

## Article

# Evaluation of the DNDC Model to Estimate Soil Parameters, Crop Yield and Nitrous Oxide Emissions for Alternative Long-Term Multi-Cropping Systems in the North China Plain

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**Abstract:** Optimizing crop rotations is one of the proposed sustainable management strategies for increasing carbon sequestration. The main aim of this study was to evaluate the DeNitrification-DeComposition (DNDC) model for estimating soil parameters (temperature, moisture and exchangeable  $\text{NO}_3^-$  and  $\text{NH}_4^+$ ), crop yield and nitrous oxide ( $\text{N}_2\text{O}$ ) emissions for long-term multi-cropping systems in Hebei, China. The model was validated using five years of data of soil parameters, crop yields and  $\text{N}_2\text{O}$  emissions. The DNDC model effectively simulated daily soil temperature, cumulative soil nitrogen and crop yields of all crops. It predicted the trends of observed daily  $\text{N}_2\text{O}$  emissions and their cumulative values well but overestimated the magnitude of some peaks. However, the model underestimated daily water filled pore space, especially in dry seasons, and had difficulties in correctly estimating daily exchangeable  $\text{NO}_3^-$  and  $\text{NH}_4^+$ . Both observed and simulated cumulative  $\text{N}_2\text{O}$  results showed that optimized and alternative cropping systems used less nitrogen fertiliser, increased grain yield and decreased  $\text{N}_2\text{O}$  emissions compared to the conventional cropping system. Our study shows that although the DNDC model (v. 9.5) is not perfect in estimating daily  $\text{N}_2\text{O}$  emissions for these long-term multi-cropping systems, it could still be an effective tool for predicting cumulative emissions.

**Keywords:** soil parameters; nitrous oxide; DNDC model; crop productivity; multi-cropping cropping system; China



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## 1. Introduction

Agricultural land accounts for about 13% of global soil greenhouse gas (GHG) emissions and one-fifth of the annual increase in radiative forcing. It represents the largest source of anthropogenic GHG emissions following the combustion of fossil fuels and industrial processes [1]. Since the pre-industrial era (around 1750), the concentrations of carbon dioxide ( $\text{CO}_2$ ), nitrous oxide ( $\text{N}_2\text{O}$ ) and methane ( $\text{CH}_4$ ) in the atmosphere have increased globally by 47, 23 and 156%, respectively [1]. According to the IPCC [1], it is possible that these human-caused higher concentrations of GHGs in the atmosphere are causing tropospheric warming and stratospheric ozone depletion and consequently, cooling of the lower stratosphere. However, management of cropland is one of the potential strategies for mitigating GHG emissions from soils [2]. Research has focused on developing sustainable field management practices that value soil resources for increasing crop productivity whilst protecting soil quality and reducing GHG emissions from soils. Management can directly influence GHG emissions from soils through soil fertility due to nitrogen (N) fertiliser inputs [3,4] or indirectly through management-induced changes in plant composition and

