulated and observed values for ammonia volatilization rate ($\ln(\varphi_{vol})$) during the calibration (A-1, and B-1) and validation (A-2, and B-2) at Fengqiu and Luancheng ecology station. Red arrow represents fertilization practice.

Uncertainty intervals of simulation performance

To evaluate quantitatively the uncertainty of simulation caused by parameter uncertainty, 10,000 parameter sets are sampled with Monte Carlo method. The ARIL and P-95CI of soil nitrate concentration, denitrification and ammonia volatilization rate are used to evaluate the uncertainty of parameters. The predicted uncertainties of soil nitrate concentration, denitrification and ammonia volatilization rates at Fengqiu station are presented in Fig. 9. The results show that the uncertainty ranges of the simulation results include most observations. The average length (ARIL) at the 95 % confidence level for soil nitrate concentration, denitrification and ammonia volatilization rate were 11.92, 0.008 and 4.26, respectively. There are about 68 %, 86 % and 92 % of observed values for soil nitrate concentration, denitrification and ammonia volatilization rates are inside the 95 % confidence interval in VIP model, indicating that individual parameter uncertainty is perhaps more important than other sources of uncertainty. The parameter uncertainty accounts for most of the deviation between the observed and the simulated.

Fig. 9 Uncertainty intervals of soil nitrate concentration (δ_{nit}), denitrification rate (ξ_{den}) and ammonia volatilization rate ($\ln(\varphi_{vol})$) at Fengqiu station from 2008 to 2009. The parameter sets are 10,000, which are sampled by the Monte Carlo method. Red arrow represents fertilization practice.

DISCUSSION

Effectiveness of sensitivity analysis methods

SA is a key step to identify sensitive parameters. It is also an effective means to comprehensively understand how the parameters affect the model performance and provides a scientific basis for further parameter optimization (Vrugt *et al.*, 2003). In this study, the Morris screening method is used to screen the parameters that have a great influence on simulations of soil nitrate concentration, denitrification and ammonia volatilization rate. The theoretical basis of Morris is based on the fundamental effect, which represents the model response to a particular parameter. The effect of each parameter is evaluated by the mean μ of the fundamental effects of each parameter (Campolongo *et al*., 2007).

The sensitivity results by the Morris method indicate that the nitrification and the decomposition of soil organic matter are the main sources of soil nitrate. Similar to this study, it has been confirmed that nitrification and soil organic matter decomposition are the main processes affecting soil nitrogen concentration (Xenakis *et al*., 2008; Liang *et al*., 2016). The denitrification rate is sensitive to potential denitrification rate and potential nitrification rate. From Michaelis-Menten equation (Equation 7), the potential denitrification rate and soil nitrate concentration are two important factors affecting the denitrification process, and the potential denitrification rate is the main parameter affecting the soil nitrate concentration, which indirectly confirms the results of sensitivity analysis. According to the results of the sensitive parameters of volatilization, it can be known that the ammonia volatilization exchange coefficient, the maximum nitrification rate and the urea hydrolysis rate have great influence on the volatilization process.

In the ammonia volatilization control equation, the gaseous ammonia concentration in the atmosphere is assumed to be zero, so the ammonia volatilization exchange coefficient will significantly affect the ammonia volatilization rate. These analysis results prove that the Morris method can effectively screen sensitive parameters.

In general, the inability to quantitatively estimate the contribution of parameters to the output variance and to distinguish the interactions between different parameters is the main limitations of the Morris algorithm (Yang, 2011). The second objective of SA is to quantitatively evaluate the influence of the selected sensitive parameters on model performance. Sobol' method is adopted to comprehensively evaluate the sensitive parameters selected by the Morris method. Sobol' sensitivity indices are ANOVA-like methods which are adopted to quantitatively assess the total indices of the parameters. In this study, the sample size of the Morris and Sobol' method are 440 and 2300, respectively. And the computational cost of the Sobol' method is about 5 times that of the Morris method. From the results of SA in this study, the potential nitrification rate has the greatest influence on soil nitrate concentration. Liang *et al.* (2016) evaluated the SA of the WHCNS model in the NCP. And the results showed that nitrogen conversion parameters, such as maximum nitrification rate and half-saturation constant, were important factors affecting soil nitrate concentration, which is similar to the results of this study. It should be pointed out that the results of the SA are only established at specific time scale and parameter range. Besides, the results of the SA depend on the parameterization scheme of the analysis method (Confalonieria *et al.*, 2010).

Effectiveness of SCE-UA algorithm on parameter optimization

There are few studies on optimizing parameters related to nitrogen cycle of agroecosystems model by SCE-UA algorithm, even widely used in hydrological models (Gelleszun *et al.*, 2017; Kan *et al.*, 2018). After the selected parameters are optimized by the SCE-UA algorithm, the simulation accuracy of nitrate concentration, denitrification and ammonia volatilization rate are significantly increased. The NSE for soil nitrate concentration increase to 0.67 after optimized in this study. By comparing the performances of multiple models, it was found that the NSE value of soil nitrate concentration varied from -0.81 to 0.20 (Kersebaum *et al.*, 2007). Relatively, the expanded VIP model simulation has a higher NSE value. For the denitrification rate, after optimized by the SCE-UA algorithm, the NSE and R^2 value increase to 0.73 and 0.78, respectively in this study, which is similar to the research conclusions (Li *et al* 2007). The correlation coefficient of N_2O emissions varied from 0.6 to 0.71 during the winter wheat-summer maize growing season using the DNDC model (Li *et al.*, 2010). Those results show that the expanded VIP model has a higher simulation accuracy. For the ammonia volatilization rate under fertilization treatments, the R^2 value is 0.62 after optimized by the SCE-UA algorithm in this study. Dubache *et al*. (2019) used the DNDC95 model to simulate the dynamics of ammonia volatilization rate after applicated urea. The statistical value R^2 value varied from 0.44 to 0.59, which is lower than the results of this paper. This indicates that, after optimized by the SCE-UA algorithm, the expanded VIP model can effectively capture the seasonal ammonia volatilization rate patterns during the wheat and maize growing periods.

