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Modeling the biogeochemical effects of rotation pattern and field management practices in a multi-crop (cotton, wheat, maize) rotation system: a case study in northern China

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Abstract. The cropping system with rotations between cotton and winter wheat−summer maize (W-M) is widely adopted in northern China. Optimizing the rotation pattern and related field management practices of this system is crucial for reducing its negative impacts on climate and environmental quality. In this study, the approach applied to identify the optimal rotation pattern with the best management practice (BMP) relied on biogeochemical model simulations to determine the negative impact potential (NIP) of individual management options/scenarios and a set of constraints. The optimal rotation pattern and related BMP are referred to as the scenario with the lowest NIP that satisfies the given constraints. All the variables of interest were generated by simulation of the DeNitrification-DeComposition 95 version (DNDC95) model. The DNDC95 model validations performed previously for a land cultivated with the W-M and presently for an adjacent area cultivated with cotton showed satisfactory performance in simulating the variables of interest with available observations. The simulations of rotation patterns indicated that proper rotation of cotton and the W-M can simultaneously benefit crop yields, soil carbon sequestration and greenhouse gas mitigation. The three-crop rotation pattern in a 6-year cycle could be optimized with 3 consecutive years of cotton and 3 continuous years of W-M cultivation. The experiments with 108 management scenarios showed that the BMP for the optimized rotation pattern involved using 15% less nitrogen fertilizer (i.e., 94 and 366 kg N ha^{-1} yr^{-1} for cotton and the W-M, respectively) and 20% less irrigation water (i.e., 60−180 and 230−410 mm yr^{-1} for cotton and the W-M, respectively) by sprinkling than the conventional practices,

fully incorporating crop residues, and adopting the current deep tillage (20−30 cm) for cotton but the reduced tillage (10 cm) for the W-M. However, field confirmation of these BMPs resulting from the model-based virtual experiments is still required.

1 Introduction

Cotton is the world's most important fiber crop (www.fao.org/faostat). In China, it was cultivated in 2.0−3.9% of the annual crop harvest areas and supported cotton lint production of 5.3−7.6 million metric tons during 2007−2016 (China Statistical Yearbook, 2017). Wheat and maize are two important cereal crops in China and the world (www.fao.org/faostat). Accounting for 39% and 26% of the cereal harvest area in China, wheat and maize produced 129 and 220 million metric tons of grains in 2016, respectively (China Statistical Yearbook, 2017). The high yields of these crops are largely supported by intensive field management practices, such as high addition rates of fertilizer, improved irrigation and application of multiple-cropping systems (e.g., Chen et al., 2014; Galloway et al., 2004; Ju et al., 2009).

Northern China contains not only the second most important area of cotton production following that of northwestern China (China Statistical Yearbook, 2017) but also the largest area of the winter wheat−summer maize double-cropping system (i.e., both crops harvested within a year, hereinafter referred to as W-M) in the country (e.g., Cui et al., 2014). Therefore, rotations of cotton and the W-M have been commonly applied in this region (e.g., Liu et al., 2010, 2014). The fiber and double-cereal systems are typically alternated every 3−5 years. This typical practice is used not only to avoid the negative effects of monoculture on cotton yields but also to maximize the economic benefits in a balance of labor costs and grain prices (e.g., Liu et al., 2010, 2014; Lv et al., 2014). Relying on intensified field management practices by increased fertilizer inputs, advanced irrigation methods and highly mechanized operations (e.g., frequent applications of pesticides and/or herbicides), cotton maintains stable yields during short-term monoculture in recent decades (Han, 2010). In addition, a recent study indicated that the cotton cropping system in northern China persistently functioned as an intensive carbon or net greenhouse gas (GHG) source compared to the W-M because of strong carbon dioxide (CO_2) emissions during the long non-growing periods (Liu et al., 2019). These previous studies revealed that the change in storage of soil organic carbon (∆SOC), net ecosystem GHG emission

(NEGE) and other biogeochemical processes of the multiple-cropping systems in northern China likely are closely related to the rotation pattern of cotton and the W-M. Thus, one can hypothesize that identifying and adopting optimal rotation pattern of cotton and the W-M are beneficial for soil carbon sequestration and mitigation of GHG emissions in the region.

To maintain high lint and grain yields for economic profits and food/feed supplies, the three-crop rotation system of cotton and the W-M in northern China are characterized by high additions of synthetic nitrogen fertilizers and irrigation water (e.g., Ju et al., 2009). A number of studies have found that cotton and the W-M receive nitrogen fertilizer(s) at 60−140 and 550−600 kg N ha^{-1} yr^{-1}, and irrigation water at 140−200 and 90−690 mm yr^{-1}, respectively (Ju et al., 2009; Liu et al., 2014; Wang et al., 2008). High nitrogen and water inputs can result in extraordinary changes in biogeochemical processes and thus excessive nitrogen remaining in the soils and high release potentials of nitrogenous pollutants. These effects can further induce a series of environmental problems (e.g., Chen et al., 2014; Collins et al., 2016). In addition to fertilization and irrigation, other field management practices, e.g., tillage and crop residue treatment, can also affect the biogeochemical processes related to emissions of GHGs or nitrogenous pollutants, thereby contributing to negative environmental effects (e.g., Zhang et al., 2017b). Therefore, the evaluation of multiple-cropping systems is shifting from a single-goal method aimed at increasing crop yields to a multi-goal approach aiming to promote sustainability (e.g., Cui et al., 2014; Garnett et al., 2013; Zhang et al., 2018). Multi-goal evaluation is especially necessary for identifying the best management practice (BMP) while optimizing the rotation pattern of cotton and the W-M.

A multi-goal strategy of multiple-cropping systems aims to not only sustain/increase crop yields but also reduce environmental costs. Specifically, it aims to simultaneously sustain/increase crop productivity to ensure food security, increase SOC contents to improve soil fertility, mitigate NEGE to alleviate climate warming, reduce ammonia (NH_3) volatilization and nitric oxide (NO) emission to secure air quality, and abate nitrate (NO_3^-) leaching to protect water quality. For an ecosystem with annual vegetation, the −ΔSOC is regarded as the net CO_2 emission assuming negligible losses through non-respiration pathways, and the residual of the annual sum of methane (CH_4) and nitrous oxide (N_2O) emissions minus the ΔSOC is regarded as the NEGE. Based on the global warming potential (GWP) of each of the three GHGs, the NEGE is expressed as a CO_2 equivalent (CO_2eq) quantity for a given time horizon, such as 100 years. The 100-year GWPs, which are 1 for CO_2, 34 for CH_4 and 298 for N_2O (IPCC, 2013), are usually applied to calculate the CO_2 equivalents.

In general, there are two methodological categories for identifying the optimal rotation pattern(s) and/or BMPs (e.g., Cui et al., 2014). One is subjective. It screens and then combines the individual single-factorial practices with the maximal benefits (e.g., Farahbakhshazad et al., 2008). The other is objective. It evaluates each decision variable with price-based proxies or other measures and then calculates the negative impact potential (NIP) of individual options while generating a set of constraints. Then, it screens the best option that has the minimal NIP among the options with the given constraints (e.g., Cui et al., 2014; Xu et al., 2017). The subjective methods are generally not applicable to complex management scenarios with opposing effects among concerned decision variables. However, it is difficult to ensure comparability for the price-based proxies or other measures involved in the objective methods among studies with different backgrounds unless protocol-based values are provided for individual decision variables. So far, however, the protocols for the price-based proxies or other measures for the decision variables, including crop yields, NEGE, emissions of NH_3 and NO, and NO_3^- leaching, have not been available.

To identify an optimal rotation pattern of a cropping system with multiple crops and its BMP using the multi-goal approach, it is essential to quantify the biogeochemical effects of various pattern options and their individual scenarios of field management practices on the multiple decision variables mentioned above. As field experiments often focus only on the decision variables of very few rotation patterns and/or management practice treatments during short periods (e.g., Ding et al., 2007; Liu et al., 2010, 2015; Wang et al., 2013a, b), these experimental studies alone are insufficient for quantifying the comprehensive biogeochemical effects concerned in a multi-goal strategy. However, process-oriented biogeochemical models have the potential to overcome this limitation of field experimental studies, such as the DNDC (e.g., Chen et al., 2016; Li, 1992, 2000; Zhang et al., 2017a), DAYCENT (e.g., Delgrosso et al., 2005) and LandscapeDNDC (e.g., Haas et al., 2012; Molina-Herrera et al., 2016) models. For instance, the DeNitrification-DeComposition (DNDC) model has bridged primary ecological drivers (e.g., climate, soil properties, vegetation and anthropogenic activities such as field

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management) and biogeochemical processes (e.g., decomposition, nitrification, denitrification and fermentation) through soil regulating variables (e.g., temperature, moisture and pH). The regulating variables resulting from the model calculations are the key regulators of soil carbon and nitrogen transformation. Thus, the model can simultaneously simulate the aforementioned decision variables, i.e., crop yields; △SOC; emissions of CH_4, N_2O, NH_3 and NO; and NO_3^- leaching (e.g., Cui et al., 2014; Li, 2000, 2007).

