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. A cropping system with rotations between cotton and winter wheat-summer maize (W-M) is widely adopted in northern China. Optimizing the crop rotation in concert with the related field management practices of this system is crucial for reducing its negative impacts on climate and environmental quality. In this study, the approach used to identify the best management practice (BMP) relied on biogeochemical model simulations to determine the negative impact potential (NIP) and a set of constraints. The BMP is referred to as the scenario with the lowest NIP that satisfies the given constraints. All the variables of interest were generated using the DeNitrification-DeComposition version 95 (DNDC95) model with minor modifications relating to the NO production during nitrification. The modified DNDC95 model showed satisfactory performance in simulating the variables of interest with the available observations for two adjacent plots cultivated with cotton and W-M. The simulations of rotation patterns indicated that the proper rotation of cotton and W-M can simultaneously benefit the crop yields, soil carbon sequestration and greenhouse gas mitigation. Monte Carlo simulations with 6000 scenarios showed that the BMP for the system involved 3 consecutive years of cotton rotating with 3 continuous years of W-M. These practices used 18% less nitrogen fertilizer (i.e., 90 and 353 kg N ha^{-1} yr^{-1} for cotton and W-M, respectively) and 18% less irrigation water (i.e., 62−189 and 238−418 mm yr^{-1} for cotton and W-M, respectively) under sprinkling than the conventional practices, incorporated 90% of crop residues, and adopted the current deep tillage (20−30 cm) for cotton but reduced tillage (10 cm) for W-M. In addition, three other alternative BMPs were also

30   screened with overlapping ranges of uncertainty. However, field confirmation of these BMPs resulting

31   from the model-based virtual experiments is still required.

1 Introduction

33   Globally, fiber crops (i.e. cotton) and cereals such as wheat and maize have long played a relevant

34   role in human society because they are primary sources of materials for the textile and food industries.

35   In China, although cotton cultivation only covers 2.0−3.9% of the annual crop harvest area (there was a

36   cotton lint production of 5.3−7.6 million metric tons from 2007−2016), the cultivation of cereals is

37   quite large. Wheat and maize accounted for 39% and 26% of the harvest area and represented 129 and

38   220 million metric tons of grain, respectively, in 2016 (China Statistical Yearbook, 2017).

39   Northern China is both the second most important area of cotton production and the largest region

40   of the winter wheat-summer maize double-cropping system (i.e., both crops are harvested within a year,

41   and they are hereinafter referred to as W-M) in the country (e.g., Cui et al., 2014). Crop rotations of

42   cotton and W-M have commonly been grown in this region, alternating every 3−5 years (e.g., Liu et al.,

43   2010, 2014). During the last few decades, the yields of cotton, wheat and maize have been increased by

44   employing intensified agricultural management practices, such as increased fertilizer inputs, advanced

45   irrigation methods and so on (Han, 2010). A recent study indicated that the cotton cropping system in

46   northern China persistently functioned as an intensive carbon or net greenhouse gas (GHG) source

47   compared to W-M (Liu et al., 2019). These previous studies have revealed that the change in the

48   storage of soil organic carbon (ΔSOC), net ecosystem GHG emissions (NEGE) and other

49   biogeochemical processes involving the multiple cropping systems in northern China are likely closely

50   related to the rotation pattern of cotton and W-M (e.g., Liu et al., 2010, 2014, 2019; Lv et al., 2014).

51   To maintain high productivity, the three-crop rotation systems for cotton and W-M in northern

52   China are characterized by large additions of synthetic nitrogen fertilizers and irrigation water (e.g.,

53   Chen et al., 2014; Galloway et al., 2004), at 60−140 and 550−600 kg N ha^{-1} yr^{-1}, and 140−200 and

54   90−690 mm yr^{-1} for cotton and W-M, respectively (Ju et al., 2009; Liu et al., 2014; Wang et al., 2008).

55   High nitrogen and water inputs can result in high release potentials for nitrogenous pollutants, and they

56   can induce a series of environmental problems, such as increased nitrate (NO_3^-) leaching for water

pollution (e.g., Collins et al., 2016). In addition, other field management practices, e.g., tillage and crop residue treatment, can also affect the emissions of reactive nitrogen and contribute to negative environmental effects (e.g., Zhang et al., 2017b; Zhao et al., 2016). Therefore, the evaluation of multiple-cropping systems (e.g., rotations of cotton and W-M) is shifting from a single-goal method aimed at increasing crop yields to a multi-goal approach (e.g., Cui et al., 2014; Garnett et al., 2013; Zhang et al., 2018). A multi-goal strategy aims to simultaneously sustain/increase crop productivity to ensure food security, increase SOC content 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 NO_3^- leaching to protect water quality.

An objective method is applied to identify the best management practice (BMP), which evaluates each decision variable with price-based proxies or other measures and screens the best option with the minimal negative impact potential (NIP) under the given constraints at an annual scale (e.g., Cui et al., 2014; Xu et al., 2017). To screen the BMP using the multi-goal approach, it is essential to quantify the biogeochemical effects of management practices at an annual scale. As field experiments often focus only on the decision variables of very few management practices during short periods (e.g., Ding et al., 2007; Liu et al., 2010, 2015; Wang et al., 2013a, b), the process-oriented biogeochemical models have the potential to overcome this limitation, through models such as the DeNitrification-DeComposition (DNDC) (e.g., Chen et al., 2016; Giltrap et al., 2010; Li, 1992, 2000; Zhang et al., 2017a), DAYCENT (e.g., Delgrosso et al., 2005) and LandscapeDNDC (e.g., Haas et al., 2012).

The DNDC model was selected in this study to investigate the biogeochemical effects of various cotton and W-M rotation patterns and their field management practices in southwestern Shanxi Province. The model version applied in this study, the DNDC95, has been modified from that of Cui et al. (2014), and it has been validated using comprehensive field measurements of cotton and W-M at the selected field site. The aim of this case study was to (i) validate the performance of the modified DNDC95 for the cotton and W-M cropping system, especially for the decision variables at an annual scale; (ii) investigate the biogeochemical effects of different rotation patterns between the cotton and W-M and those of the field management practices; and, (iii) identify the BMP by considering the rotation pattern and field management using a multi-goal strategy. These efforts were undertaken to test

85 the hypothesis that the sustainable intensification of the three-crop cultivation system that is focused on

86 enhancing crop yields and simultaneously reducing environmentally negative impacts can be achieved

87 through the optimization of the rotation pattern and associated field management practices.

88 **2 Materials and methods**

89 **2.1 Brief introduction to the DNDC95 and its modification**

90 The DNDC95 model used in this study is one of the latest DNDC versions

91 (www.dndc.sr.unh.edu/model/GuideDNDC95.pdf). This model consists of two components with six

92 modules in total. Driven by the given primary ecological factors, the former component simulates the

93 field states of a soil-plant system, such as the soil chemical and physical status, vegetation growth and

94 organic matter decomposition. Driven by the soil-regulating variables yielded by the former component,

95 the latter component simulates the core biogeochemical processes of carbon and nitrogen

96 transformations and the physical processes of liquid and gas transportations and thus the annual

97 dynamics of net ecosystem exchanges of carbon dioxide (CO_2) (NEE); emissions of methane (CH_4),

98 nitrous oxide (N_2O), NH_3 and NO; and NO_3^- leaching and the inter-annual dynamics of SOC and

99 NEGE. These features enable the model to investigate the integrative biogeochemical effects of the

100 rotation patterns of multiple crops and/or other management practices based on comprehensive

101 validation. The minimum inputs used to facilitate the model simulation include (i) the meteorological

102 variables of daily precipitation and maximum/minimum temperature; (ii) the soil (cultivated horizon)

103 properties of the clay fraction, bulk density, SOC content and pH; (iii) the crop parameters for the yield

104 potential, thermal degree days (TDD) for maturity, and the mass fractions and carbon-to-nitrogen (C/N)

105 ratios of the grain, root and leaf plus stem; (iv) the management practice variables of sowing and

106 harvest (dates), fraction of incorporated/retained residue at harvest, tillage (date and depth), irrigation

107 (date, method and water amount), and fertilization (date, type, method, nitrogen amount and C/N ratio

108 of organic manure); and (v) other variables (annual means of the NH_3 concentration in the atmosphere

109 and the ammonium plus NO_3^- concentration in rain water). For more details about the model, please

110 see Li et al. (1992) and Li (2000, 2007, 2016).