Model parameter values of different model

In this study, the potential nitrification rate and its half-saturation constant, which the parameter range of the potential nitrification rates and half-saturation constants are 6.4 – 9.6 g m^{-3} day^{-1} and 44 – 66 g m^{-3} day^{-1}, have higher sensitivity in soil nitrate concentration, and the optimization values are 9.5 g m^{-3} day^{-1} and 44.0 g m^{-3} day^{-1}, respectively. Liang *et al.* (2016) studied the WHCNS model in the application of agroecosystems in the NCP and optimized the nitrogen conversion parameters by PEST. The potential nitrification rate and its half-saturation constant are 10.2 g m^{-3} day^{-1} and 51.7 g m^{-3} day^{-1}. The vales are slightly larger than the results of this study. Parameter optimization is closely related to the range of parameter values. The values of the above two parameters in the WHCNS model are 10 – 30 g m^{-3} day^{-1} and 25 – 75 g m^{-3} day^{-1}, respectively, which are larger than the range set in this study during the optimization process. This may be the reason why the above two parameters values are larger than this study. Besides, the objective function and the difference of the optimization algorithm are also the reasons for the different optimized values. The denitrification rate in the expanded VIP model is based on the NEMIS scheme (Henault and Germon, 2000), in which the denitrification rate and its half-saturation constant are important parameters influencing the denitrification rate, and the results optimized by the SCE-UA algorithm are 2.46 kg hm^{-2} day^{-1} and 22.3 mg kg^{-1}. Gu *et al*. (2016) simulated the denitrification rate of a maize-wheat rotation system in southwestern China by NOEv2 model. The denitrification rate is 2.96 kg hm^{-2} day^{-1}, which is similar to the value of this study. From the results of parameter optimization, some parameter's optimization results are unchanged. How to set the threshold of parameter sensitivity and determine the range of values of optimization parameters requires further research.

CONCLUSIONS

In this study, Morris and Sobol' algorithm are used to conduct global sensitivity analysis (SA) of the nitrogen cycle module. And the selected sensitive parameters, which are based on the previous global SA results, are optimized by SCE-UA algorithm to improve the simulation accuracy of expanded VIP model. Several conclusions are as follows:

According to the results of sensitivity indices, Morris and Sobol' algorithm could effectively identify sensitive parameters of soil nitrogen cycle module at three ecology stations. And the sensitive parameters related to soil nitrate concentration are potential nitrification rate, Michaelis constant, microbial carbon-nitrogen ratio and slow humus carbon-nitrogen ratio; the sensitive parameters related to denitrification rate are potential denitrification rate, Michaelis constant and N_2O production rate; the sensitive parameters for ammonia volatilization rate include ammonia volatilization exchange coefficient and potential nitrification rate.

After optimization by SCE-UA algorithm, the expanded VIP model may effectively simulate the dynamics of the soil nitrate concentration, denitrification and ammonia volatilization rate during the winter wheat and summer maize growing periods. Besides, the optimized value of each parameter is within a reasonable range. Furthermore, more than 68 % of observed values are inside the 95 % confidence interval.

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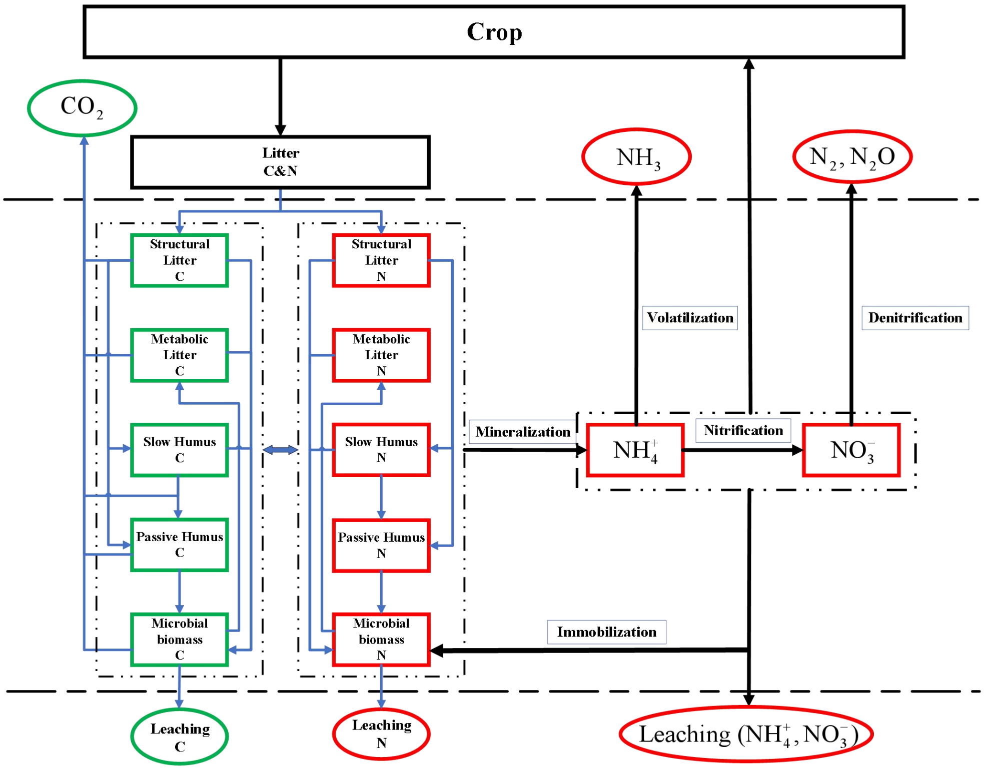


Fig. 1 Carbon and nitrogen pools and fluxes in expanded VIP model. The green and red shapes represent variables associated with carbon (C) and nitrogen (N), respectively.