The DNDC model was selected in this work to perform a modeling case study at a field site located in the most southwestern region of Shanxi Province. Model simulations were conducted to investigate the biogeochemical effects of various options of cotton and the W-M rotation patterns and their field management practices. The model version applied in this study, DNDC95, has been validated with comprehensive field measurements of the W-M at the selected field site (Cui et al., 2014), but not with the cotton cropping system. This case study aimed to (i) validate the performance of DNDC95 for the cotton cropping system with comprehensive field observations; (ii) simulate the abovementioned decision variables for individual scenarios of rotation pattern options and field management practices; (iii) investigate the biogeochemical effects of different patterns of the rotation between cotton and the W-M and those of the field management practice options; and, (iv) identify the optimal rotation pattern and its BMP in light of a multi-goal strategy. These efforts were undertaken to test the hypothesis that the sustainable intensification of the three-crop cultivation system aiming to enhance crop yields and simultaneously reduce environmentally negative impacts can be realized through the optimization of the rotation pattern and its field management practices.

2 Materials and methods

2.1 Brief introduction to the selected field site

The field site (34°55.50′N, 110°42.59′E, altitude of 348 m) selected for this modeling case study is situated at the Dongcun farm, near Yongji County, Shanxi Province, northern China. It is subjected to a temperate continental monsoon climate, with an annual precipitation of 580 mm and a mean air temperature of 14.4 ℃ in 1986–2010 (Cui et al., 2014). Cotton, winter wheat and summer maize are the major crops grown in this farm and its surrounding regions. Field experiments were carried out in two adjacent lands (each 100 m wide and 200 long) of the farm, in which comprehensive observations were performed for some of the multiple decision variables and some other related factors in 2007−2010. Both lands were used for long-term cultivation of the three crops, rotating from cotton to the W-M, or the opposite every 3−8 years until 2004. In the following 6 years (2005−2010), cotton was consecutively cultivated in one of the lands, while the W-M was used in the other. The soil of the land cultivated with cotton during the experimental period was a clay loam, with approximately 38% clay (< 0.002 mm), 57% silt (0.002−0.05 mm), 5% sand (0.05−2 mm), 10.0 g kg^{-1} SOC, 1.1 g kg^{-1} total nitrogen and a pH (H_2O) of 8.0 at 0−10 cm depth and a bulk density (0−6 cm depth) of 1.20 g cm^{-3} (Liu et al., 2010). The soil of the land cultivated with the W-M during the experimental period was also a clay loam, with approximately 32% clay, 50% silt, 18% sand, 11.3 g kg^{-1} SOC, 1.12 g kg^{-1} total nitrogen, a pH(H_2O) of 8.7 and a bulk density of 1.17 g cm^{-3} (Liu et al., 2011, 2012). A sprinkler system was applied in both lands. For more detailed information on both experimental lands, experimental design, field management practices, crop yields and data from comprehensive observations, please refer to Cui et al. (2014), Liu et al. (2010, 2011, 2014, 2015) and Wang et al. (2013a, b).

2.2 Brief introduction to the DNDC95 model

The DNDC95 model used in this study is one of the latest DNDC versions (www.dndc.sr.unh.edu/model/GuideDNDC95.pdf). Like the earlier and later versions, the DNDC95 model consists of two components with six modules in total. One component includes the soil climate, crop growth and decomposition modules while the other contains the nitrification, denitrification and fermentation modules. Driven by given primary ecological factors, the former component simulates the field states of a soil-plant system, such as soil chemical and physical status, vegetation growth and organic matter decomposition. Driven by the soil regulating variables yielded and provided by the former component, the latter component simulates the core biogeochemical processes of carbon and nitrogen transformations and physical processes of liquid and gas transportations and thus the annual dynamics of net ecosystem exchanges of CO_2 (NEE); emissions of CH_4, N_2O, NH_3 and NO; and NO_3^- leaching and the inter-annual dynamics of SOC and NEGE. These features enable the model

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simulations to investigate the integrative biogeochemical effects of the changes in rotation patterns of multiple crops and/or other management practices at the site or even regional scales, provided the model is validated with comprehensive field observations. The inputs used to facilitate the model simulation include (i) least meteorological variables of daily precipitation and maximum/minimum temperature; (ii) least soil (cultivated horizon) properties of the clay fraction, bulk density, SOC content and pH; (iii) least crop parameters of yield potential, thermal degree days (TDD) for maturity, and the mass fractions and carbon−to−nitrogen (C/N) ratios of grain, root and leaf plus stem; (iv) management practice variables of sowing and harvest (dates), fraction of incorporated/retained residue at harvest, tillage (date and depth), irrigation (date, method and water amount), and fertilization (date, type, method, nitrogen amount and C/N ratio of organic manure); and (v) other variables (annual means of NH_3 concentration in the atmosphere and ammonium plus NO_3^- concentration in rain water). For more details of the model, please see Li et al. (1992) and Li (2000, 2007, 2016).

2.3 Model validation for the cotton cropping system

Various DNDC versions have been widely applied in cropping systems across different regions of the world to assess the changes in a single decision variable of SOC variation, N_2O emission, NO release, or NO_3^- leaching (e.g., Chen et al., 2016; Giltrap et al., 2010; Li et al., 2017). So far, however, validation of any version with comprehensive observations of the multiple decision variables and their regulating factors has been scarce. Cui et al. (2014) validated the DNDC95 model using very intensive observations for most of the multiple decision variables and their related factors in the experimental land cultivated with the W-M (Liu et al., 2011, 2014, 2015; Wang et al., 2013a, b). Based on the work of Cui and her colleagues, the authors were able to further validate the performance of this model version in simulating the similar regulating factors and decision variables of the experimental land cultivated with cotton.

To validate the model for the cotton cultivation system, the observational data of the input items and those of some of the multiple decision variables and their related factors were collected from Liu et al. (2010, 2014) and Wang et al. (2013a, b). The daily meteorological data of 2004−2010 were directly obtained from Cui et al. (2014). Measured data (described in Sect. 2.1) were directly used for the least required soil properties. The field capacity and wilting point in water-filled pore space (WFPS) used as model inputs, being 0.65 and 0.2, respectively, were cited from Cui et al. (2014), who calibrated both values using the observations in the adjacent land cultivated with the W-M. The crop parameters for cotton were directly determined by the field measurements. The potential grain (seeds plus lint) yield was 1900 kg C ha^{-1}, which was given as 1.2 times the mean of the measured values. The mass fractions and C/N ratios of grain, root and leaf plus stem were 0.41 and 25, 0.16 and 40, and 0.43 and 40, respectively. The TDD from seeding to maturity was 3600 ℃, which was given as the sum of those daily averages of air temperature greater than 0 ℃ during the period from sowing to final grain harvest. The detailed management practices, including dates of operations; tillage depth; fertilizer type, amount and depth; and irrigation water amount and method (Table S1), were obtained from Li et al. (2009) and Liu et al. (2014). Compared with the conventional fertilizer application rate of 110−140 kg N ha^{-1} yr^{-1} for the cotton cropping system, the fertilizer doses of 2007 and 2008 were reduced to 66−75 kg N ha^{-1} yr^{-1} by local farmers to avoid the overgrowth of leaves instead of seeds or lint. The measured data used to validate the model outputs were available for soil (5 cm depth) temperature and topsoil (0−6 cm) moisture as major regulating factors and for those used as decision variables including N_2O and NO emissions in 2007−2009 (Liu et al., 2010, 2014), CH_4 uptake fluxes during the period from March to November 2010 (unpublished data of the authors), grain yields, and NEE during the period from November 2008 to November 2009 (Wang et al., 2013a). For the W-M, the crop parameters and other inputs used by Cui et al. (2014) were directly adopted in this study. As the validation of the model outputs for the W-M was reported by Cui et al. (2014), it was not repeated in this paper.

2.4 Scenario settings of rotation patterns and management practices

To investigate the biogeochemical effects of rotation pattern and management practices with the goal of identifying the optimal pattern and its BMP, two levels of scenarios were explored.