111 To improve the model performance during daily NO simulations for cotton cropping system, the

112 production process for NO (NO_p) during nitrification was modified. For the original version by Cui et

113 al. (2014), the NO production was simply quantified as a fixed fraction (0.003) of nitrification (Fni),

114 which reflected a constant production rate of NO during nitrification. For the modified version, the

115 effect of the soil moisture (SM in water-filled pore space (WFPS)) on NO production was incorporated

116 in view of that applied during the N_2O production process in nitrification (Eq. (1)). The maximum NO

117 production rate (K_n) was calibrated as 0.03 using the observed daily NO fluxes from 2007−2008 for the

118 cotton cropping system. The incorporated soil moisture effects indicated that high soil moisture

119 facilitated the production of NO during nitrification under the concept of an "anaerobic balloon".

$$NO_p = K_n FniSM^{5.0} \tag{1}$$

120 **2.2 Brief introduction to the selected field site and model validation**

121   The field site (34 °55.50′N, 110 °42.59′E, altitude of 348 m) selected for this modeling case study is

122 located at Dongcun Farm, near Yongji County, Shanxi Province, in northern China. The site is subject

123 to a temperate continental monsoon climate, and it had an annual precipitation of 580 mm and a mean

124 air temperature of 14.4 °C from 1986−2010 (Cui et al., 2014). Cotton, winter wheat and summer maize

125 are the major crops grown at this farm and the surrounding regions. Field experiments were performed

126 on two adjacent plots (each of which was 100 m wide and 200 long) for cotton and W-M in 2007−2010.

127 The soil of the land cultivated with cotton and W-M was clay loam, with approximately 38% and 32%

128 clay (< 0.002 mm), 57% and 50% silt (0.002−0.05 mm), 5% and 18% sand (0.05−2 mm), 10.0 and 11.3

129 g kg^{-1} SOC, 1.1 and 1.1 g kg^{-1} total nitrogen and pH (in H_2O) of 8.0 and 8.7 at a 0−10 cm depth and

130 bulk densities (0−6 cm depth) of 1.20 and 1.17 g cm^{-3} (Liu et al., 2010, 2011, 2012). A sprinkler system

131 was applied to both plots. For more detailed information on the field experiments and observed data,

132 please refer to Cui et al. (2014), Liu et al. (2010, 2011, 2014, 2015) and Wang et al. (2013a, b).

133   The modified model was validated in the plot cultivated with cotton. The daily meteorological

134 data from 2004−2010 were obtained directly from Cui et al. (2014). The measured data were used

135 directly for the minimum required soil properties. The input data on the field capacity and wilting point

136 in the WFPS were 0.65 and 0.2, respectively, as cited from Cui et al. (2014). The crop parameters for

137 cotton were directly determined by the field measurements, which were 1900 kg C ha^{-1} for potential

138   grain (1.2 times the mean of the measured values), 0.41 and 25, 0.16 and 40, and 0.43 and 40 for the

139   mass fractions and C/N ratios of the grain, root and leaf plus stem, respectively, and 3600 ℃ for the

140   TDD. Detailed management practices (Table S1) were obtained from Li et al. (2009) and Liu et al.

141   (2014). Compared with the conventional fertilizer application rate of 110−140 kg N ha^{-1} yr^{-1} for the

142   cotton, the fertilizer doses for 2007 and 2008 were reduced to 66−75 kg N ha^{-1} yr^{-1} by local farmers to

143   avoid the overgrowth of the leaves in place of seeds or lint. The measured data used for calibration and

144   validation were available for the soil (5 cm depth) temperature, topsoil (0−6 cm) moisture and N_2O and

145   NO (the daily NO fluxes from 2007−2008 were used for the K_n calibration and the data from

146   2008−2009 were used for validation) emissions from 2007−2009 (Liu et al., 2010, 2014), CH_4 uptake

147   fluxes (Liu et al., 2019), grain yields, and NEE (Liu et al., 2019). In addition, because the model has

148   been modified from the version used by Cui et al. (2014) for W-M in the adjacent plot, the W-M

149   simulations were performed with the modified version again, using the crop parameters and other

150   inputs adopted by Cui et al. (2014). The cotton and W-M validation data are detailed in Table S2. Thus,

151   to identify the BMP, both the validations of cotton and W-M for the cumulative N_2O, NO and CH_4

152   under various field managements, NH_3 and NEE were also analyzed in this study.

153   **2.3 Scenario settings and simulations**

154   To investigate the biogeochemical effects of the rotation pattern and management practices, two

155   levels of scenarios were explored. The level-I scenarios considered the rotation patterns. These patterns

156   were set for a 6-year cycle based on surveys of local farmers (Liu et al., 2010, 2011, 2014). There were

157   six level-I scenarios in total, which are hereinafter referred to as R_0, R_1..., R_5, and the number of the

158   rotation indicated the years of consecutive cotton planting. For instance, R_0 denotes a 6-year

159   monoculture of W-M; R_2 represents 2-year continuous cotton cropping rotated with 4 years of

160   consecutive W-M; etc. Because the local farmers typically did not cultivate cotton monocultures in this

161   region for longer than five years, the longest cotton monoculture was set as 5 years for the level-I

162   scenarios. The transitions between cotton and W-M are detailed in Table S3. To study the

163   biogeochemical effects of the rotation pattern, the baseline simulations of the level-II scenario (Tables

164   S3−4) for each rotation pattern were analyzed.

165   The level-II scenarios addressed five field management factors, which were the (i) fertilizer dose,

166 (ii) water amount and (iii) method of irrigation, (iv) incorporated/retained fraction of crop residues, and

167 (v) depth of tillage. The values of the five factors used for the baseline were known as the observations

168 for the conventional management practices in the experimental region (Tables S1, S3 and S4). The

169 nitrogen application rates of the baseline were 110 and 430 kg N ha^{-1} yr^{-1} for cotton and W-M,

170 respectively. Over the last few decades, the fields in this region have mostly been flood-irrigated (Liu et

171 al., 2010), which was chosen as the baseline condition. The baseline timings and water amounts were

172 established by referring to the 10- to 30-d cumulative precipitation prior to the individual irrigations

173 and the recorded timings and water amounts of conventional management practices in both plots. Thus,

174 the irrigation frequencies and annual cumulative water amounts of the baseline during the 18-year

175 period (Table S4) vary from 1 to 3 times and 75 to 230 mm yr^{-1} for cotton and 4 to 6 times and 290 to

176 510 mm yr^{-1} for W-M. In addition, 100% residue incorporation and conventional tillage to a depth of

177 20−30 cm were applied for the baseline conditions. To screen the BMP of six rotation patterns in the

178 interaction with all the considered management practices, the variation in the fertilizer amount,

179 irrigation amount and residue incorporation rate was set as 40% of the baseline to the baseline

180 (N44/172 to N110/430), 40% of the baseline to the baseline (I40 to I100) and 0 to 100% (RI0 to RI100).