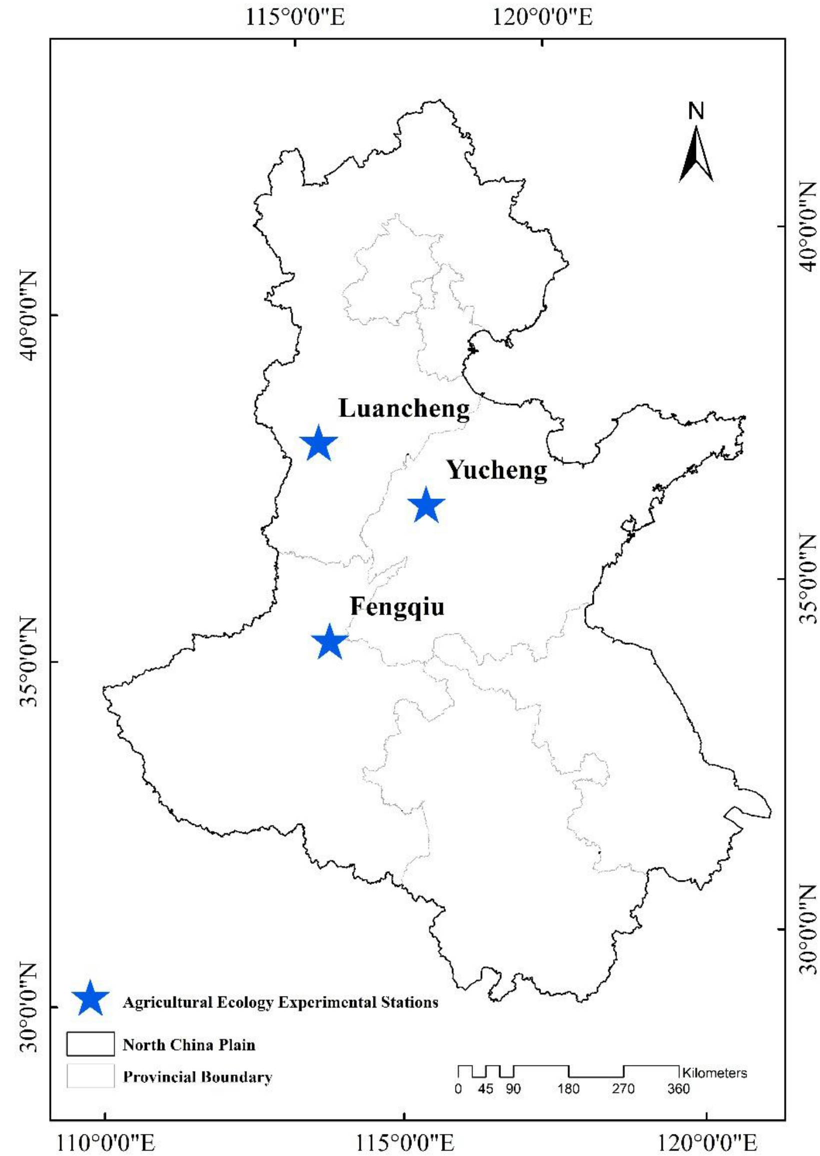


Fig. 2 Location map of the study area and the spatial distributions of agricultural ecology experimental stations.