The level-I scenarios considered rotation patterns. They were set for a 6-year cycle based on surveys of local farmers (Liu et al., 2010, 2011, 2014). These pattern scenarios included all the rotation combinations between cotton and the W-M as well as the monoculture of the latter cropping system. Thus, there were six level-I scenarios in total, hereinafter referred to as R_0, R_1,..., R_5, from which the optimal pattern was selected. Among these scenarios, R_0 denotes the 6-year monoculture of the W-M; R_1 represents the 1-year cotton rotated with the 5-year W-M; and so on. Some years ago, the local farmers typically did not cultivate cotton monocultures for longer than five years in the region. However, heavy applications of herbicides, pesticides and germicides are often required to stabilize the cotton yields of long-term monocultures. To reduce the negative environmental effects of these chemicals, the longest cotton monoculture was set as 5 years in the level-I scenarios. For the transition from cotton to the W-M in each pattern scenario, winter wheat sowing occurs in late October of the same year, immediately following the last harvest of cotton grain. Prior to this winter wheat sowing, the cotton residues are cut with machinery operations and fully incorporated into the soil by plow tillage (30 cm depth). In the non-transition year, the cutting and incorporation of cotton residues occur in early November (Table S2). For the opposite transition, the cotton grown after the last maize is sown in the middle of April of the following year, with a bare-soil fallow period of nearly 5 months between the growing seasons of the two crops. In screening for the optimal rotation pattern, the management practices of the baseline level-II scenario (Tables S2−3) were adopted to drive the simulations for all the level-I scenarios.

The level-II scenarios considered the field management practices of fertilization, irrigation, crop residue treatment and tillage. From these scenarios, the BMP was identified for the optimal rotation pattern. In this regard, the level-II scenarios were set only for the optimal rotation pattern chosen from the level-I scenarios. In setting these level-II scenarios, five factors were considered, including (i) fertilizer dose, (ii) water amount and (iii) method of irrigation, (iv) incorporated/retained fraction of crop residues, and (v) depth of tillage. This resulted in 108 level-II scenarios in total, of which one was used as the baseline for all five factors, eight were used for the single-factorial settings (Table 1), and the remaining ninety-nine were the multi-factorial scenarios that were generated by fully combining the settings of the baseline and single-factor scenarios (details of combinations not shown). In each single-factor scenario, one of the five factors was exclusively modified, i.e., improved from its baseline level.

The values of the five factors were set for the baseline level-II scenario (Tables S2-3) by referring to the observations for the conventional management practices in both experimental lands (Liu et al., 2010, 2011, 2014; Wang et al., 2013a, b). These baseline management practices were widely adopted in the region (Cui et al., 2014). Specifically, the dates of sowing and final harvest were set as 14 April and 23 October, respectively, for cotton; as 24 October and 3 June, respectively, for wheat; and as 6 June and 14 October, respectively, for maize. Doses of nitrogen fertilizers were set as 110 and 430 kg N ha^{-1} yr^{-1} for cotton and the W-M, respectively. The fertilizer types, application methods and timings of the conventional management practices (Liu et al., 2010, 2011, Wang et al., 2013a) were adopted for the baseline scenario (Tables S1−2). Over the last few decades, the fields in the region have been mostly flood-irrigated (Liu et al., 2010). Therefore, flood irrigation was chosen for the baseline. The baseline timings and water amounts were set by referring to the 10- to 30-d cumulative precipitation prior to individual irrigations and the recorded timings and water amounts of conventional management practices in both lands during the experimental periods. Thus, the irrigation frequencies and annual cumulative water amounts during the three consecutive 6-year rotation cycles for the baseline scenario (Table S3) vary from 1 to 3 times and 75 to 230 mm yr^{-1} for cotton and 4 to 6 times and 290 to 510 mm yr^{-1} for the W-M, respectively. As the incorporation of crop residues has been widely adopted in northern China, full incorporation following the final harvest of each crop was set as the baseline. Two tillage depths were set in the baseline level-II scenario based on the conventional practices of the region. One is approximately 20 cm, which occurs immediately prior to the sowing of each crop. The other is 30 cm. This depth is used following the cutting of cotton stems immediately or shortly after the last grain harvest of this crop. Table S2 lists in detail the baseline management practices excluding those of irrigation.

The five non-baseline level-II scenarios include: (i) N94/366 and N77/301, which use 15% and 30% lower fertilizer nitrogen doses, respectively, than the single-factor baseline scenario (i.e., N110/430); (ii) I08 and I06, which reduce the water amounts of each irrigation event by 20% and 40%, respectively, relative to the single-factor baseline scenario (i.e., I10); (iii) IS, which adopts sprinkling instead of flood irrigation as the baseline method (i.e., IF); (iv) RI0, with no incorporation/retention of aboveground residues instead of the full incorporation/retention as in the baseline (i.e., RI1); and, (v) T10 and T0, which apply reduced tillage (to 10 cm depth) and no-tillage practices, respectively, for the W-M, instead of the conventional tillage depth of 20 cm used as the baseline (i.e., T20).

Table 1 summarizes the different settings of the five management factors among the basic level-II scenarios.

2.5 Operation of model simulation

For all the scenarios of both levels, the average outputs of individual decision variables for 18-year simulations, including three consecutive 6-year rotation cycles of each level-I scenario, were used to assess the biogeochemical effects of rotation patterns and management practices. The simulations were driven by the meteorological data observed at the Yuncheng station (approximately 60 km east to the experimental site) in 1996−2013, which were provided by the China Meteorological Data Service Center (http://data.cma.cn/data/cdcindex/cid/6d1b5efbdcbf9a58.html). To stabilize the carbon and nitrogen dynamics and reduce the residual effects of initial conditions (Zhang et al., 2015), especially to establish the carbon and nitrogen equilibriums among different pools, a spin-up of at least 10 years is usually required (Palosuo et al., 2012). For this reason, the model applied a spin-up of 12 years (i.e., a period of two 6-year rotation cycles) before performing the 18-year simulations for each scenario. The spin-up was driven by the same rotation pattern and field management practices as each scenario. The average yields were the averages of cotton, wheat and maize yields of all three 6-year rotation cycles, while the average values of other decision variables explicitly or implicitly involved in Eq. (1) were the averages of 18-year simulations for each scenario.

2.6 Method for identifying the best management practices

An objective method jointly relying on three constraints and NIPs was adopted in this study to identify the optimal rotation pattern and BMP. These constraints included (i) stable or increased crop yields, (ii) stable or increased SOC (identical with the SOC definition of Cui et al. 2014), and (iii) reduced NEGE. In the present study, the NEGE was quantified as a CO_2eq based on the 100-year GWPs provided by the IPCC (2013). The NIP was used to evaluate the potential for a climatically and environmentally integrative impact exerted by a rotation pattern with a given level-II scenario. The NIP was measured in this study by a price-based proxy quantity in USD ha^{-1} yr^{-1}, even though other alternative units were used in other similar studies. The NIP was determined by the quantities of

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individual decision variables and their coefficients as mass-scaled price-based proxies (Eq. (1)).

$$\mathrm{NIP} = k_1\mathrm{NEGE} + k_2\mathrm{NH_3} + k_3\mathrm{NO} + k_4\mathrm{N_2O_{ODM}} + k_5\mathrm{NL} \quad (1)$$

In Eq. (1), NEGE, NH_3, NO, N_2O_{ODM}, and NL represent the multi-goal decision variables of net ecosystem GHG emission (Mg CO_2eq ha^{-1} yr^{-1}), NH_3 volatilization, NO emission, release of N_2O as ozone layer depletion matter and hydrological nitrogen loss (mainly by NO_3^- leaching), respectively (kg N ha^{-1} yr^{-1} for all the variables of nitrogen compounds). The coefficients k_1, k_2, k_3, k_4 and k_5 are mass-scaled price-based proxies of NEGE, NH_3, NO, N_2O_{ODM}, and NL, respectively. Their values presented in Cui et al. (2014) were directly used in this study, which were 7.00 USD Mg^{-1} CO_2eq, and 5.02, 25.78, 1.33 and 1.92 USD kg^{-1} N for k_1, k_2, k_3, k_4 and k_5, respectively.

In Eq. (1), a lower NIP indicates a better set of management practices that can exert smaller negative impacts on the climate and environment. Accordingly, the optimal rotation pattern with the BMP was identified as the scenario with the lowest NIP among those scenarios satisfying all three constraints.