amounts and quality of plant residue added to soils [5,6]. There are many management mitigation strategies to sequester carbon (C) or reduce emissions from soils such as reduced N fertilisation, reduced water irrigation, applying non-inversion tillage and optimizing crop rotations [7,8]. These field management practices offer great opportunity for reducing N<sub>2</sub>O emissions and achieving national mitigation targets [4,9]. Nitrous oxide is a powerful GHG, which has a global warming potential 273 times that of CO<sub>2</sub> on a 100-year time scale. Moreover, it is potent in destroying stratospheric ozone. The concentration level of N<sub>2</sub>O in the atmosphere in the year 2019 was 332 ppb [1]. Emissions of N<sub>2</sub>O to the atmosphere are mostly derived from microbial nitrification and denitrification in soils due to human activities such as nitrogen fertilisation, irrigation, biomass burning and industry [10–12]. These emissions are often enhanced by the conditions of low oxygen in soils [13] and where the N available exceeds plant requirements, especially following the application of N fertiliser [14,15]. Many factors are responsible for regulating N<sub>2</sub>O emissions during the processes of nitrification and denitrification. Among others, these factors include soil N concentration, N fertiliser application amounts, soil temperature, soil moisture and land use and management [16]. All these factors should be entirely examined to avoid higher N<sub>2</sub>O emissions. Agriculture is one of the main sources of N<sub>2</sub>O emissions to the atmosphere in China due to widespread and overuse of N fertiliser in intensive cropping systems [17]; however, in 2020, the government set a policy of zero growth in N fertiliser and pesticide use [18]. Additionally, optimization/re-structurization of crop rotation systems can increase crop yield and soil carbon and represents a sustainable strategy for crop production compared to monoculture systems [19,20]. Previous studies reported that crop rotations could enhance interactions between diverse plants and microbes in the soils [21,22], which could benefit the following crops in the rotation [23]. They improve soil physical and chemical properties and enhance soil health [24–26]. In order to sequester carbon atmospheric CO<sub>2</sub> into plant biomass, a widespread of crop rotations has been suggested [27]. However, unoptimized crop rotation could increase N<sub>2</sub>O emissions if soil mineral N is increased. Moreover, soil microorganisms responsible for N<sub>2</sub>O consumption or production are influenced by these crop rotations and their associated higher soil organic matter (SOM) [28]. They can convert N<sub>2</sub>O to N<sub>2</sub> (i.e., complete denitrification) and thereby reduce the emissions of N<sub>2</sub>O from soils [29,30]. The DeNitrification-DeComposition (DNDC) model [31,32] is a widely used ecosystem biogeochemistry model to assess N<sub>2</sub>O and other GHG emissions from agricultural soils. The DNDC model was originally developed for simulating GHG emissions from USA conditions but have been calibrated and used worldwide [33–35]. The model is dynamic and can capture complex agroecosystem interactions for simulating GHG emissions from croplands and other ecosystems [35,36]. The main aim of this study was to evaluate the DNDC model for simulating soil parameters, crop yield and N<sub>2</sub>O emissions for conventional, optimal and alternative long-term multi-cropping systems in Hebei, China.

## 2. Materials and Methods

### 2.1. Experimental Site

This study is part of a process to calibrate and validate the DNDC model for estimating N<sub>2</sub>O emissions from different crop rotations in China [35–38]. The experiment was established in 2007 at Quzhou Station (36.87° N, 115.02° E). The soil is a calcareous fluvo-aquic soil, and the main cropping system at the site is winter wheat-summer maize. The average annual air temperature and precipitation over the experimental period were 13.2 °C and 440 mm, respectively. A detailed description of the experimental site can be found in Gao et al. [37,38].

### 2.2. Cropping Systems

A completely randomized plot design with five treatments and four replicates was used in this study. Cropping systems applied were as follows: (a) control—conventional winter wheat-summer maize double-cropping system (Chem. W/M) using the local N

fertilisation rates; (b) optimized winter wheat-summer maize double-cropping system (Opt. W/M); (c) winter wheat-summer maize-fallow-spring maize system (W/M-M); (d) winter wheat-summer soybean-fallow-spring maize system (W/S-M); and (e) a single spring maize system with one crop per year (M). The last four cropping systems were alternative systems designed with crops, water and fertiliser optimizations. The cropping systems, N fertiliser rates and tillage, irrigation practices and crop yields are shown in Tables S1–S3, respectively. Winter wheat was irrigated two or three times whilst summer maize was irrigated once or twice. The amount of irrigation water added to winter wheat and summer maize ranged from 60 to 100 mm depending on previous farming practice in the Chem. W/M. However, for the alternative cropping systems, only 45 to 80% of plant available water was determined, by measuring field water holding capacity and the corresponding wilting point [39], and maintained. More details about the cropping systems can be found in [37,38].

### 2.3. Field Measurements and N<sub>2</sub>O Fluxes

Measurements of N<sub>2</sub>O fluxes in every cropping system were carried out from June 2009 to June 2013. The daily N<sub>2</sub>O fluxes for each crop season are shown in Table S4. The closed static chamber method described by [40] was used for the measurements. The fluxes were measured on a daily basis for 10 days after N fertiliser application and for 3 to 5 days after irrigation or heavy rainfall (>10 mm). However, for the rest of the growing season, N<sub>2</sub>O fluxes were observed twice per week or once per week when the soil was frozen. More details about the chamber used, flux measurements and analysis and calculation of the N<sub>2</sub>O can be found in Gao et al. [37,38].