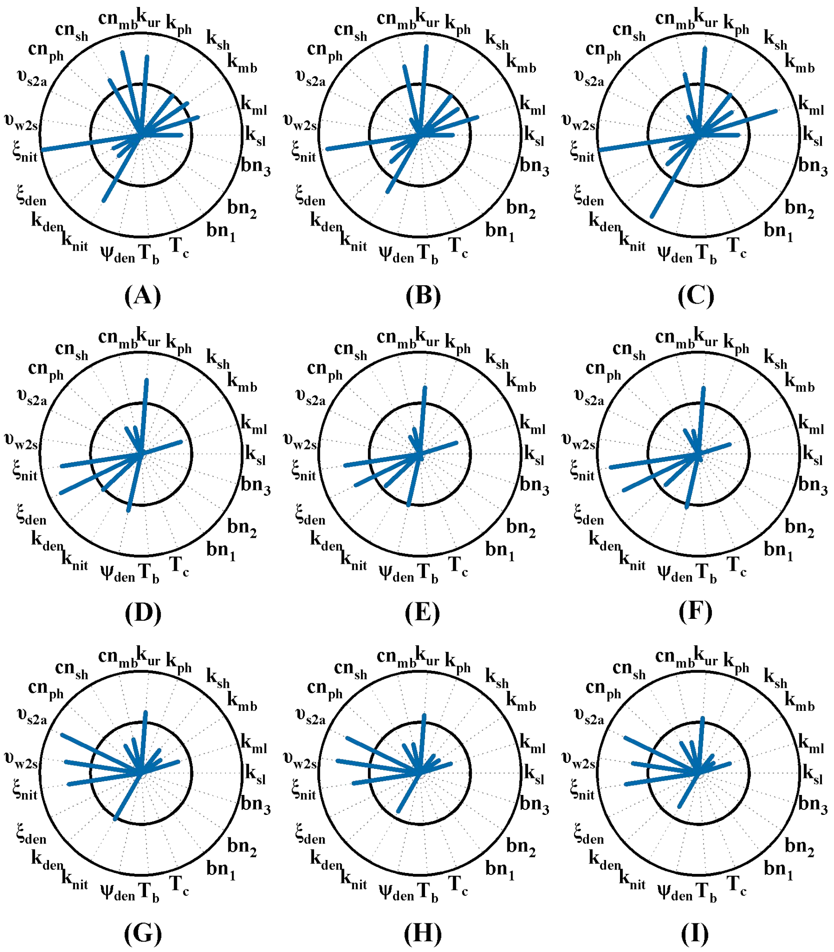
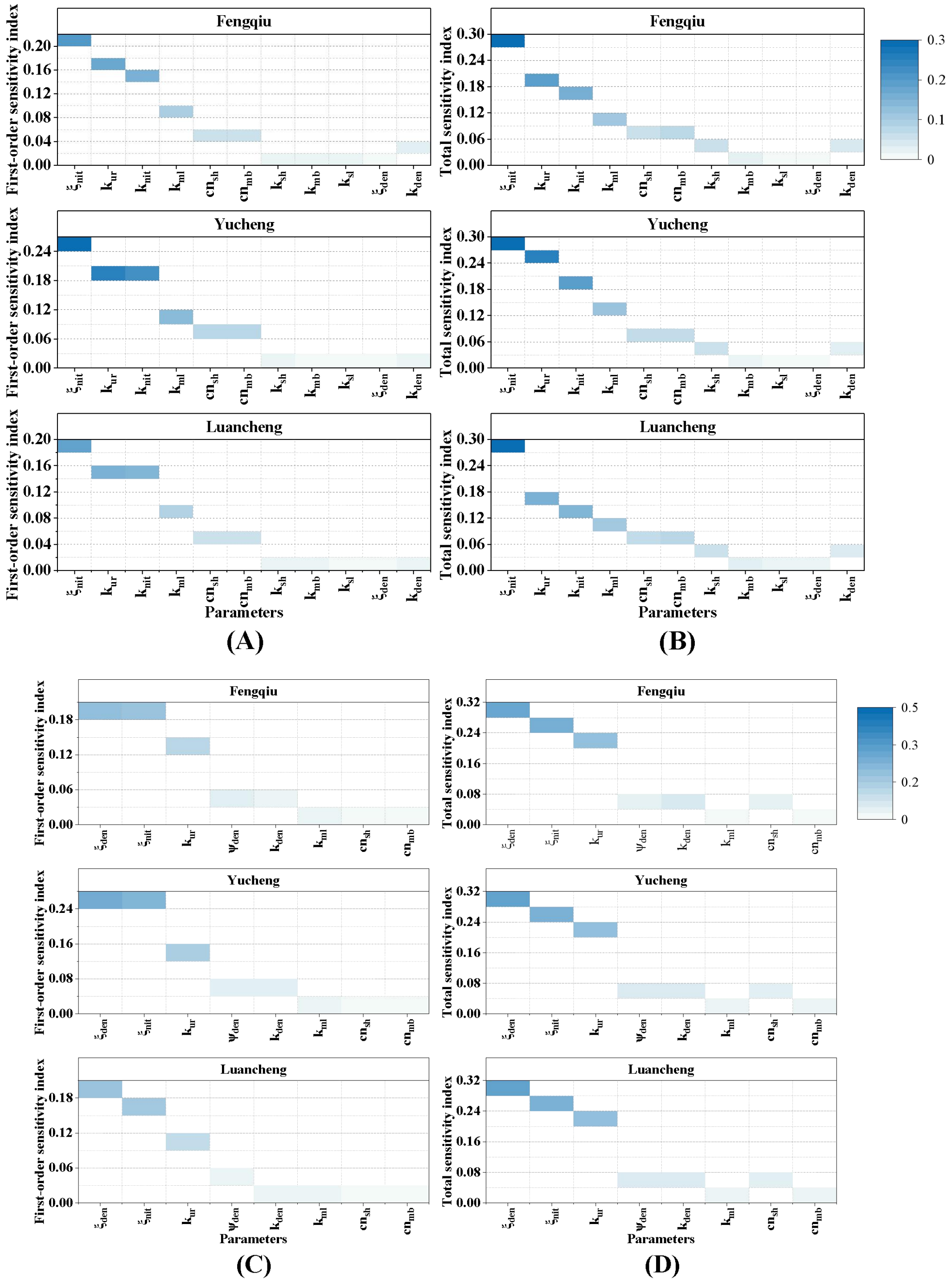


Fig.3 Sensitivity analyzing results of Morris for soil nitrate concentration (A-C), denitrification rate (D-F) and ammonia volatilization rate (G-I) at Fengqiu, Yucheng and Luancheng ecology stations. Sample size, which is calculated by $N = (n + 1) \times r$, is 440 in this study (n number parameter and replication times r is 20).


Fengqiu
Yucheng
Luancheng
First-order sensitivity index
Total sensitivity index
Parameters
(A)
(B)
(C)
(D)