2.7 Statistics and analysis

The statistical criteria of the (i) index of agreement (IA) (Eq. (2)), (ii) Nash-Sutcliffe efficiency (NSI) (Eq. (3)) evaluating modeling efficiency (e.g., Moriasi et al., 2007; Nash and Sutcliffe, 1970), (iii) determination coefficient (R^2), slope and significance level of a zero-intercept univariate linear regression (ZIR) of observations (o) against simulations (s) and (iv) model relative bias (MRB) (e.g., Congreves et al., 2016; Willmott and Matsuura, 2005) were simultaneously used to evaluate model validity. In Eqs. 2−4, k and n (k = 1, 2,..., n) denote the kth pair and the total pair number of the values, respectively, and $\bar{o}$ represents the mean of observations. The IA index falls between 0 and 1, with a value closer to 1 indicating better simulation, and vice versa. An NSI value between 0 and 1 shows acceptable model performance and otherwise, worse. The R^2 value of a ZIR, which has the same meaning as that of a univariate linear regression including an intercept, is also calculated by Eq. (4) (Jiang, 2010), wherein $\hat{o}$ denotes the s-based prediction using the ZIR. The F-test was used to determine the significance level of a ZIR. Better model performance is indicated by a significant ZIR at $P < 0.05$ and a slope and an R^2 value being closer to 1, and vice versa. A slope less than 1 indicates an overestimation by simulations and the opposite underestimation. The MRB, which is expressed as a percentage, is defined by Eq. (5), wherein $\bar{s}$ denotes the average of simulations. In this study, an absolute MRB greater than two times the coefficient of variation (CV) (or a simulation falling outside of the range of mean ± two standard deviations) of spatially replicated observations is used to represent a significant discrepancy based on the 95% confidence interval (CI); the opposite indicates a good agreement or an insignificant discrepancy based on the CI. A positive MRB value indicates overestimation by modeling whereas a negative value indicates underestimation.

$$\mathrm{IA} = 1 - \frac{\sum_{k=1}^{n}(s_k - o_k)^2}{\sum_{k=1}^{n}(|s_k - \bar{o}| + |o_k - \bar{o}|)^2} \tag{2}$$

$$\mathrm{NSI} = 1 - \frac{\sum_{k=1}^{n}(o_k - s_k)^2}{\sum_{k=1}^{n}(o_k - \bar{o})^2} \tag{3}$$

$$R^2 = 1 - \frac{\sum_{k=1}^{n}(o_k - \hat{o}_k)^2}{\sum_{k=1}^{n}(o_k - \bar{o})^2} \tag{4}$$

$$\mathrm{MRB} = 100\,\frac{\bar{s} - \bar{o}}{\bar{o}} \tag{5}$$

In this study, ZIR analysis, variance analysis, and graphical comparison were performed with SPSS Statistics Client 19.0 (SPSS Inc., Chicago, USA) and Origin 8.0 (OriginLab, Northampton, MA, USA) software.

3 Results

3.1 Model validation of the cotton cropping system

The seasonal dynamics and magnitudes of soil (5 cm) temperature and topsoil (0−6 cm) moisture were predicted well by the model simulations (Figs. 1a−b). The sound model performance was indicated by the IA, NSI, and ZIR slope and R^2 of 0.99 and 0.81, 0.95 and 0.24, 1.05 and 0.93, and 0.95 (n = 677, P < 0.001) and 0.29 (n = 432, P < 0.001) for the temperature and moisture, respectively.

For the comparison of cotton yields (seeds plus lint) for two consecutive years, the simulations

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and observations also agreed well, with an absolute MRB of 7%, which was less than two times the spatial CVs (37−44%) for the measurements (adapted from Liu et al., 2014).

The simulated seasonal patterns and peak emissions of N_2O and NO generally matched the observations (Figs. 1c−d). The simulations showed a relatively low modeling efficiency for daily fluxes, as indicated by the IA, NSI, and ZIR slope and R^2 of 0.77, < 0, 0.48 and 0.40 (n = 592, P < 0.001), respectively, for N_2O and of 0.62, < 0, 0.37 and 0.09 (n = 614, P < 0.001), respectively, for NO. Nevertheless, the simulated annual N_2O and NO emissions in the two consecutive experimental years were comparable with the observations, with absolute MRBs of less than 3% and 6%, respectively, both of which were less than two times the spatial CVs (24−50%) for the measurements (adapted from Liu et al., 2014).

The simulated NEE fluxes suggested that the model captured the seasonal fluctuations, which were negative in the cotton growing season, but positive or neutral during the remaining periods (Fig. 1e). The IA, NSI, and ZIR slope and R^2 were 0.72, 0.29, 0.79 and 0.31 (n = 365, P < 0.001), respectively, for the daily NEE simulation. For the annual cumulative NEE, the model simulation showed an absolute MRB of 2%, which was less than the reported uncertainty (25%) of observations (Wang et al., 2013a)

For CH_4 uptake, the observations and simulations showed similar seasonal variations (Fig. 1f), with the IA, NSI and ZIR slope and R^2 of 0.71, < 0, 0.76 and 0.16 (n = 69, P < 0.01), respectively. The model simulation yielded an absolute MRB of 8% for the cumulative CH_4 uptake, which was smaller than two times the spatial CVs (12%) of observations (adapted from the unpublished data).

These results suggest that the DNDC95 model could be applicable for investigating the biogeochemical effects of different rotation patterns between cotton and the W-M and those of different management practices under a given rotation pattern.

3.2 Biogeochemical effects of different cotton and wheat−maize rotation patterns

Figure 2 illustrates the dynamics of crop yields and each decision variable resulting from the consecutive simulations over 18 years for all rotation pattern options subject to the field management practices of the baseline scenario. Figure 3 shows the relationship between the annual average of each decision variable and the number of consecutive years of cotton monoculture within the rotation pattern options.

The average grain yields of cotton, wheat and maize were not significantly different among various rotation pattern options, with averages of 3.0, 5.0 and 7.0 kg dry matter ha^{-1} for cotton, wheat and maize, respectively (Figs. 2a−c).

For the dynamic changes in annual SOC stocks, the values were positive for the W-M, but negative for the cotton, except for the first year after the transition to this fiber crop. As Fig. 2d indicates, the simulated SOC contents over the 18-year period increased for R_0, R_1, R_2 and R_3 but decreased for R_4 and R_5. The annual average −ΔSOC significantly increased ($P < 0.001$) with an increase in the consecutive years of cotton monoculture from 0 to 5 within the 6-year rotation cycle (Fig. 3a). Rotation pattern options with baseline management showed small variations in CH_4 uptake (Fig. 2e), with the annual uptake ranging from 1.80 to 1.89 kg C ha^{-1}. However, the annual averages of CH_4 uptake significantly increased ($P < 0.001$) with an increase in the consecutive years of cotton monoculture from 0 to 5 within the 6-year rotation cycle (Fig. 3b). For N_2O, the annual emission of the rotation options with the management baselines showed large inter-annual variations (Fig. 2f), with a CV of 21−45%. Meanwhile, the annual average emissions of this gas significantly decreased from 4.3 to 2.6 kg N ha^{-1} (Fig. 3c) with an increase in the consecutive years of cotton monoculture ($P < 0.001$). As a result, increasing the consecutive years of cotton monoculture from 0 to 5 within a 6-year rotation significantly promoted ($P < 0.01$) the NEGE (Figs. 2g and 3d).

As for the gaseous air pollutants of NH_3 and NO, the simulated annual emissions ranged from 17 to 104 and 0.5 to 3.5 kg N ha^{-1}, respectively (Figs. 2h−i). Figures 3e and f show that the averages of annual emissions of both gases were significantly reduced by increasing the consecutive years of cotton monoculture from 0 to 5 within the 6-year rotation cycle ($P < 0.001$).

The annual NO_3^- leaching of different rotation pattern options displayed significant inter-annual variations (Fig. 2j), with CVs of 40−68%. Thus, the annual averages of NO_3^- leaching insignificantly changed in response to the consecutive years of cotton monoculture within the 6-year rotation cycle (Fig. 3g).

The NIP significantly varied among the various rotation pattern options ($P < 0.001$), declining

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from 609 to 320 USD ha^{-1} yr^{-1} with an increase in the consecutive years of cotton monoculture within the 6-year rotation cycle (Fig. 3h). For the three constraints, the one for crop yields was not used in screening the optimal rotation pattern as the simulations showed no obvious difference among the options. Both R_0 and R_5 represent the typical rotation patterns in the region. The simulations for the former indicate the greatest increase in SOC and lowest NEGE but the highest NIP, and those for the latter show the greatest SOC loss and largest NEGE but the lowest NIP (Figs. 3a and d). These patterns indicate that neither typical rotation pattern is optimal. Considering the trade-offs between NIP and both ΔSOC and NEGE, R_3 was chosen as the optimal rotation pattern that can balance economic benefit (crop yields), soil fertility and environmental safety well.