### 2.4. Soil Temperature, WFPS (%) and Soil Mineral N (Exchangeable NH<sub>4</sub><sup>+</sup> and NO<sub>3</sub><sup>-</sup>)

Soil temperature (°C) at 0–10 cm depth was measured during gas sampling. Soil samples for measurements of WFPS (%) and soil mineral N (exchangeable NH<sub>4</sub><sup>+</sup> and NO<sub>3</sub><sup>-</sup>) were collected and calculated as described in [37].

### 2.5. Model Description, Validation and Statistical Evaluation

The DNDC model accommodates six sub-models and describes soil C and N cycles in agricultural systems [31,32]. DNDC (v. 9.5) was calibrated to simulate summer maize–winter wheat cropping system, and the sensitivity of the model to different input parameters was investigated as described in [35]. The parameters of this calibrated model were adopted to simulate summer maize–winter wheat in this study whilst default values were used for the spring maize and soybean. We validated the model using five-year field data collected from all cropping systems (Chem. W/M; Opt. W/M; W/M-M; W/S-M and M) between June 2009 to June 2013. The model was assessed by calculating the root mean square error (RMSE; Equation (1)), normalized RMSE (nRMSE; Equation (2)), index of agreement (d; Equation (3)) and relative deviation (RD; Equation (4)). More details about the model description can be found in [35]:

$$\text{RMSE} = \sqrt{[\Sigma(S_i - M_i)^2/n]} \quad (1)$$

$$\text{nRMSE} = (\text{RMSE}/\bar{X}) * 100 \quad (2)$$

$$d = 1 - \Sigma(S_i - M_i)^2 / \Sigma[(S_i - \bar{X}) + (M_i - \bar{X})]^2 \quad (3)$$

$$\text{RD} = (M_i - S_i)/M_i \quad (4)$$

where  $M_i$  and  $S_i$  are the measured and simulated values, respectively.  $n$  is the number of measured values and  $\bar{X}$  is the average of the measured values. The annual cumulative N<sub>2</sub>O flux for model results was determined by the summation of daily emissions [41]. The coefficient of determination ( $r^2$ ) was also calculated to observe whether simulated and observed values follow the same pattern.

### 3. Results and Discussion

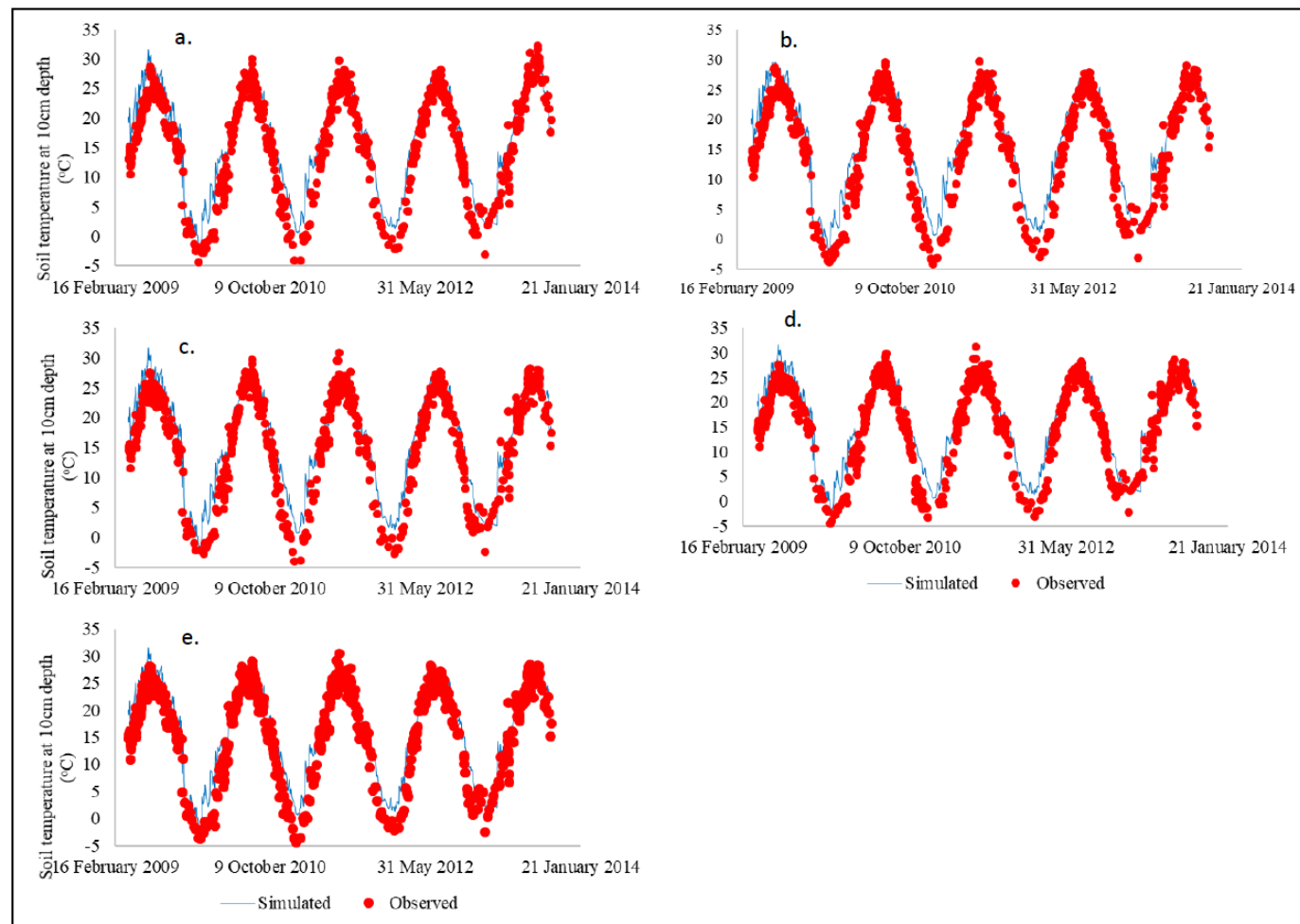
#### 3.1. Evaluation of the DNDC Model to Estimate Soil Parameters