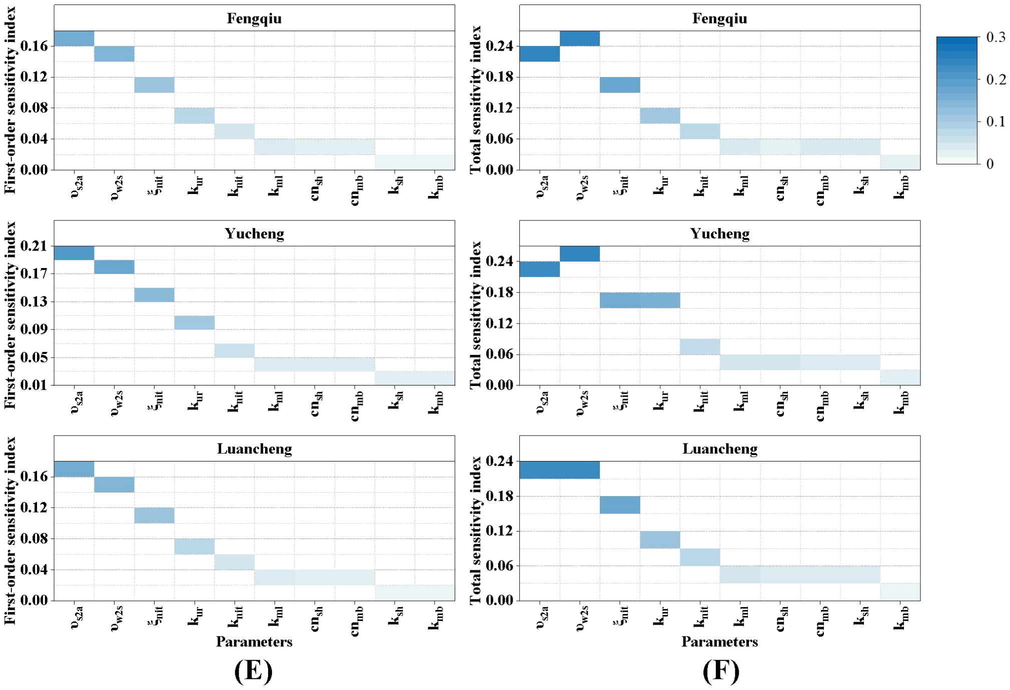


Fig. 4 Sensitivity analysis results of Sobol' first-order and total index for soil nitrate concentration (A and B), denitrification rate (C and D) and ammonia volatilization rate (E and F) at Fengqiu, Yucheng and Luancheng ecology stations. Samples size of Sobol' can be estimated by $N = (n + 2) \times r$ (n represents number parameter and r represents replication times).

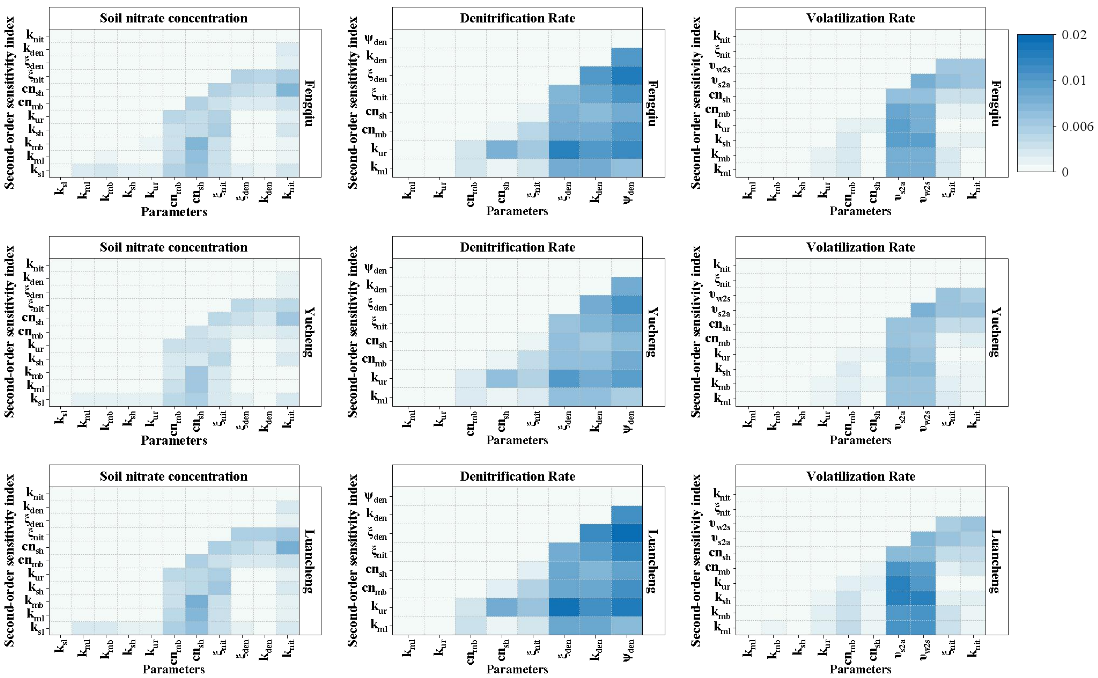


Fig. 5 Sensitivity analysis results of Sobol' second-order for soil nitrate concentration, denitrification rate and ammonia volatilization rate at Fengqiu, Yucheng and Luancheng ecology station.