3.3 Biogeochemical effects of single-factor management alternatives

Under the screened optimal rotation pattern of R_3, the biogeochemical effects of each single field management practice were evaluated.

N94/366 had no obvious effects on annual average yields compared to N110/430 based on the single-factor baseline of nitrogen doses. However, N77/301, with a further 15% reduction in doses, reduced the annual averages of crop yields, especially for the W-M, by more than 10% ($P < 0.05$; Fig. 4a). The annual averages of ΔSOC and N_2O emission tended to decline by 2% and 3%, respectively, for N94/366 and by 10% and 10%, respectively, for N77/301. As a result, the NEGE for nitrogen reduction scenarios was reduced by 13−15% (Fig. 3b). For NH_3, NO emissions and NO_3^- leaching, the annual averages were reduced by 19%, 10% and 29%, respectively, for N94/366 and 37%, 20% and 49%, respectively, for N77/301 (Fig. 4c). Compared with N110/430, the lower emissions of gaseous or dissolved nitrogen pollutants from these two scenarios with reduced nitrogen doses resulted in a 15% and 33% ($P < 0.05$) lower NIP, respectively (Fig. 4a).

In comparison with I10 as the baseline, I08 slightly decreased the annual average yields by less than 4% (Fig. 4a), but the annual average yield of maize was reduced by more than 10% for I06. The effects of the reduced irrigation water amount on annual ΔSOC, CH_4 uptake, and N_2O, NH_3 and NO emissions were not consistent among simulations during the 18-year period. Thus, the annual averages of these decision variables for both I08 and I06 were not significantly different from those of I10. The

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annual averages of NO_3^- leaching also showed insignificant response to the reduced irrigation water amount. Therefore, saving water did not lead to an obviously modified NIP compared to the conventional amount of irrigation water used as the single-factor baseline (Figs. 4b and c).

The IS tended to increase crop yields very slightly (by 0.4−2%) while showing negligible effects on the decision variables and thus the NIP compared to IF as the baseline irrigation method.

In comparison with RI1 as the baseline, the annual averages of crop yields of the RI0 tended to decrease slightly (< 3%). However, the SOC contents of RI0 were generally lower than those of the baseline and showed a ΔSOC of −0.18 Mg C ha^{-1} yr^{-1} on average (Figs. 4a−b). Meanwhile, the annual N_2O and NO emissions of RI0 were consistently lower than those of RI1, with annual averages of 2.2 versus 3.6 kg N ha^{-1} yr^{-1} for N_2O ($P < 0.05$) and 1.4 versus 1.9 kg N ha^{-1} yr^{-1} for NO (Figs. 4b−c). The large decreases in both ΔSOC and N_2O emissions resulted in a 56% higher annual average NEGE than that of the baseline. In addition, RI0 decreased the annual average of NO_3^- leaching by approximately 31% compared to RI1. The trade-off between NEGE and NO_3^- leaching resulted in approximately comparable NIP values between RI0 and RI1 (Figs. 4a−c).

For both T10 and T0, the annual averages of crop yields were not significant changed from those of T20 as the baseline with a conventional tillage depth of 20−30 cm (Fig. 4a). However, both T10 and T0 enlarged the annual averages of ΔSOC and N_2O emission to different extents compared to the baseline, with 0.21−0.18 versus 0.12 Mg C ha^{-1} yr^{-1} for the former and 3.9−4.2 versus 3.6 kg N ha^{-1} yr^{-1} for the latter (Fig. 4b). Further, T10 and T0 led to a lower annual CH_4 uptake than T20, with the effect of the no-tillage scenario being very significantly in particular ($P < 0.01$). As the increases in ΔSOC could offset the decrease in CH_4 uptake and the increases in N_2O emission, the annual average of NEGE for T10 decreased by 19%. Moreover, T10 and T0 showed no obvious effects on the emissions of NH_3 and NO and leaching of NO_3^-. Nevertheless, no statistically significant difference in NIP was detected between T10 or T0 and the baseline.

According to the results above on the single-factor scenarios under the optimal rotation pattern, the following insights were obtained: reducing nitrogen fertilizer doses by 15% does not significantly affect the crop yields but obviously reduces the decision variables, thus leading to reduced NIPs; full incorporation/retention of crop residues decreases NEGE but increases NO_3^- leaching, thus showing no

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obvious effect on the NIP due to the trade-off between these two opposing effects; shifting conventional tillage to the reduced tillage or no-tillage practices benefits ∆SOC while increasing N_2O emission.

3.4 Identification of best management practices

To achieve the BMP under the optimal rotation pattern (i.e., R_3), all multifactorial scenarios were simulated. The simulated results of all 108 scenarios were compared to evaluate the integrative biogeochemical effects based on the three constraints and NIPs.

To screen the BMP, the annual averages for the 18-year simulations of the examined variables, including crop yield, NEGE, NH_3 volatilization, N_2O and NO emissions, and NO_3^- leaching, for each single- and multifactorial scenario of various management practices were analyzed. In consideration of the two constraints that crop yields and SOC stocks are no less than those of the baseline, only five out of the 107 scenarios, excluding that of the baseline, met these requirements. Further taking into account the third constraint that the NEGE should be reduced compared with that of the baseline, only four of the 107 scenarios were screened. According to the final objective quantitative criteria, one of these four scenarios, i.e., N94/366_I08_IS_RI1_T10, which showed the minimal NIP (23% lower than that of the baseline), was identified as the BMP under R_3.

The identified BMP for the investigated crop rotation system showed the following management features: (i) each of the cotton and W-M is cultivated for three consecutive years within a 6-year rotation cycle; (ii) the present crops and the current schedules of planting, harvesting, fertilization (date, depth, and splits) and irrigation (date and times) are adopted; (iii) urea is applied at a 15% lower rate, namely, 94 and 366 kg N ha^{-1} yr^{-1} for cotton and the W-M, respectively; (iv) 20% less water than the conventional level is irrigated by sprinkling; (v) crop residues are fully incorporated at harvest; and (vi) conventional tillage (20−30 cm depth) for cotton but reduced tillage (10 cm depth) for the W-M are applied.

In comparison to the baseline, i.e., the currently applied field management practices, the identified BMP could produce stable crop yields (increase by 1% on average) and enlarge ∆SOC (by 75% on average) while decreasing NEGE (by −26% on average), NH_3 volatilization (by −19% on average), NO emission (by −2% on average) and NO_3^- leaching (by −43% on average) (Table 2).

4 Discussion

4.1 Model performance

The DNDC model has been widely applied in agricultural systems across the world. The model version used in this study has been comprehensively validated with measurements of soil environmental variables, crop yields, and fluxes of NEE, NH_3, CH_4, N_2O and NO under various field management treatments for the double-cropping system of W-M (Cui et al., 2014). Cui and her colleagues reported satisfying model performance in simulating the variables of interest of the W-M. The validation in the present study also showed satisfying performance of the DNDC95 model in simulating the crop yields, NEE, CH_4 uptake, emissions of N_2O and NO and related soil factors of the land cultivated with cotton. Both validations, namely those by Cui et al. (2014) and those by this study, suggest that the DNDC95 model can be applied to quantify the decision variables and related factors of the cotton and W-M rotation system under different management practices.

The model effectively captured the dynamics of topsoil temperature and moisture as responses to seasonal variations in precipitation or irrigation events. Furthermore, the well-simulated crop yields combined with the soil environmental factors provided a solid basis for further simulating the decision variables to quantify the NIP under any condition. The crop yields and soil environmental factors are the indicators of essential processes of plant nitrogen uptake and the key factors regulating the biogeochemical processes of a cropping system (Chirinda et al., 2010; Kröbel et al., 2010). For the simulations of N_2O and NO emissions, discrepancies in daily emissions generally occur in DNDC models and other current biogeochemical models due to the complex interactions among soil environmental factors and carbon and nitrogen processes (Zhang et al., 2015). For the case of cotton in this study, underestimations of daily NO fluxes mostly occurred during the spring period of both experimental years. This under-prediction may have been caused by the overestimated topsoil moisture, which facilitated the reduction of NO to N_2O via denitrification (del Prado et al., 2006). These negative biases in simulating daily NO fluxes resulted in worse statistical evaluations. The temporal variations in both observed and simulated NEE indicated that the cotton field frequently assimilated atmospheric

CO_2 during the vigorous growth stages but emitted CO_2 to the atmosphere during the other periods. However, the abrupt NEE increases during the growing season on cloudy or rainy days were still not well simulated due to the calculation of plant growth relying on cumulative daily temperature over 0 ℃ and the parameter TDD (e.g., Cui et al., 2014). For the simulations of other nitrogen losses from the cotton field, the NH_3 volatilization and NO_3^- leaching accounted for 18−24% and 6−13%, respectively, of the applied fertilizer nitrogen during the 2-year period used for model validation. These loss rates were comparable with the field measurements of 10−23% for NH_3 volatilization (Li et al., 2016) and 16−17% for NO_3^- leaching (Liu et al., 2014).