##### 3.1.1. Soil Temperature

In this study, the DNDC model effectively estimated trends and values of daily soil temperature ( $^{\circ}\text{C}$ ; 0–10 cm depth) throughout the experimental period and for the five investigated cropping systems, with few variations between the observed and simulated results (Figure 1). The correlations between observed and simulated values ( $r^2$ ) ranged from 0.94 to 0.95 and the overall  $r^2$  and RD were 0.94 and 12%, respectively. The average measured temperature was  $17.8^{\circ}\text{C}$ , RMSE ranged from  $3.73^{\circ}\text{C}$  to  $4.36^{\circ}\text{C}$ ; nRMSE ranged from 19 to 24% and d values ranged from 0.92 to 0.95 (Table 1). The model simulated the temperature fluctuations for both dry and wet seasons well but had better estimates for the dry season (Figure 1). Many previously published studies showed that DNDC successfully simulated soil temperature under multiple cropping systems, e.g., [35,42–44]. Interestingly, the simulations of soil temperature for the long-term multiple cropping systems, in this study, are equally good as that of a double cropping system reported by [35] where  $r^2$  was 0.97 and better than that for a single spring barley crop where  $r^2$  was 0.83 [45]. Other studies on multiple cropping systems also reported high  $r^2$  values ranging from 0.89 to 1.0 [42,44]. This result confirms our previous finding that the current algorithm in the DNDC model is capable of accurately simulating soil temperature for a single as well as for a multiple cropping system [35]. The correct estimation of soil temperature by the DNDC is important for a reliable model-estimation for crop yield and  $\text{N}_2\text{O}$  emissions as the soil temperature influences decomposition of soil organic carbon, soil microorganism activities and plant growth [46,47]. Soil temperature also influences  $\text{N}_2\text{O}$  emissions by affecting the ratio of  $\text{N}_2/\text{N}_2\text{O}$  [48] and freeze–thaw cycles [49]. The  $\text{N}_2/\text{N}_2\text{O}$  ratio increases exponentially with increasing soil temperature [50].