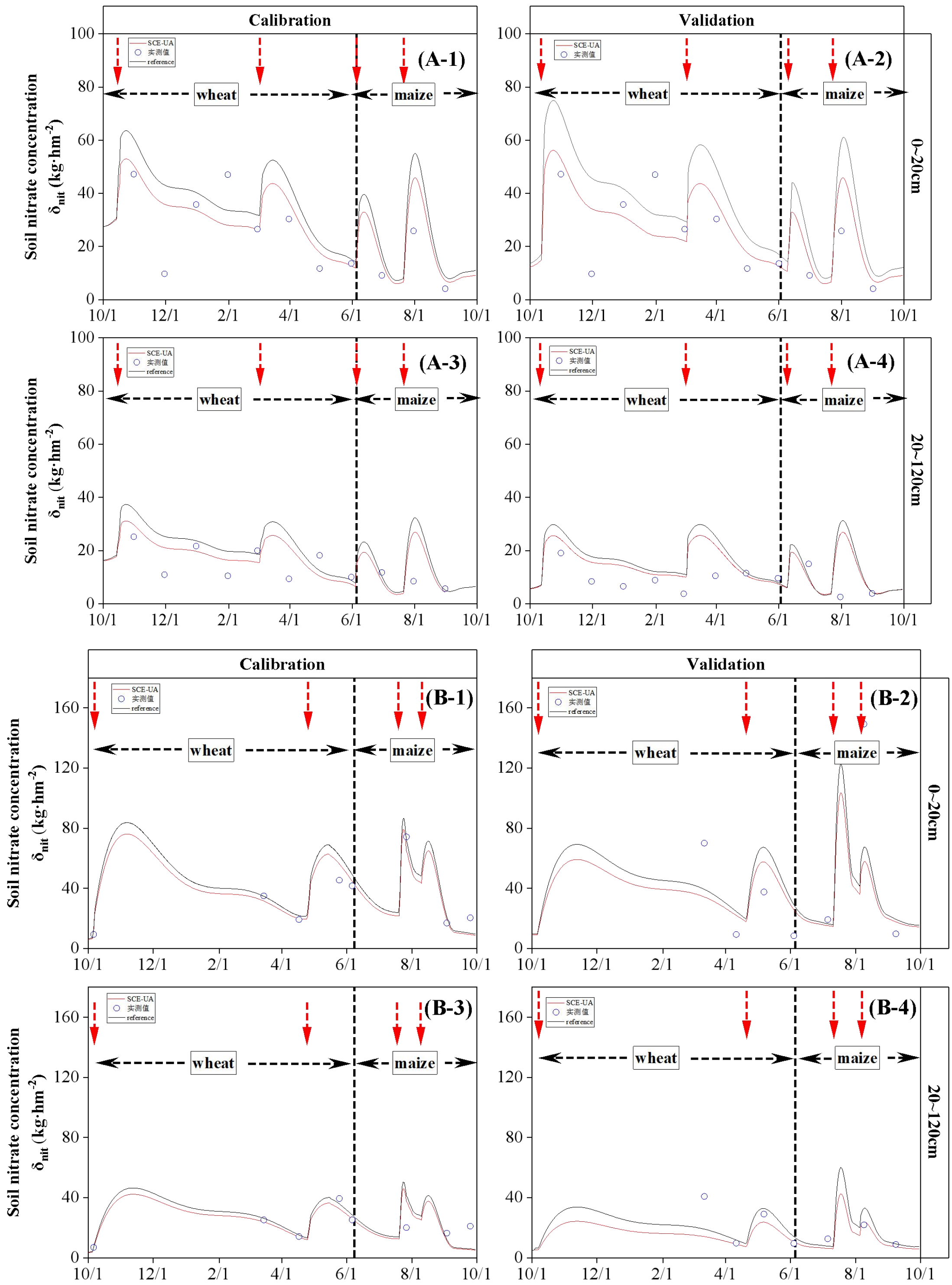


Fig. 6 Simulated and observed values for soil nitrate concentration (δ_{nit}) in soil surface (0-20cm) and bottom layer (20-120cm) during the growth periods of wheat and maize at Fengqiu and Yucheng ecology station during the calibration (A-1, A-3, B-1 and B-3) and validation (A-2, A-4, B-2 and B-4). Red arrow represents fertilization practice.

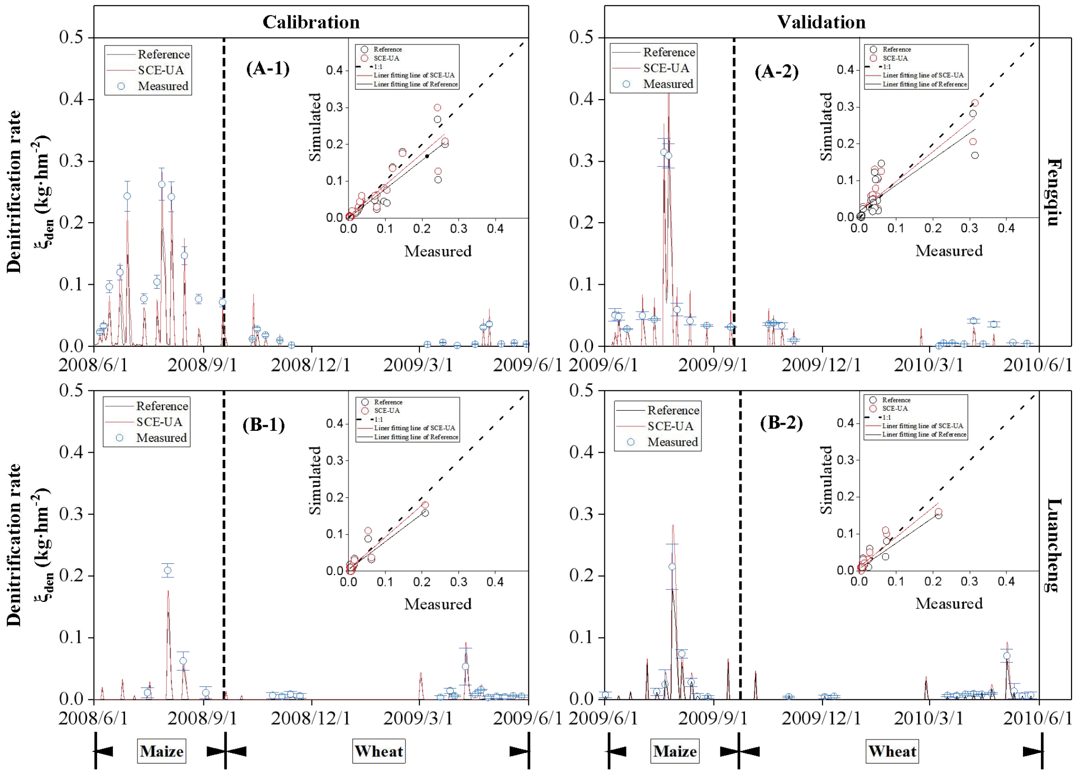


Fig. 7 Simulated and observed values for denitrification rate (ξ_{den}) during the calibration (A-1, and B-1) and validation (A-2, and B-2) at Fengqiu and Luancheng ecology station.