181 The irrigated method and tillage factors consisted of flood (IF) and sprinkle (IS) irrigation and

182 no-tillage (T0) and reduced tillage (5 cm and 10 cm, T5 and T10) for W-M and conventional tillage

183 (20−30 cm, T20). We assumed that the frequency distributions of all the factors were uniform. Monte

184 Carlo simulations, at 1000 combined field management scenarios, were used to screen the BMP for

185 each rotation pattern, and the final BMP was selected from the BMPs of six rotation patterns in light of

186 the 6000 combined scenarios.

187   An 18-year simulation was performed to assess the biogeochemical effects of the rotation patterns

188 and management practices. These simulations were driven by the meteorological data observed at the

189 Yuncheng station (approximately 60 km east to the experimental site) from 1996−2013

190 (http://data.cma.cn/data/cdcindex/cid/6d1b5efbdcbf9a58.html). To stabilize the carbon and nitrogen

191 dynamics and reduce the residual effects of the initial conditions (Zhang et al., 2015), a spin-up of 12

192 years was performed (i.e., a period of two 6-year rotation cycles) before the 18-year simulations

193 (Palosuo et al., 2012). The spin-up was driven by the same rotation pattern and field management

194 practices as each scenario. For each scenario, the average values for each crop yield and the other

195 decision variables were the averages of the 18-year simulations.

2.4 Method for identifying the best management practices

197 An objective method jointly relying on three constraints and NIPs was adopted in this study to

198 identify the BMP. These constraints included (i) stable or increased crop yields, (ii) stable or increased

199 SOC, and (iii) reduced NEGE. In the present study, the NEGE was the residual of the annual sum for

200 the CH_4 and N_2O emissions minus the ΔSOC and was quantified as a CO_2 equivalent (CO_2eq) quantity

201 for the 100-year time horizon, at 1 for CO_2, 34 for CH_4 and 298 for N_2O (IPCC, 2013). The NIP was

202 used to evaluate the potential for a climatically and environmentally integrative impact, which was a

203 price-based proxy quantity in USD ha^{-1} yr^{-1}. The NIP was determined by using the quantities of

204 individual decision variables and their coefficients as mass-scaled price-based proxies (Eq. (2)).

$$NIP = k_1 NEGE + k_2 NH_3 + k_3 NO + k_4 N_2O_{ODM} + k_5 NL \qquad (2)$$

205 In Eq. (2), the NEGE, NH_3, NO, N_2O_{ODM}, and NL represent the multi-goal decision variables of

206 the net ecosystem GHG emission (Mg CO_2eq ha^{-1} yr^{-1}), NH_3 volatilization, NO emission, release of

207 N_2O as depleted ozone layer matter and hydrological nitrogen loss (mainly by NO_3^- leaching),

208 respectively (kg N ha^{-1} yr^{-1} for all the nitrogen compound variables). The coefficients k_1, k_2, k_3, k_4 and

209 k_5 are mass-scaled price-based proxies for the NEGE, NH_3, NO, N_2O_{ODM}, and NL, respectively. Their

210 values as presented in Cui et al. (2014) were directly used in this study, and they were 7.00 USD Mg^{-1}

211 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.

212 In Eq. (2), a lower NIP indicates a better set of management practices that can exert smaller

213 negative impacts on the climate and environment. Accordingly, the BMP was identified as the scenario

214 with the lowest NIP among the scenarios that could satisfy all three constraints. According to the BMP

215 screening method used in this study, a solid validation of the cumulative emissions of N_2O, NO, NEE

216 and CH_4 was the basis for identifying the BMP, rather than those at the daily scale.

 2.5 Statistics and analysis

218   The statistical criteria of the (i) index of agreement (IA) (Eq. (3)), (ii) Nash-Sutcliffe efficiency

219   index (NSI) (Eq. (4)) (e.g., Moriasi et al., 2007; Nash and Sutcliffe, 1970), (iii) determination

220   coefficient (R^2) (Eq. (5)) and slope of a zero-intercept univariate linear regression (ZIR) of observations

221   (o) against simulations (s) (Jiang, 2010) and (iv) model relative bias (MRB) (Eq. (6)) (e.g., Congreves

222   et al., 2016; Willmott and Matsuura, 2005) were simultaneously used to evaluate the model validity. In

223   Eqs. (3−6), k and n (k = 1, 2..., n) denote the kth pair and the total pair number of the values,

224   respectively, and $\bar{o}$ represents the mean of the observations. The IA index falls between 0 and 1, with a

225   value closer to 1 indicating a better simulation, and vice versa. An NSI value between 0 and 1 shows

226   acceptable model performance. Better model performance is indicated by a slope and an R^2 value that is

227   closer to 1, and vice versa. The MRB is expressed as a percentage, wherein $\bar{s}$ denotes the average of

228   the simulations. In this study, the MRBs of the cumulative N_2O, NO, NEE and CH_4 amounts were

229   regarded as the relative uncertainty of the model validation, and they were further used to estimate the

230   relative uncertainty of each scenario based on the error transfer formula (Eqs. (S1−4)).

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

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

$$R^2 = 1 - \frac{\sum_{k=1}^{n}(o_k - \hat{o}_k)^2}{\sum_{k=1}^{n}(o_k - \bar{o})^2} \tag{5}$$

$$MRB = 100\frac{|\bar{s} - \bar{o}|}{\bar{o}} \tag{6}$$

231   In this study, the ZIR analysis, variance analysis, and graphical comparison were performed with

232   SPSS Statistics Client 19.0 (SPSS Inc., Chicago, USA) and Origin 8.0 (OriginLab, Northampton, MA,

233   USA) software.

3 Results

3.1 Model validation

3.1.1 Validation for the cotton cropping system

The seasonal dynamics and magnitudes of the 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 the R^2 values of 0.98 and 0.83, 0.93 and 0.15, 0.93 and 0.83, and 0.95 (n = 677, P < 0.001) and 0.42 (n = 432, P < 0.001) for the temperature and moisture, respectively.

To compare the cotton yields (seeds plus lint) over three consecutive years (2008−2010), the simulations and observations were also highly consistent, with an MRB of 6%, which was less than two times the spatial coefficient of variations (CVs) (39−56%) for the measurements (Liu et al., 2014, 2019).

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 the R^2 values of 0.77, < 0, 0.48 and 0.40 (n = 592, P < 0.001), respectively, for N_2O and the values of 0.78, < 0, 0.54 and 0.39 (n = 333, P < 0.001), respectively, for NO. In comparison, the modified model significantly improved the model performance for the daily NO fluxes, especially for emissions in the spring. The IA, NSI, and ZIR slope and the R^2 values increased from 0.62 to 0.78, -1.03 to -0.04, 0.37 to 0.54 and 0.09 to 0.39, respectively. In addition, the simulated annual N_2O and NO emissions during the two consecutive experimental years were comparable with the observations, with MRBs of 2% and 11%, respectively, both of which were less than two times the spatial CVs (23−50%) for the measurements (Liu et al., 2014).