##### 3.1.2. Soil Water Filled Pore Space (WFPS)

For all cropping systems, the DNDC model was able to satisfactorily simulate the trends of daily WFPS (%) but underestimated their magnitude values, especially during the dry season (Figure 2). The correlations between the observed and simulated WFPS values ( $r^2$ ) for different cropping systems ranged from 0.23 to 0.42, the overall  $r^2$  was 0.33 and RD was 43% (Table 1 and Figure 2). The average measured WFPS in this study was 51.44%; RMSE ranged from 23.34 to 27.43; nRMSE = 47% to 51%; and d = 0.33 to 0.44 (Table 1). Similar variations are available in the literature, e.g., a correlation value ( $r^2$ ) between the observed and DNDC-simulated soil moisture of 0.35 was reported [45] whilst another study found an  $r^2$  value of 0.29 [42]. The higher discrepancy was not in the entire crop rotation but in the summer maize phase only [44]. Moreover, the model overestimated water content near the soil surface but underestimated it at deeper layers [51]. The cascade model approach of DNDC was not suitable for estimating soil water at certain sites [52]. In order to improve the performance of the DNDC to simulate WFPS, water module should be improved [35]. Further improvements of data input to the model, e.g., root density and root penetration functions, soil profile and usage of fluctuating water table were suggested [51]. This is because a correct estimation of WFPS by the DNDC model is important for the prediction of reliable  $\text{N}_2\text{O}$  emissions by the model. WFPS influences the concentration and transport of oxygen in soil matrix and, thereby, production of  $\text{N}_2\text{O}$  from denitrification [53,54]. The impacts of WFPS, between 40% and 98%, on  $\text{N}_2\text{O}$  emissions from a fine-loamy soil in Germany were investigated [55]. The results revealed that  $\text{N}_2\text{O}$  emissions by denitrification increased when WFPS rose above 60–70%.