The model validation suggests that the scientific processes determining the NO fluxes during the spring period before nitrogen fertilization in cotton fields and those determining the photosynthesis and ecosystem respiration in CO_2 fluxes (both as the NEE components) on cloudy and rainy days still require improvement in the future study. As there was no observation of NH_3 volatilization and NO_3^- leaching from the experimental cotton field, this validation study did not include both decision variables. Thus, future study still requires further validation of model performance using comprehensive observations covering both decision variables as well as others.

4.2 Biogeochemical effects of rotation pattern and management practices

The monoculture effect is neglected in the DNDC model. However, this neglect did not affect the simulated crop yields and thus the decision variables as results of biogeochemical interactions. For the W-M, the two crops are cultivated in rotation instead of the monoculture of either of them. Therefore, the W-M has been cultivated over the long term in many lands in northern China. The monoculture effect may manifest as changes in cotton yields if this crop is continuously cultivated for a long time. In practice, a period of 5 consecutive years is usually applied for the longest cotton monoculture to stabilize its yields while avoiding heavy uses of herbicides, pesticides and germicides, which benefit the environment. Meanwhile, balanced elemental nutrients have been applied in cotton cultivation, in which the crop residues remain in the field after the final seed harvest to avoid nutrient deficit. In this way, the negative effect of monoculture on cotton yields can be offset (Han, 2010). This fact is reflected by the DNDC model that assumes balanced nutrient supplies for any crops (e.g., Li, 2017).

The definition of modeled SOC of Cui et al. (2014) was applied in this study, which represents the total organic pool including the carbon in microbes, active humus (namely, humads) and resistant (or inactive) humus and excludes visible biomass residues in any form. In fact, this definition is identical to that of the SOC measured by the classic method in soil science. The simulated positive annual changes in SOC for the W-M were mainly attributed to the incorporation of full aboveground residues (at rates of 5.1−7.0 Mg C ha^{-1} yr^{-1}), which were favorable for carbon sequestration (Han et al., 2016). However, the negative annual changes in SOC for the cotton cropping system resulted from the shorter growing season relative to that of the W-M. The longer fallow season stimulated a notable amount of CO_2 emission from the soil, thereby reducing soil carbon sequestration (Liu et al., 2019). As a remarkable carbon sink, the W-M with incorporation of full crop residues could even totally compensate for the SOC lost during the first cotton-planting year following cultivation of the W-M for some years. Thus, the annual change in SOC was generally positive in the first cotton-cultivation year of the investigated rotation patterns. Therefore, an appropriate rotation pattern of cotton and the W-M could balance the ecosystem organic carbon budget of a 6-year cycle as well as gain an economic benefit from growing the non-cereal cash crop. The rotation patterns of R_0 and R_1 acted as net GHG sinks since the increased SOC exceed the increased N_2O emission related to the W-M cultivation. In comparison, the other rotation pattern options all functioned as net GHG sources. The higher application rate of fertilizer for the W-M than for cotton resulted in more reactive nitrogen remained in the soil (Chen et al., 2014; Ju et al., 2009), thereby stimulating more emissions of the nitrogenous air pollutants and N_2O under the scenarios with fewer cotton planting years. Therefore, the R_3 should be proposed as the appropriate rotation pattern of cotton and the W-M, which, among the six examined options, can allow the sustainable intensification with maximal yield benefits and minimal negative impacts on the environment.

Northern China, as the most important agricultural region, experienced an increase in crop yields by a factor of 2.8 in 1980−2008, during which the application of mineral fertilizers increased by a factor of 5.1. The rapid increase in fertilizer inputs has resulted in excessive nitrogen remaining in soil, posing potential risks for the environment (Chen et al., 2011; Zhang et al., 2017b). To solve this problem, the reduction of fertilizer application was proposed in several previous studies (e.g., Chen et al., 2011, 2014; Liu et al., 2012). The results of scenario analysis in this study indicated that, for the optimal rotation pattern, further reducing the farmer-optimized nitrogen doses by 15% (to 94 and 366 kg N ha^{-1} yr^{-1} for cotton and the W-M, respectively) could sustain the crop yields while greatly decreasing the emissions of nitrogenous gases.

In addition to fertilization, over-irrigation in northern China has also been ubiquitous for a long time, which threatens the water security of this region due to the sharply declining groundwater table and water pollution (Gao et al., 2015; Ju et al., 2009). For this reason, only management options with a reduced irrigation water amount should be considered under the severe shortage of water resources, even though the yields for these scenarios slightly decreased. In addition, adopting sprinkling instead of flood irrigation for an equal water amount showed positive effects on crop yields, indicating irrigation efficiency improvement (Zhang et al., 2017b). This result means that rather than blindly using larger nitrogen doses, increasing water-use efficiency through the application of alternative irrigation techniques could be a pathway to sustain crop yields with reduced nitrogen addition.

Through a ban on burning crop residues in fields, returning the residues to the field is strongly suggested by the government. The simulated results for incorporation of full residues indicated that this practice can simultaneously increase crop yields, soil carbon storage and emissions of N_2O and NO while decreasing the NEGE. These simulations were consistent with the results of field observations (Liu et al., 2011). The consistent results indicate the beneficial effect of residue incorporation on GHG balance.

Reduced tillage and no-tillage practices have been promoted in China in recent decades. To facilitate decomposition of woody cotton residues and avoid outbreaks of diseases and pests due to the continuous implementation of the no-tillage practice, adjustment of tillage practices was only applied in the W-M, while deep tillage for cotton was maintained when setting the tillage scenarios. As the no-tillage practice reduces gas permeability, it significantly decreases CH_4 uptake (Zhao et al., 2016). However, as shown by the model simulations, the contribution of this effect on CH_4 uptake to the change in NEGE was much smaller compared to that of the no-tillage effect on SOC stock. Similar to previous experimental studies (e.g., Zhao et al., 2016), the scenario analysis relying on model simulations in this study showed that the reduced tillage or no-tillage practice could sustain crop yields and increase carbon sequestration in the soil while reducing NH_3 volatilization and NO_3^- leaching.

As shown above, the influences of various field management practices on crop yields and the decision variables were different from each other in most cases. This implies that an appropriate combination of the single-factor management practices must exist for the rotation cropping system of cotton and the W-M. The biogeochemical effects of such an appropriate combination should satisfy the three constraints while resulting in the lowest NIP. Direct observations in field experiments, which often have very few treatments, measure very few variables and/or parameters for each treatment and represent very few conditions, are usually far less sufficient for screening such an appropriate combination. However, identifying such an appropriate combination is one of the purposes of developing a biogeochemical model, such as the DNDC model. The biogeochemical model validated with limited observations from field experiments is in principle capable of fulfilling this task.

4.3 Evaluation of the best management practice

The scenario analysis succeeded in screening for the BMP. The BMP could sustain the crop yields of cotton, winter wheat and summer maize of the three-crop rotation system, increase SOC stock, mitigate N_2O emission and NEGE, reduce emissions of NH_3 and NO, and reduce NO_3^- leaching due to the enhanced resource use efficiency in response to the reduced nitrogen-fertilizer dose and irrigation water amount. Hence, the BMP could result in a more drastically reduced NIP than the other examined management options. In the face of the scarcity of water resources and the pollution of underground water in northern China, reducing the irrigation water amount is an important pathway for adapting and alleviating these challenges (Gao et al., 2015; Ju et al., 2009; Zhang et al., 2017b). Therefore, in addition to the BMP, another scenario, in which the irrigation water amount is further reduced to 60% of the conventional level of farmer practices, could also be chosen if the loss of maize yield by 9% on average is tolerable. The model simulations for this management practice combination with 25% less irrigation water than the identified BMP showed similar effects on the cotton and wheat yields and all the decision variables compared to the BMP.

The uncertainties of the screened BMP mainly stem from three aspects.

The first aspect is the possible limitation of the applied model, which cannot simulate the effects of monoculture on cotton yields. However, some studies have demonstrated that the negative effects of cotton monoculture can be compensated for by improved field management (Han, 2010; Liu et al., 2014). This solution has been considered as much as possible in developing the scenario settings to avoid the unexpected monoculture influences.