The simulated NEE flux is one component of the ∆SOC, which is a key factor that is considered during BMP identification. The simulation suggested that the model captured the seasonal fluctuations, which were negative during the cotton-growing season, but positive or neutral during the remaining periods (Fig. 1e). The IA, NSI, and ZIR slope and R^2 were 0.76, 0.38, 0.85 and 0.39 (n = 365, P < 0.001), respectively, for the daily NEE simulation. For the annual cumulative NEE in 2009 and 2010,

261   the model simulation showed an MRB of 10%, which was less than the reported uncertainty (25%) of

262   the observations (Wang et al., 2013a).

263   For the CH_4 uptake, the observations and simulations showed similar seasonal variations (Fig. 1f),

264   with the IA, NSI and ZIR slope and an R^2 of 0.68, < 0, 0.72 and 0.15 ($n = 69$, P < 0.01), respectively.

265   The model simulation of the annual cumulative CH_4 uptake in 2009 and 2010 yielded an MRB of 2%,

266   which was less than two times the spatial CVs (13−17%) of the observations (Liu et al., 2019).

267   **3.1.2 Validation of the cumulative emissions of both cropping systems used for BMP identification**

268   To screen the BMP of the cotton and W-M rotation system under various management practices

269   based on the annual simulation results, the model performances for the cumulative N_2O, NO, NEE and

270   CH_4 were required for validation. According to the updated results of Cui et al. (2014) and this study

271   using the modified model, the model showed satisfactory performances for simulating the cumulative

272   variables, with ZIR slope and the R^2 values of 0.90 and 0.83 ($n = 12$, P < 0.001), 0.90 and 0.94 ($n = 11$,

273   P < 0.001), 0.98 and 0.99 ($n = 5$, P < 0.001), and 0.99 and 0.91 ($n = 7$, P < 0.001) for the cumulative

274   N_2O, NO, NEE and CH_4, respectively, which provided a solid basis for the BMP identification at this

275   site scale (Fig. 2). These results suggested that the DNDC95 model could be applicable in investigating

276   the biogeochemical effects of different rotation patterns between the cotton and W-M and the effects of

277   different management practices.

278   **3.2 Biogeochemical effects of different cotton and wheat-maize rotation patterns**

279   Figure 3 illustrates the dynamics of the crop yields and each decision variable resulting from the

280   consecutive simulations over 18 years for all the rotation pattern options subject to the field

281   management practices of the baseline scenario (Table S5). Figure 4 shows the relationship between the

282   annual average of each decision variable and the number of consecutive years of cotton monoculture

283   within the rotation pattern options.

284   The average grain yields for the cotton, wheat and maize were not significantly different among

285   the various rotation pattern options, with averages of 3.5, 4.8 and 6.7 kg dry matter ha^{-1} for cotton,

286   wheat and maize, respectively (Figs. 3a−c).

287   For the dynamic changes in the annual SOC stocks, the values were generally positive for W-M

but negative for the cotton, except for the first year after the transition to this fiber crop. As indicated by Fig. 3d, 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 $-\triangle SOC$ increased significantly (P < 0.001) with an increase in the consecutive years of cotton monoculture from 0 to 5 within the 6-year rotation cycle (Fig. 4a). The rotation pattern options with baseline management showed small variations in the CH_4 uptake (Fig. 3e), with the annual uptakes ranging from 1.6 to 2.1 kg C ha^{-1}. However, the annual averages for the CH_4 uptake increased significantly (P < 0.001) with the increased consecutive years of cotton monoculture (Fig. 4b). For N_2O, the annual emissions showed large inter-annual variations (Fig. 3f), with a CV of 26−48%. In addition, the annual average emissions of this gas decreased significantly from 4.6 to 2.6 kg N ha^{-1} (Fig. 4c) after increasing consecutive years of cotton monoculture (P < 0.001). As a result, the NEGE was significantly promoted (P < 0.01) (Figs. 3g and 4d).

Regarding the gaseous air pollutants NH_3 and NO, the simulated annual emissions ranged from 17 to 103 and 0.5 to 3.3 kg N ha^{-1}, respectively (Figs. 3h−i). Figures 4e and f show that the average annual emissions of both gases were significantly reduced after increasing the consecutive years of cotton monoculture (P < 0.001). The annual NO_3^- leaching of the different rotation patterns displayed significant inter-annual variations (Fig. 3j), with CVs of 41−69%. Thus, the annual averages for NO_3^- leaching changed insignificantly in response to the consecutive years of cotton monoculture (Fig. 4g).

The NIP varied significantly among the various rotation pattern options (P < 0.001), declining from 610 to 324 USD ha^{-1} yr^{-1} with increased consecutive years of cotton monoculture (Fig. 4h). For the three constraints, the crop yields showed no obvious differences among the various rotation patterns. 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 the lowest NEGE but the highest NIP, while those for the latter show the greatest SOC loss and the largest NEGE but the lowest NIP (Figs. 4a, d and h). These patterns indicate that neither typical rotation pattern is sustainable.

3.3 Identification of best management practices

The Monte Carlo simulation showed that only 51, 22, 16, 9 and 16 of the 1000 combined scenarios from R_0 to R_4 simultaneously satisfied the three constraints, while no scenario met all the

requirements for R_5. The screened BMPs for the five rotation patterns indicated that a reduction in the amount of fertilizer and irrigation water can be applied for all the rotation patterns, with the declines of 15−21% and 18−27% for the BMPs (87−94 and 334−367 kg N ha^{-1} yr^{-1}, and 55−189 and 211−418 mm yr^{-1} for the cotton and W-M, respectively). In addition, when compared with flood irrigation, sprinkle irrigation was adopted for all the BMPs except that for R_4. The rate of residue incorporation for the BMPs ranged from 55−90%, which increased with the increased consecutive cotton monoculture years. Regarding the depth of tillage, except for the 10 cm and no-tillage treatment for the BMPs of R_3 and R_4, the depths of other rotation patterns were all 5 cm. Compared with the baseline of each rotation excluding the R_5, the NEGE, NH$_3$ volatilization, NO$_3^-$ leaching and NIP of the BMPs decreased by more than 4%, 20% 41% and 27%, respectively. When ranking the NIPs of each rotation BMP, the final BMP was identified as the BMP of R_3 (N90/353_I82_IS_RI90_T10), with an NIP of 327 USD ha^{-1} yr^{-1}. Although the NIP of the BMP for R_4 was slightly lower than that for R_3, the NEGE and ΔSOC were 20% higher and 71% lower than that of the final BMP, respectively, and the technology required for no-tillage, such as planting, was not widely available.

The identified BMP for the cotton and W-M rotation system showed the following management features: (i) both cotton and W-M are 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 18% lower rate, namely, 90 and 353 kg N ha^{-1} yr^{-1} for cotton and W-M, respectively; (iv) 18% less water is used for irrigation by sprinkling than the conventional level; (v) the rate of crop residue incorporation is 90% at harvest; and (vi) conventional tillage (20−30 cm depth) for cotton but reduced tillage (10 cm depth) for W-M are applied. In comparison to the R_3 baseline, i.e., the currently applied field management practices, the identified BMP could produce stable crop yields and enlarge the ΔSOC (by 4% on average) while decreasing the NEGE (by −4% on average), NH$_3$ volatilization (by −23% on average), NO emissions (by −9% on average) and NO$_3^-$ leaching (by −44% on average) (Table 1).

3.4 The uncertainty of the best management practice

Compared with the simulation results by the model version of Cui et al. (2014), the R^2 of ZIR by

4 Discussion

4.1 Model performance

The DNDC model has been widely applied in agricultural systems around the world. The modified model version used in this study showed good performance in simulating the crop yields, NEE, NH_3, CH_4 uptake, emissions of N_2O and NO and related soil factors for the land cultivated with cotton and W-M under various field management treatments. The satisfying validations of both cropping systems, especially for the decision variables at an annual scale used for the scenario analysis, suggest that the DNDC95 model can be applied to quantify the decision variables and related factors for the cotton and W-M rotation system under different management practices.