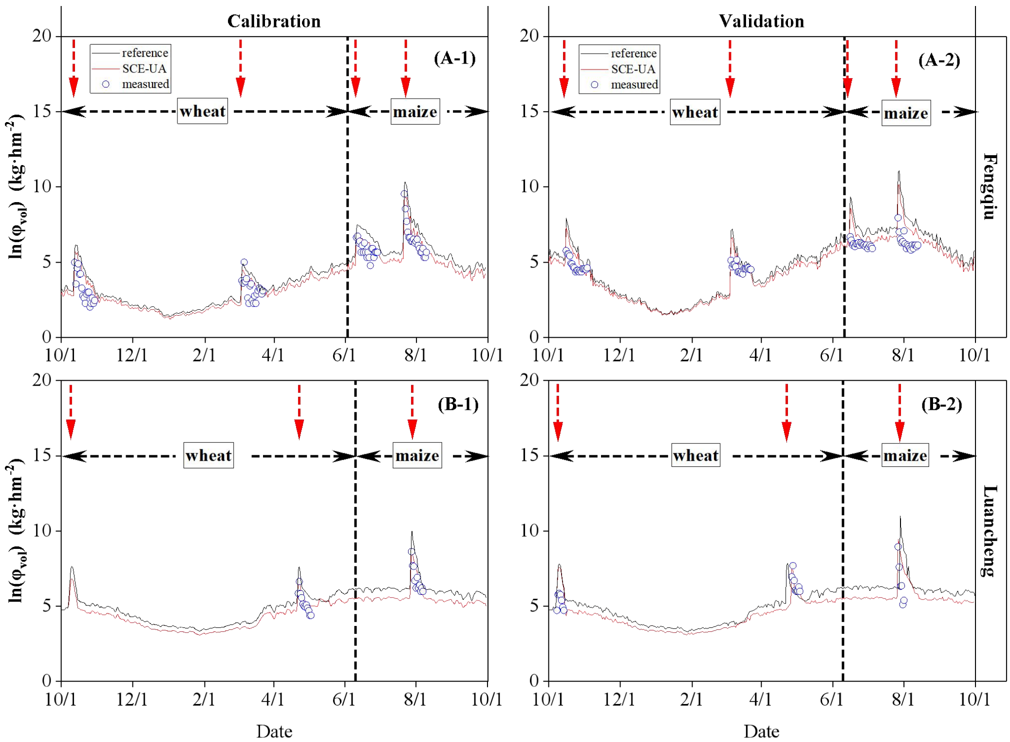
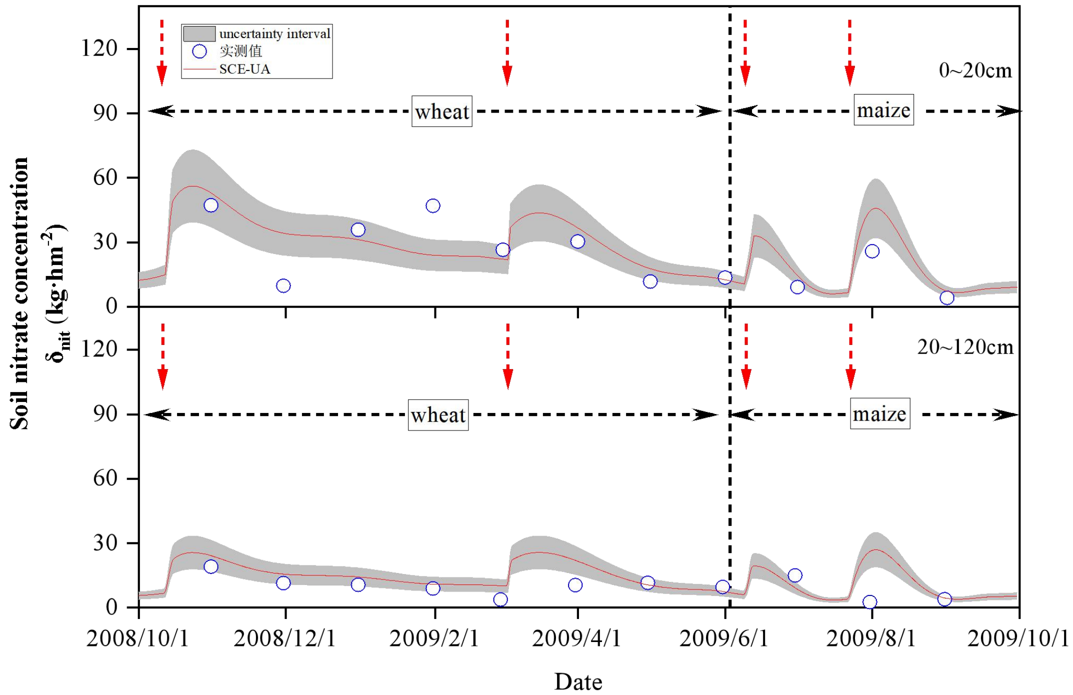
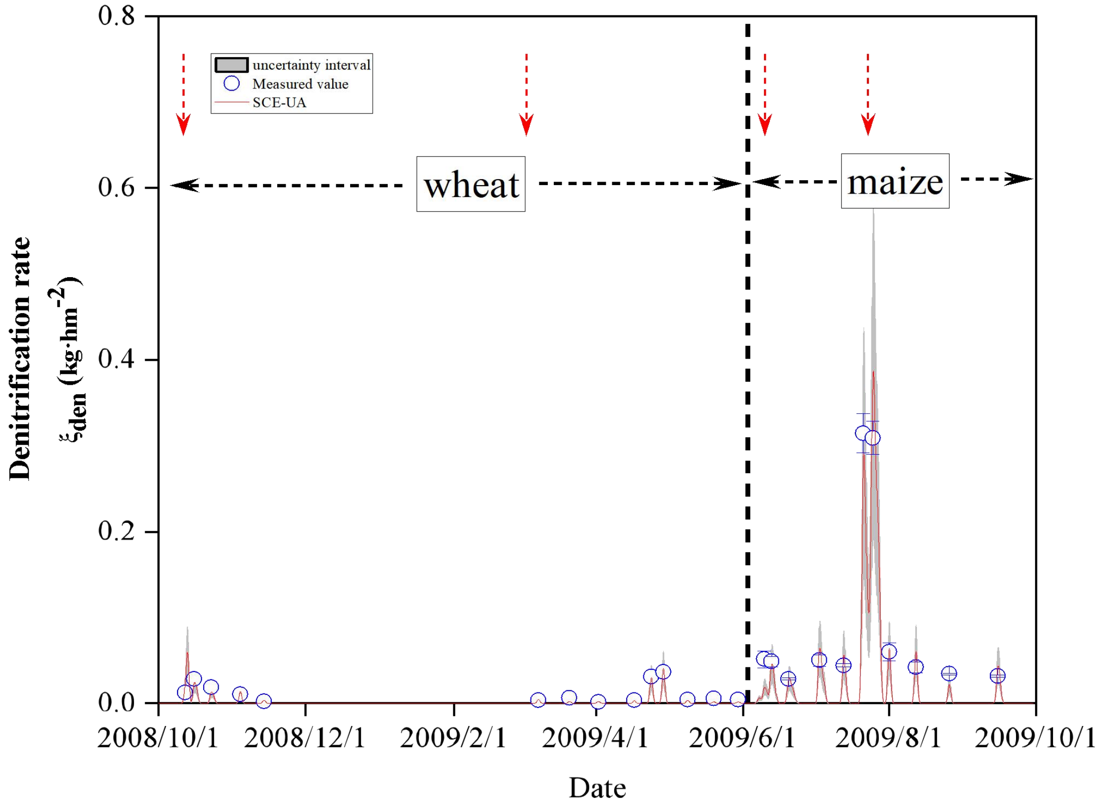