The second aspect is the insufficient data for model validation. Due to the lack of observations, the model simulations on NH_3 fluxes for cotton cultivation and those on NO_3^- leaching in both cotton and the W-M cropping systems were not validated (Cui et al., 2014; this study). The DNDC model has been established by following the mass conservation law. In other words, it can reflect the mass balance of the nitrogen budget for the simulated soil layer (0−50 cm depth) well. This model principle implies that only one budget item could be allowed to not be validated. The item is usually soil nitrogen loss through the production of dinitrogen gas (N_2) mainly by denitrification, which is very difficult to measure *in situ* (e.g., Wang et al., 2013). For both cropping systems, the nitrogen lost through this pathway could be almost fully inhibited in the topsoil, wherein the soil moisture contents were often lower than 60% WFPS (Linn and Doran, 1984; Liu et al., 2011, 2014). However, most likely, N_2 lost could not be neglected in lower soil due to higher groundwater tables of approximately 1 m in depth. The model principle also implies that the uncertainty for the simulation of NO_3^- leaching during cotton cultivation might have been larger than that of the W-M cropping system since the former has one more decision variable (i.e., NH_3 volatilization) not directly validated by observations. These situations suggest that the current uncertainties in identifying the BMP may not be reduced unless the simulations of both NH_3 volatilization and NO_3^- leaching can be validated in addition to the other validated variables.

The last aspect is the method applied for the identification of the BMP. The current method only considers the biogeochemical effects on decision variables and crop yields as one of the three constraints. It excluded other factors, such as those related to the costs of management practices, thereby likely resulting in uncertainty. Although the method applied in this study still has some deficiencies, this case study shows its potential application in more comprehensive situations, which can be easily and automatically implemented as long as the simulations for all the decision variables and crop yields can be validated with comprehensive observations.

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5 Conclusions

An approach was proposed and applied to identify the optimal rotation pattern with the best other field management practice (BMP) based on the negative impact potentials (NIPs) of individual options/scenarios and a set of constraints. The NIP of an option or a scenario was defined as the linear function of five decision variables, including net ecosystem greenhouse gas emission (NEGE), ammonia volatilization, nitric oxide release, emission of nitrous oxide in the form of ozone layer depletion matter, and nitrate leaching. This study used three variables, i.e., crop yield, soil organic carbon (SOC) content, and NEGE, to specify the applied constraints that were stable/increased crop yields and SOC contents and reduced NEGE. All the decision variables and those related to constraints were generated through model simulation. The optimal management option was referred to as the scenario with the lowest NIP among those simultaneously satisfying the three constraints.

This case study focuses on a multi-crop cultivation system with rotation between cotton and winter wheat−summer maize (W-M) alternations, which has been widely adopted in northern China. As previously indicated by the validation studies for a land cultivated with the W-M and presently indicated for an adjacent area cultivated with cotton, version 95 of the DeNitrification-DeComposition (DNDC95) model showed satisfactory performance in simulating the decision and constraint variables with available field observations. This indicates a solid basis for using simulations of the model to evaluate the biogeochemical effects of rotation pattern and other field management practices of the multi-cropping system. Relying on the DNDC95 simulations driven by 113 management scenarios, the effect of various field management options on the variables of interest were investigated, and the optimal rotation pattern and its BMP were identified. The simulation results of rotation patterns indicated that proper rotation of cotton and the W-M can simultaneously be beneficial for the economic benefit (crop yields), soil fertility (soil carbon sequestration) and climate (GHG mitigation). Thus, the three-crop rotation pattern of a 6-year cycle could be optimized with 3 consecutive years of cotton with 3 continuous years of W-M. The BMP under this rotation pattern could use 15% less fertilizer and 20% less irrigation water by sprinkling compared to the currently adopted conventional practices, fully incorporate crop residues and adopt conventional deep tillage (to 20−30 cm) for cotton but reduced tillage (to 10 cm) for the W-M. This study emphasizes the necessity of comprehensive observations that fully cover the decision and constraint variables and related soil factors to facilitate effective BMP screening relying on virtual experiments using a biogeochemical model such as the DNDC model.

Author contribution

Xunhua Zheng and Chunyan Liu contributed to the further development in data management and enhanced scientific efficacy and effectiveness. Wei Zhang performed the simulations and prepared the manuscript with contributions from all co-authors. Chunyan Liu, Kai Wang, Rui Wang and Zhisheng Yao designed and carried out the experiments. Feng Cui and Siqi Li applied the model in adjacent land of winter wheat−summer maize cropping system.

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Table 1 Detailed management practices for each level-II scenario.

Scenarios	N [a]	RI [b]	Tillage [c]	IrrA [d]	IrrM [e]
Baseline	C: 110; W-M: 430 (N110/430)	Full (RI1)	C: 20/30; W-M: 20 (T20)	C: 1−3 times, 75−230 mm yr^{-1} MW: 4−6 times, 290−510 mm yr^{-1} (I10)	IF (IF)
N94/366	C: 94; W-M: 366	s.a.b	s.a.b	s.a.b	s.a.b
N77/301	C: 77; W-M: 301	s.a.b	s.a.b	s.a.b	s.a.b
I08	s.a.b	s.a.b	s.a.b	20% less	s.a.b
I06	s.a.b	s.a.b	s.a.b	40% less	s.a.b
IS	s.a.b	s.a.b	s.a.b	s.a.b	IS
RI0	s.a.b	Zero	s.a.b	s.a.b	s.a.b
T10	s.a.b	s.a.b	C: 20/30; W-M: 10	s.a.b	s.a.b
T0	s.a.b	s.a.b	C: 20/30; W-M: 0	s.a.b	s.a.b

[a] C, cotton; W-M, wheat−maize; N, nitrogen application rate (kg N ha^{-1} yr^{-1});
[b] RI, residue incorporation;
[c] Tillage, tillage depth (cm);
[d] IrrA, irrigation water amount;
[e] IrrM, irrigation method; IF, flood irrigation; IS, sprinkling. s.a.b, same as the baseline. The management practices other than those listed in this table were the same for all the scenarios and described in the text and Tables S2−3. The code in each pair of parentheses denotes the abbreviation of baseline for each management factor.

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Table 2 Simulated decision and constraint variables and negative impact potential (NIP) for the management practices under the optimal rotation pattern.

Scenarios [a]	CY	WY	MY	∆SOC	CH_4	N_2O	NEGE	NH_3	NO	NL	NIP
BAS	3.54	4.98	6.91	0.12	-1.86	3.59	1.16	56	1.85	59	453
BMP	**3.59**	**5.06**	**6.99**	**0.21**	**-1.82**	**3.64**	**0.86**	**45**	**1.82**	**34**	**348**
BMP_a	3.55	5.01	6.31	0.20	-1.83	3.62	0.89	45	1.84	38	359

[a] BMP, best management practice. CY, WY and MY, yields of cotton, wheat and maize, respectively (Mg dry matter ha^{-1} yr^{-1}). For the other variable names and units, refer to the footnotes of Fig. 2. BAS, BMP and BMP_a, baseline management practices, the best management practices (BMP) and the BMP alternative, which are encoded as N110/430_I10_IF_RI1_T20, N94/366_I08_IS_RI1_T10, N94/366_I06_IS_RI1_T10, respectively. For the meanings of these codes, refer to Table 1.

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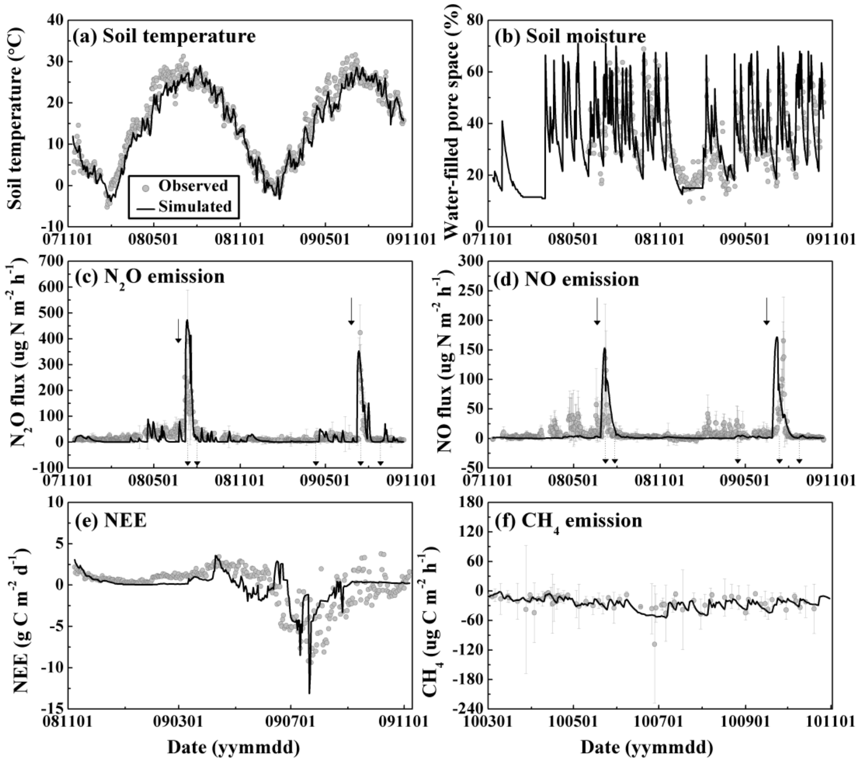