The well-simulated soil environmental factors (soil temperature and moisture) and crop yields provided a solid basis for further simulating the decision variables to quantify the NIP under any

369 condition. The soil environmental factors and crop yields are the key factors regulating the

370 biogeochemical processes and indicator of essential processes in plant nitrogen uptake (Chirinda et al.,

371 2011; Kröbel et al., 2010). For the simulations of the N_2O and NO emissions, discrepancies in daily

372 emissions generally occur in DNDC models and other current biogeochemical models due to the

373 complex interactions among soil environmental factors and carbon and nitrogen processes (e.g., Bell et

374 al., 2012; Chirinda et al., 2011; Cui et al., 2014; Lehuger et al., 2011; Zhang et al., 2015), which

375 resulted in the time lags between the observations and simulations. For the cotton in this study, the

376 underestimated daily NO fluxes in the spring in the model from Cui et al. (2014) was improved by the

377 modified model. However, the improvements in the daily NO fluxes did not significantly affect the

378 annual cumulative emissions, which were not major contributors to the annual emissions (Liu et al.,

379 2015). The temporal variations in both the observed and simulated NEE indicated that the cotton field

380 frequently assimilated atmospheric CO_2 during the vigorous growth stages but emitted CO_2 to the

381 atmosphere during the other periods. However, the abrupt NEE increases during the growing season on

382 cloudy or rainy days were still not well simulated due to the calculation of plant growth relying on

383 cumulative daily temperatures over 0 ℃ and the TDD parameter (e.g., Cui et al., 2014). However, this

384 defect did not result in significant biases in the cumulative NEE. Therefore, the identified BMPs that

385 depended on the simulated annual NEE were reliable. For the simulations of other nitrogen losses from

386 the cotton field, the NO_3^- leaching accounted for 9−12% of the applied fertilizer nitrogen for model

387 validation, which was comparable with the field measurements of 16−17% (Liu et al., 2014).

388   The model validation suggests that the satisfactory simulation of decision variables at an annual

389 scale provided a solid basis for the BMP identification, but the scientific processes for determining the

390 photosynthesis and ecosystem respiration in CO_2 fluxes (both as the NEE components) on cloudy and

391 rainy days still require improvements in future studies. Because there were no observations of NH_3

392 volatilization and NO_3^- leaching from the experimental cotton field, this validation study did not

393 include both decision variables. Thus, future studies still required further validation of the model

394 performance using comprehensive observations covering both decision variables as well as others.

4.2 Biogeochemical effects of the rotation pattern and management practices

The scenario analysis relying on model simulations in this study showed that environmental contamination can be reduced while i) sustaining crop yields, ii) increasing soil carbon sequestration and iii) decreasing the net ecosystem GHG emissions. Reductions in environmental contamination are attributed to the better synchronization of crop nitrogen requirements and soil nitrogen availability.

For cotton, a period of 5 consecutive years is usually applied as the longest cotton monoculture to stabilize its yields. In addition, balanced elemental nutrients have been applied during cotton cultivation, and thus the negative effect of monoculture on cotton yields can be offset in practice (Han, 2010). Because the DNDC model assumes balanced nutrient supplies for any crops as well as optimum phytosanitary conditions, the negative effects of monoculture are not accounted for here (e.g., Li, 2017). The simulated positive annual changes in the SOC for W-M were mainly attributed to the incorporation of the full aboveground residues (at rates of $5.1-7.0$ Mg C ha^{-1} yr^{-1}), which favored for carbon sequestration (Han et al., 2016). However, the negative annual changes in the SOC for the cotton cropping system resulted from notable CO_2 emissions over a long fallow season relative to that of W-M (Liu et al., 2019). As a remarkable carbon sink, the W-M under the incorporation of the full crop residues could completely compensate for the SOC lost during the first cotton-planting year following the W-M cultivation. Thus, the annual change in the SOC was generally positive during the first cotton cultivation year. The rotation patterns of R_0 acted as net GHG sinks since the increased SOC exceeds the increased N_2O emission related to W-M cultivation, while the others all functioned as net GHG sources. The higher fertilizer application rate for W-M than for cotton resulted in the more reactive nitrogen remaining in the soil (Chen et al., 2014; Ju et al., 2009), thereby stimulating higher emissions of nitrogenous air pollutants and N_2O in the trials with fewer cotton cultivation years. Therefore, the appropriate rotation pattern of cotton and W-M can realize sustainable intensification with maximum yield and economic benefits, a balanced soil organic carbon budget 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 from 1980−2008, during which the application of mineral fertilizers increased by a factor of 5.1. The rapid increase in fertilizer use has resulted in excessive nitrogen remaining in the soil,

423   posing potential risks for the environment (Chen et al., 2011; Zhang et al., 2017b). To solve this

424   problem, a reduction in fertilizer application was proposed in several previous studies (e.g., Chen et al.,

425   2011, 2014; Liu et al., 2012). The results of the scenario analysis in this study indicated that, for all the

426   rotation patterns, further reducing the farmer-optimized nitrogen doses by 15−21% (87−94 and

427   334−367 kg N ha^{-1} yr^{-1} for the cotton and W-M, respectively) could sustain the crop yields while

428   greatly decreasing the emissions of nitrogenous gases. In addition to fertilization, over-irrigation has

429   also been ubiquitous in northern China for a long time, and it threatens the water security of this region

430   due to the sharply declining groundwater table and water pollution (Gao et al., 2015; Ju et al., 2009).

431   For this reason, only management options for reducing the amount of irrigation water should be

432   considered under the severe shortage of water resources. In addition, adopting sprinkling irrigation

433   instead of flood irrigation for an equal amount of water showed positive effects on the crop yields,

434   indicating improved irrigation efficiency (Zhang et al., 2017b). This result indicates that rather than

435   blindly using larger nitrogen doses, increasing the water-use efficiency through the application of

436   alternative irrigation techniques could be a pathway to sustaining crop yields with reduced nitrogen

437   addition. Through a ban on burning crop residues in fields, the return of these residues to the field is

438   strongly suggested by the government. The simulated results indicated that this practice can

439   simultaneously increase crop yields, soil carbon storage and emissions of N_2O and NO while

440   decreasing the NEGE. These simulations were consistent with the results of field observations (Liu et

441   al., 2011). Reduced tillage practices have been promoted in China in recent decades. To facilitate the

442   decomposition of woody cotton residues and avoid outbreaks of diseases and pests due to the

443   continuous implementation of reduced tillage or no-tillage practices, the tillage practices were only

444   adjusted in the W-M plots, while deep tillage was maintained for cotton when setting the tillage

445   scenarios. The simulations showed that the reduced tillage or no-tillage practices could sustain the crop

446   yields and reduce the NH_3 volatilization and NO_3^- leaching (e.g., Zhao et al., 2016).

447   As shown above, an appropriate combination of the rotation pattern and management practices can

448   satisfy the three constraints while resulting in the lowest NIP. The direct observations from the field

449   experiments are usually far less sufficient for screening this type of appropriate combination due to

450   limited resources and labor. However, identifying the appropriate combination is one of the purposes of

451   developing a biogeochemical model, such as the DNDC. A biogeochemical model that is validated with

452   limited observations from field experiments is, in principle, capable of fulfilling this task.