Fig. 8 Simulated and observed values for ammonia volatilization rate (ln (φ_{vol})) during the calibration (A-1, and B-1) and validation (A-2, and B-2) at Fengqiu and Luancheng ecology station. Red arrow represents fertilization practice.


uncertainty interval
实测值
SCE-UA
0~20cm
20~120cm
wheat
maize
Soil nitrate concentration
δnit (kg·hm-2)
120
90
60
30
0
2008/10/1
2008/12/1
2009/2/1
2009/4/1
2009/6/1
2009/8/1
2009/10/1
Date


uncertainty interval
Measured value
SCE-UA
wheat
maize
Denitrification rate
ξden (kg·hm-2)
0.8
0.6
0.4
0.2
0.0
2008/10/1
2008/12/1
2009/2/1
2009/4/1
2009/6/1
2009/8/1
2009/10/1
Date

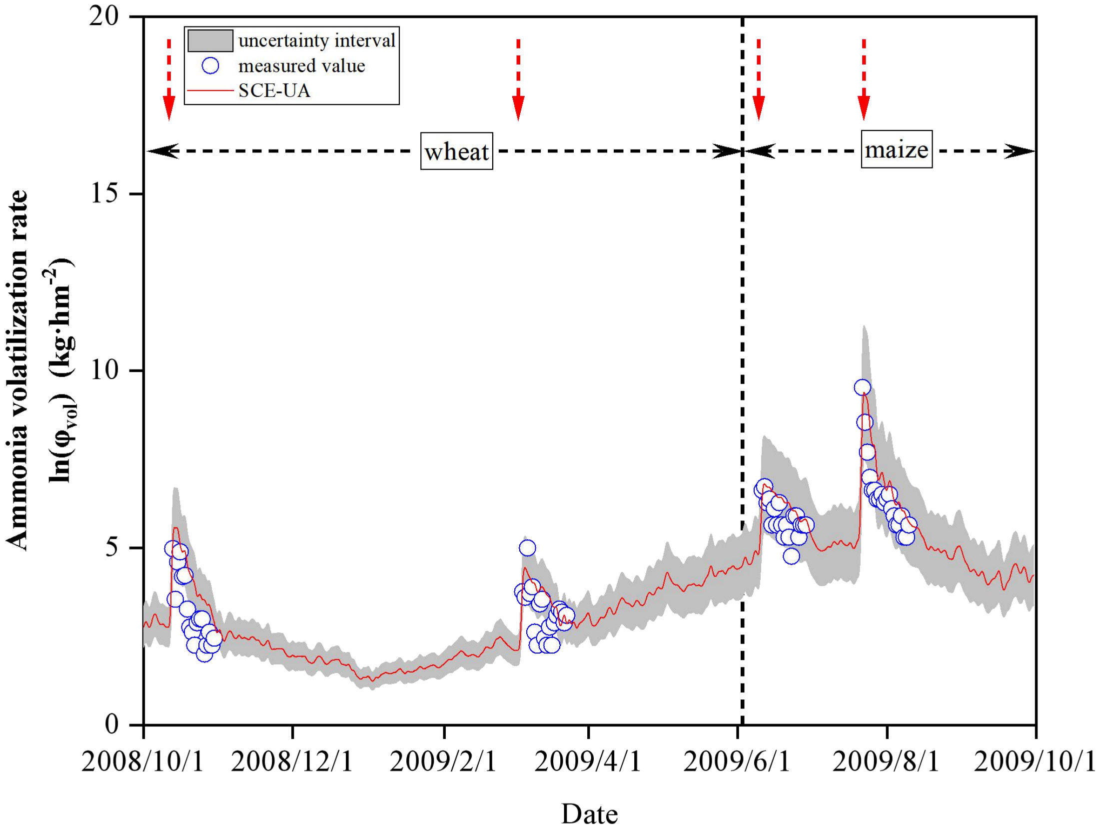


Fig. 9 Uncertainty intervals of soil nitrate concentration (δ_{nit}), denitrification rate (ξ_{den}) and ammonia volatilization rate ($\ln(\varphi_{vol})$) at Fengqiu station from 2008 to 2009. parameter sets, which are sampled by the Monte Carlo method, are 10,000. Red arrow represents fertilization practice.