Figure 1: Observed and simulated daily mean soil (5 cm) temperature, soil (0−6 cm) moisture, nitrous oxide (N_2O) and nitric oxide (NO) fluxes, net ecosystem exchanges of carbon dioxide (NEE), and methane (CH_4) emissions. The solid- and dashed-line arrows indicate the dates of fertilization and irrigation, respectively. The measurement errors were not shown in panels a, b and e. The vertical bar for each observation in panels c, d and f indicates two times standard deviations to represent the uncertain range at the 95% confidence interval. The legend in panel a applies for all subfigures.

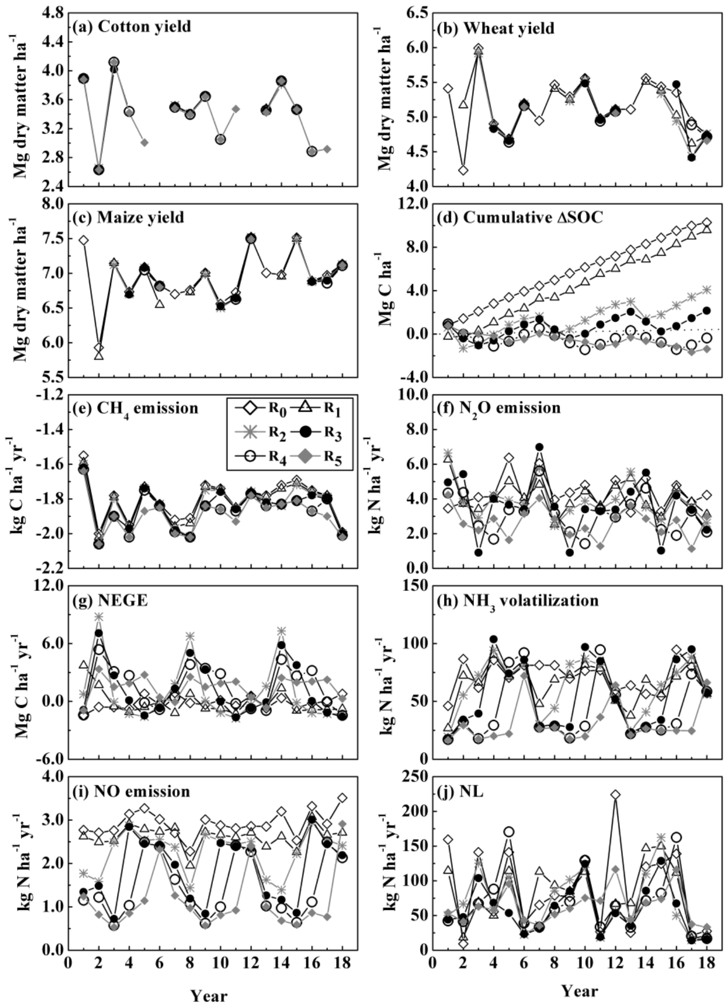

Figure 2: Simulated crop yields, cumulative changes in soil organic carbon (ΔSOC), methane (CH_4) and, nitrous oxide (N_2O) release, net ecosystem greenhouse gases emission (NEGE), ammonia (NH_3) volatilization, nitric oxide (NO) emission and nitrate leaching (NL) over a 18-year period (spanning three 6-year rotation cycles) for each rotation pattern scenario. For the definitions of the rotation pattern options, i.e., R_0, R_1,..., R_5, refer to the text in Sect. 2.4. The legend in panel e applies for all subfigures.

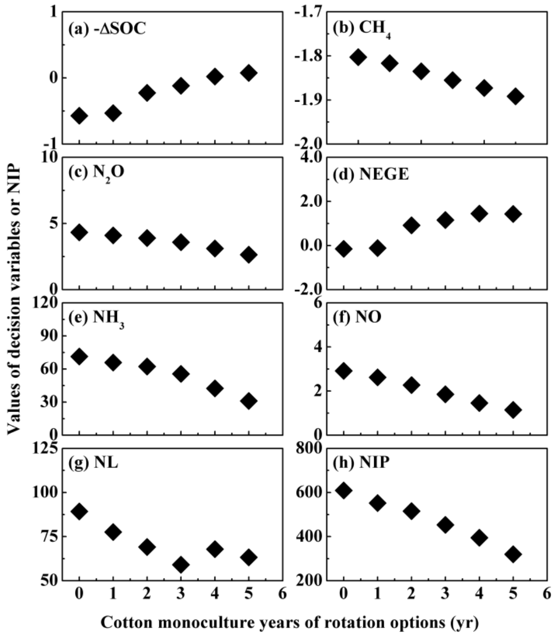

Figure 3: Simulated effects of rotation options under the baseline management practices on decision variables and negative impact potential (NIP). For the definitions of the rotation pattern options, i.e., R_0, R_1,..., R_5, refer to the text in Sect. 2.4. The y-axis units are Mg C ha^{-1} yr^{-1} for the opposite of mean annual increase in soil organic carbon stock (−ΔSOC), kg C ha^{-1} yr^{-1} for methane (CH_4) emission, kg N ha^{-1} yr^{-1} for emissions of nitrous oxide (N_2O), ammonia (NH_3) and nitrous oxide (NO), and nitrate leaching (NL), Mg CO_2eq ha^{-1} yr^{-1} for net ecosystem greenhouse gas emission (NEGE), and USD ha^{-1} yr^{-1} for NIP. The CO_2eq was based on the 100-year global warming potentials, i.e., 34 for CH_4 and 298 for N_2O (IPCC, 2013). The NIP was calculated using Eq. (1) presented in the text.

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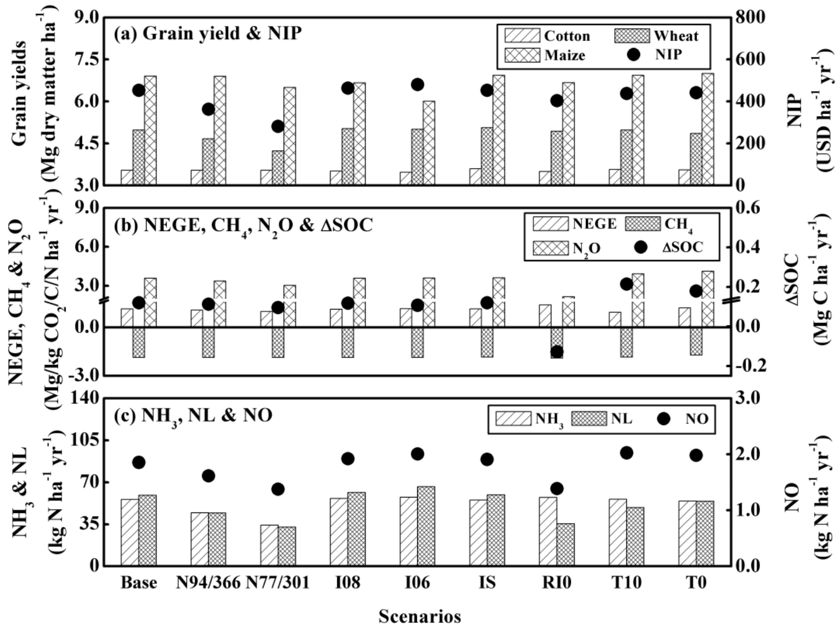

Figure 4: Averages of crop grain yields and negative impact potential (NIP), soil organic carbon change (ΔSOC), emissions of methane (CH_4) and nitrous oxide (N_2O), and net ecosystem greenhouse gases emission (NEGE), ammonia (NH_3) volatilization, nitrate leaching (NL) and nitric oxide (NO) emission over a 18-year period for different management scenarios under the optimal rotation pattern (i.e., R_3, see Fig. 2 for its details). For the definitions of each scenario, refer to Table 1. Each NIP was calculated using Eq. (1) presented in the text.