453   **4.3 Evaluation of the best management practice**

454   The scenario analysis was effective at screening for the BMP. The BMP could sustain the crop

455   yields of the three-crop rotation system, increase the SOC stock, mitigate the N_2O emissions and

456   NEGE, reduce the emissions of NH_3 and NO, and reduce the NO_3^- leaching due to the enhanced

457   resource use efficiency in response to the reduced nitrogen-fertilizer dose and irrigation water amount.

458   Hence, the BMP could result in a more dramatically reduced NIP than the others. In addition, the

459   alternative scenarios with overlapping ranges of uncertainty were also chosen as BMP alternatives,

460   although the increase in fertilizer and irrigation increased the negative effects to some extent. Because

461   the identified BMP was based on the sufficient validation only at this site, it should be the potential

462   BMP in this region, but additional validations for other sites in this region are still required to confirm

463   the BMP.

464   The uncertainty of the model validation for the screened BMP was evaluated in this study (3.1%).

465   However, there are three other unquantifiable factors. The first is the possible limitation of the applied

466   model, which cannot simulate the potential effects of monoculture on weeds and diseases, as well as

467   yields. The continuous cultivation of these crops, especially for cotton, could lead to challenges in

468   weed and disease management. In addition, the continuous no-tillage scenarios for W-M could also

469   increase the weed and disease pressure. However, these effects could not be adequately addressed by

470   the current model. Thus, the proper parameterization of the monoculture and no-tillage effects on the

471   weeds and diseases as well as the yields would be beneficial for screening the more realistic and

472   effective BMP.

473   The second concern is the insufficient data for model validation. Due to the lack of observations,

474   the model simulations on NH_3 fluxes for cotton cultivation and those on NO_3^- leaching in both the

475   cotton and W-M cropping systems were not validated. The DNDC model has been established by

476   following the mass conservation law. In other words, this model can accurately reflect the mass balance

477   of the nitrogen budget for the simulated soil layer (0−50 cm depth). This model principle implies that

478   only one budget item could be omitted for validation. This item is usually soil nitrogen loss through the

479   production of dinitrogen gas, mainly by denitrification, which is very difficult to measure *in situ* (e.g.,

480   Wang et al., 2013). For both cropping systems, the nitrogen lost through this pathway could be almost

481   fully inhibited in the topsoil, wherein the soil moisture contents were often lower than 60% WFPS

482   (Linn and Doran, 1984; Liu et al., 2011, 2014). The model principle also implies that the uncertainty in

483   the NO_3^- leaching simulation during cotton cultivation might have been larger than that of W-M

484   cropping system since the former has one more decision variable (i.e., NH_3 volatilization) not directly

485   validated by observations. These situations suggest that the current uncertainties may not be reduced

486   unless the simulations of both NH_3 volatilization and NO_3^- leaching can be validated in addition to the

487   other validated variables.

488   The third consideration is the method applied for identifying of the BMP. The current method only

489   considers the biogeochemical effects on the decision variables and crop yields as one of the three

490   constraints. This method excludes other factors, such as those related to the costs of the management

491   practices, thereby likely resulting in uncertainty. Although the method applied in this study still has

492   some deficiencies, this case study has potential application to more comprehensive situations, which

493   can be easily and automatically implemented as long as the simulations for all the decision variables

494   and crop yields can be validated using comprehensive observations.

495   **5 Conclusions**

496   An approach was proposed and applied to identify the best management practice of crop rotation

497   in the interaction with field management practices based on the negative impact potentials and a set of

498   constraints. The NIP of a scenario was defined as the linear function of five decision variables,

499   including the NEGE, ammonia volatilization, nitric oxide release, emission of nitrous oxide in the form

500   of depleted ozone layer matter, and nitrate leaching. This study used three variables, i.e., the crop yield,

501   SOC content, and NEGE, to specify the applied constraints that were stable/increased the crop yields

502   and SOC contents and reduced the NEGE. All the decision variables and those related to constraints

503   were generated through model simulation. The BMP was referred to as the scenario with the lowest

504   NIP among the possibilities capable of simultaneously satisfying the three constraints.

505   This case study focuses on a multi-crop cultivation system with a rotation between cotton and

506   W-M, which has been widely adopted in northern China. Version 95 of the

507   DeNitrification-DeComposition (DNDC95) model, with minor modifications of NO production during

508   nitrification, was used to validate two adjacent plots cultivated with cotton and W-M. The modified

509   model exhibited a satisfactory performance in simulating the decision and constraint variables under

510   the available field observations. When relying on the Monte Carlo simulations driven by 6000

511   management scenarios, the effects of various rotation patterns and field management choices on the

512   variables of interest were investigated, and the BMP for each rotation pattern and the final BMP for the

513   cropping system were identified. The simulation results of the rotation patterns indicated that the proper

514   rotation of the cotton and W-M can be simultaneously beneficial for the economy (crop yields), soil

515   fertility (soil carbon sequestration) and climate (GHG mitigation). The final BMP for the system could

516   be a rotation of 3 consecutive years of cotton rotated with 3 continuous years of W-M that uses 18%

517   less fertilizer and 18% less irrigation water through sprinkling compared to the current conventional

518   practices. This BMP would incorporate 90% of the crop residues and adopt conventional deep tillage

519   (20−30 cm) for cotton but reduced tillage (10 cm) for W-M. This study emphasizes the need to make

520   comprehensive observations that fully cover the decision and constraint variables and related soil

521   factors to facilitate effective BMP screening by relying on virtual experiments using a biogeochemical

522   model such as the DNDC model.

523   **Author contribution**

524   Xunhua Zheng, Chunyan Liu and Jiang Zhu contributed to the further development in data

525   management and enhanced scientific efficacy and effectiveness. Wei Zhang performed the simulations

526   and prepared the manuscript with contributions from all co-authors. Chunyan Liu, Kai Wang, Rui Wang

527   and Zhisheng Yao designed and carried out the experiments. Feng Cui and Siqi Li applied the

528   un-modified model in adjacent plot of winter wheat-summer maize cropping system.

529   **Acknowledgement**

530   This study was jointly supported by the National Key R&D Program of China (2016YFA0602303) and

531   the National Natural Science Foundation of China (41603075, 41761144054).

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680   Table 1 Simulated decision variables, negative impact potential (NIP; USD ha^{-1} yr^{-1}) and relative

681   uncertainty of NIP (NIP$_u$) for the best management practices and alternatives.

Scenarios [a]	R	ΔSOC	CH$_4$	N$_2$O	NEGE	NH$_3$	NO	NL	NIP	NIP$_u$
BAS	R$_3$	0.14	-1.9	3.6	1.06	57	1.6	58	453	3.0%
BMP	**R$_3$**	**0.15**	**-1.9**	**3.5**	**1.01**	**44**	**1.5**	**33**	**327**	**3.1%**
BMP$_{a1}$	R$_3$	0.07	-1.9	3.0	1.06	46	1.4	36	339	3.2%
BMP$_{a2}$	R$_3$	0.16	-1.9	3.7	1.03	46	1.5	37	347	3.1%
BMP$_{a3}$	R$_3$	0.11	-1.8	3.3	1.05	48	1.5	33	348	3.2%

682   [a] BMP, best management practice. BAS, BMP, BMP$_{a1}$, BMP$_{a2}$ and BMP$_{a3}$, baseline management practices, the best

683   management practices (BMP) and the three BMP alternatives, which are encoded as

684   N110/430_I100_IF_RI100_T20, N90/353_I82_IS_RI90_T10, N94/366_I94_IS_RI75_T20,

685   N94/366_I91_IS_RI95_T10 and N97/378_I88_IS_RI70_T5, respectively. For the meanings of these codes, refer

686   to section 2.3. R$_3$, 3 consecutive years of cotton rotated with 3 continuous years of W-M. The decision variables

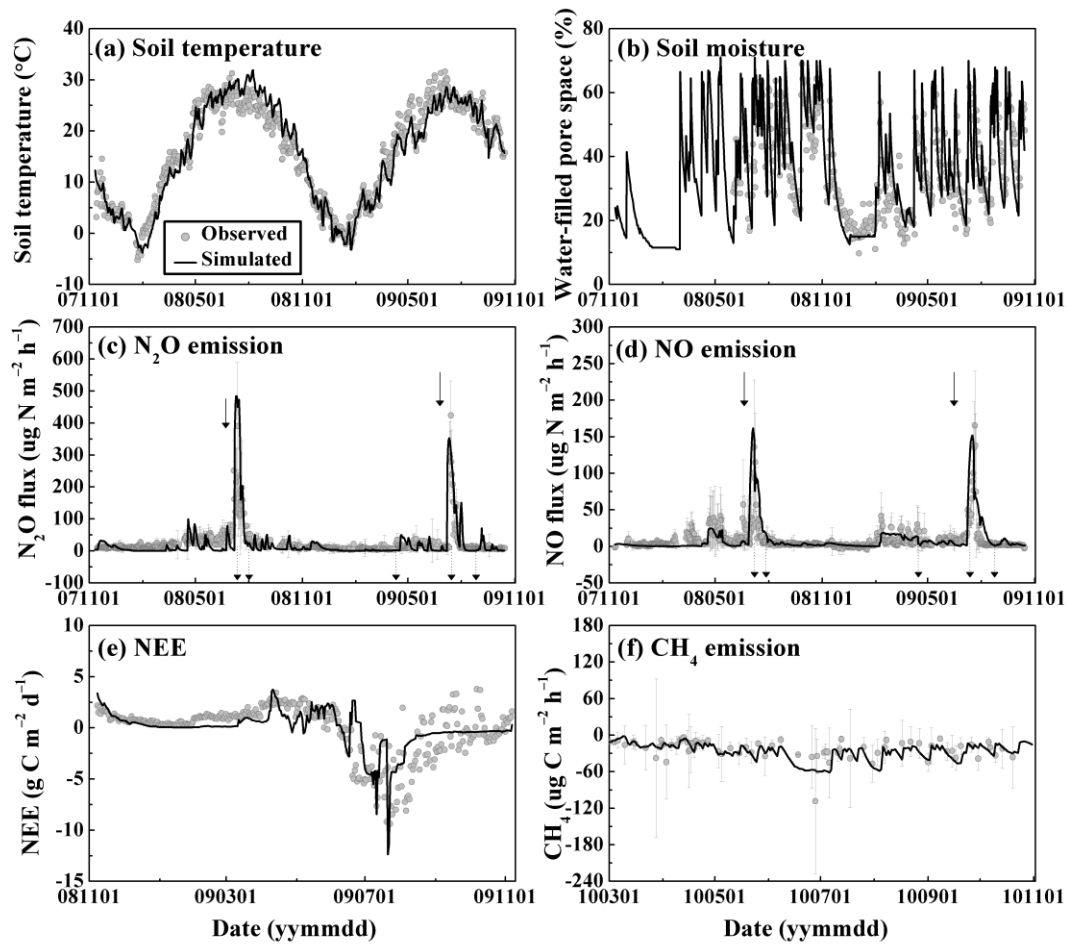
687   include annual change in soil organic carbon (ΔSOC; Mg C ha^{-1} yr^{-1}), methane (CH$_4$; kg C ha^{-1} yr^{-1}) and, nitrous

688   oxide (N$_2$O) releases, net ecosystem greenhouse gases emission (NEGE; Mg CO$_2$eq ha^{-1}), ammonia (NH$_3$)

689   volatilization, nitric oxide (NO) emission and nitrate leaching (NL) (kg N ha^{-1} yr^{-1}). The CO$_2$eq was based on the

690   100-year global warming potentials, i.e., 34 for CH$_4$ and 298 for N$_2$O (IPCC, 2013). The NIP was calculated using

691   Eq. (2) presented in the text.

692

693 **Figure 1: Observed and simulated daily mean soil (5 cm) temperature, soil (0−6 cm) moisture, nitrous oxide**

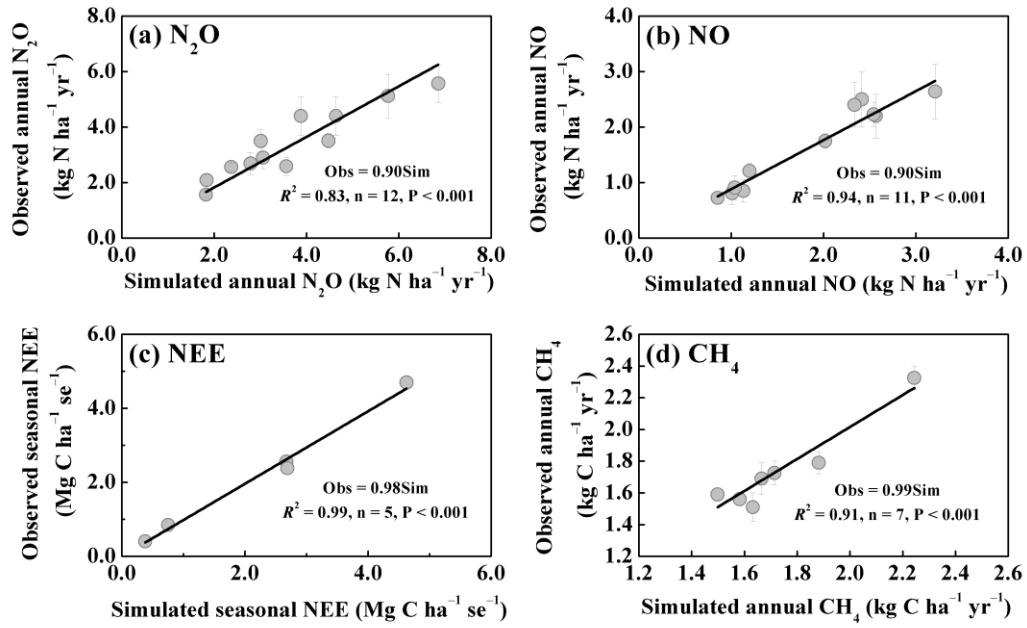
694 **(N₂O) and nitric oxide (NO) fluxes, net ecosystem exchanges of carbon dioxide (NEE), and methane (CH₄)**

695 **emissions. The solid- and dashed-line arrows indicate the dates of fertilization and irrigation, respectively.**

696 **The measurement errors were not shown in panels a, b and e. The vertical bar for each observation in**

697 **panels c, d and f indicates two times standard deviations to represent the uncertain range at the 95%**

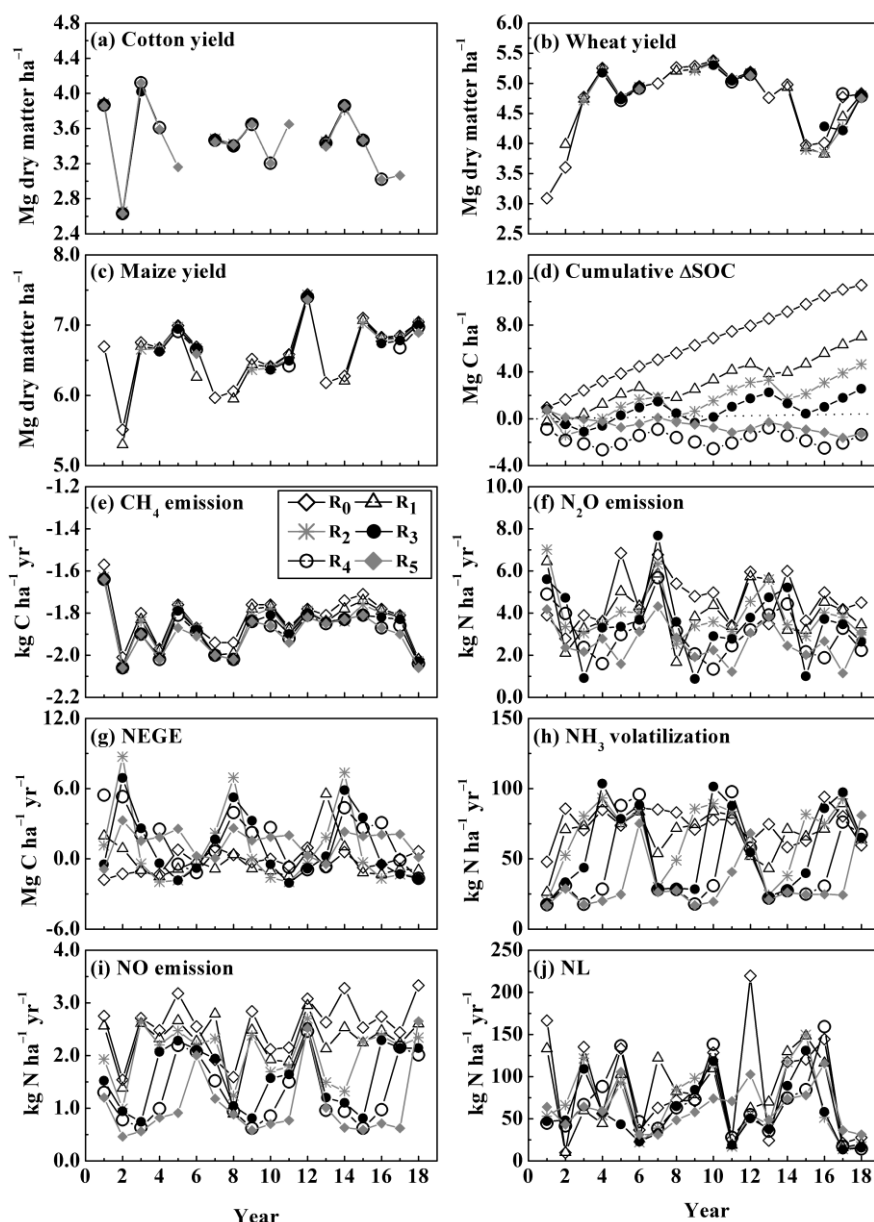
698 **confidence interval. The legend in panel a applies for all subfigures.**

699

700 **Figure 2: Comparison between observations and simulations of annual nitrous oxide (N_2O) (a) and nitric**

701 **oxide (NO) (b) emissions, seasonal net ecosystem exchanges of carbon dioxide (NEE) (c), and annual**

702 **methane (CH_4) uptake (d). The black solid lines are the zero-intercept linear regression lines. The vertical**

703 **bars indicate the standard error of four spatial replicates.**

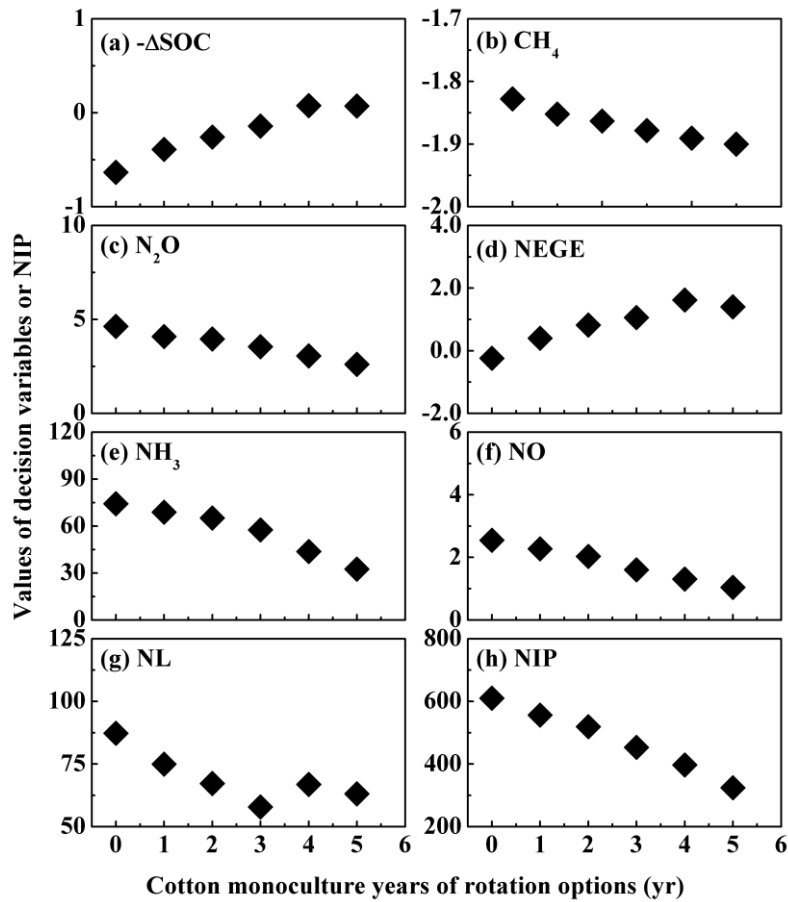
704

705 **Figure 3: Simulated crop yields, cumulative changes in soil organic carbon (ΔSOC), methane (CH₄) and,**

706 **nitrous oxide (N₂O) release, net ecosystem greenhouse gases emission (NEGE), ammonia (NH₃) volatilization,**

707 **nitric oxide (NO) emission and nitrate leaching (NL) over a 18-year period (spanning three 6-year rotation**

708 **cycles) for each rotation pattern scenario. For the definitions of the rotation pattern options, i.e., R₀, R₁..., R₅,**

709 **refer to the text in section 2.3. The legend in panel e applies for all subfigures.**

710

711 **Figure 4: Simulated effects of rotation options under the baseline management practices on decision**

712 **variables and negative impact potential (NIP). For the definitions of the rotation pattern options, i.e., R_0,**

713 **R_1..., R_5, refer to the text in section 2.3. The y-axis units are Mg C ha^{-1} yr^{-1} for the opposite of mean annual**

714 **increase in soil organic carbon stock ($-\Delta SOC$), kg C ha^{-1} yr^{-1} for methane (CH_4) emission, kg N ha^{-1} yr^{-1}**

715 **for emissions of nitrous oxide (N_2O), ammonia (NH_3) and nitrous oxide (NO), and nitrate leaching (NL), Mg**

716 **CO_2eq ha^{-1} yr^{-1} for net ecosystem greenhouse gas emission (NEGE), and USD ha^{-1} yr^{-1} for NIP. The CO_2eq**

717 **was based on the 100-year global warming potentials, i.e., 34 for CH_4 and 298 for N_2O (IPCC, 2013). The**

718 **NIP was calculated using Eq. (2) presented in the text.**