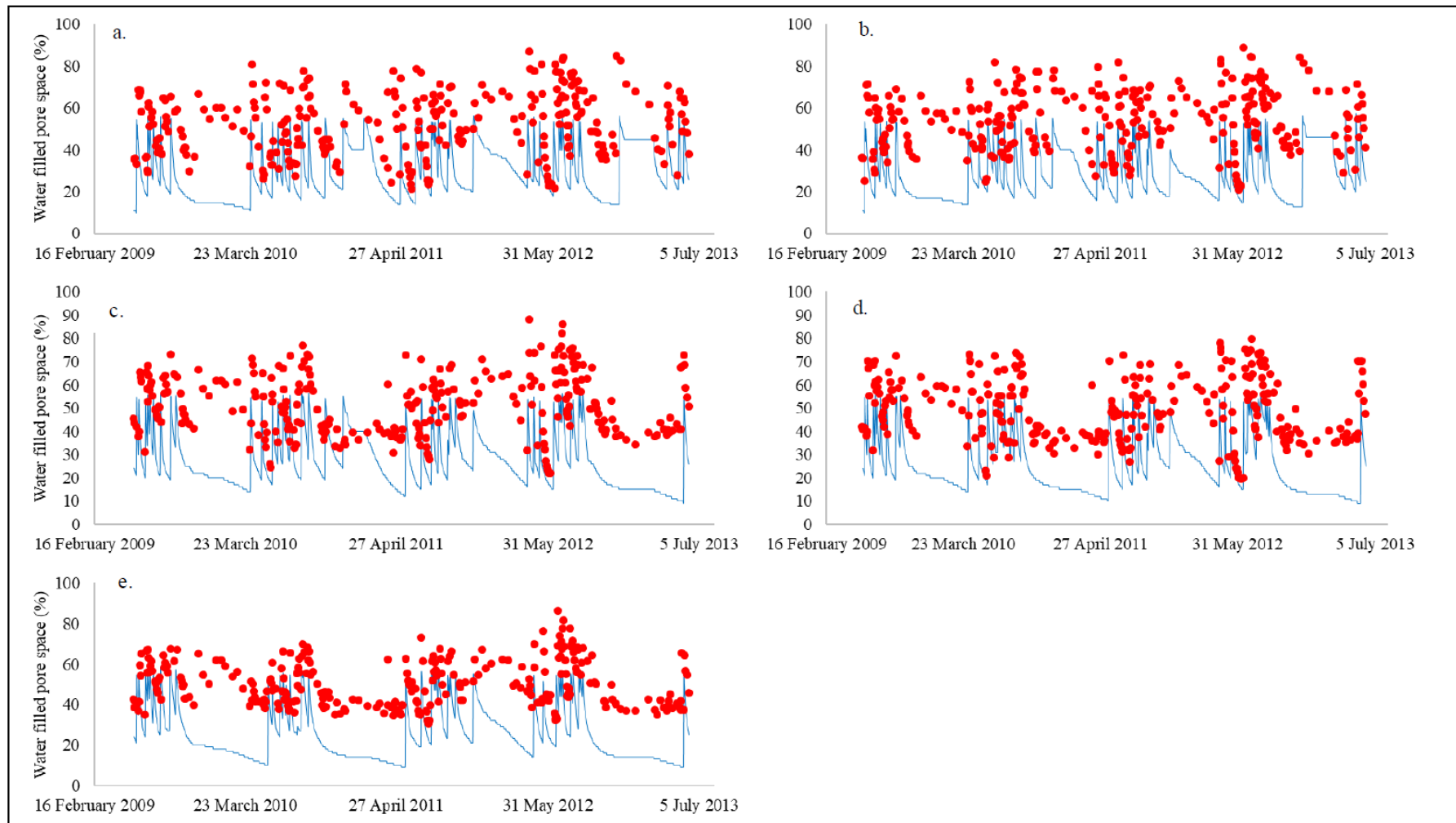


**Figure 1.** Comparisons between field observed (●) and DNDC simulated (line) daily soil temperatures (°C) at the conventional winter wheat-summer maize double-cropping system (Chem. W/M; a.), optimized winter wheat-summer maize double-cropping system (Opt. W/M; b.), winter wheat-summer maize-fallow-spring maize system (W/M-M; c.), winter wheat-summer soybean-fallow-spring maize system (W/S-M; d.), and spring maize system (M; e.) over the experimental period from June 2009 to June 2013. The  $r^2$  ranged from 0.94 to 0.95 and the overall  $r^2$  is 0.94.

**Table 1.** Statistical evaluations of simulated daily soil temperature, WFPS, soil nitrogen and cumulative N<sub>2</sub>O fluxes compared with the observed values under different cropping systems.

Treatment/Parameter	Observed	Simulated	RD (%)	RMSE	nRMSE (%)	d
Chem. W/M						
Average daily soil temperature (°C)	17.71	19.96	13	3.38	19	0.95
Average daily WFPS (%)	52.02	29.55	−43	26.44	51	0.33
Average daily soil N (kg N ha <sup>−1</sup> )	98.14	155.49	58	124.23	>100	0.00
N <sub>2</sub> O emissions	7.85	8.32	5	54.48	>100	0.16
Opt. W/M						
Average daily soil temperature (°C)	17.57	19.95	14	3.73	21	0.94
Average daily WFPS (%)	53.91	29.01	−46	27.43	51	0.35
Average daily soil N (kg N ha <sup>−1</sup> )	63.97	119.29	86	73.66	>100	−0.60
N <sub>2</sub> O emissions	7.37	7.87	6	50.23	>100	0.08
W/M-M						
Average daily soil temperature (°C)	17.69	19.91	13	3.83	22	0.94
Average daily WFPS (%)	51.59	29.29	−43	25.26	49	0.35
Average daily soil N (kg N ha <sup>−1</sup> )	67.26	66.12	−1	48.47	72	0.22
N <sub>2</sub> O emissions	5.46	5.25	−3	35.70	>100	0.14
W/S-M						
Average daily soil temperature (°C)	17.72	19.92	12	3.94	22	0.94
Average daily WFPS (%)	49.42	29.01	−41	23.34	47	0.44
Average daily soil N (kg N ha <sup>−1</sup> )	53.72	89.46	66	68.77	>100	−0.13
N <sub>2</sub> O emissions	3.96	6.18	56	42.02	>100	0.13
M						
Average daily soil temperature (°C)	18.10	19.85	10	4.36	24	0.92
Average daily WFPS (%)	50.24	29.01	−42	23.79	47	0.41
Average daily soil N (kg N ha <sup>−1</sup> )	57.46	41.59	−27	50.08	87	0.27
N <sub>2</sub> O emissions	6.18	4.51	−26	33.42	>100	0.38

Chem. W/M = conventional winter wheat-summer maize double-cropping system using the local N fertilisation rates; Opt. W/M = optimized winter wheat-summer maize double-cropping system; W/M-M = winter wheat-summer maize-fallow-spring maize system; W/S-M = winter wheat-summer soybean-fallow-spring maize system; and M = a single spring maize system with one crop per year.



**Figure 2.** Comparisons between field observed (●) and DNDC simulated (line) daily WFPS (%) at the conventional winter wheat-summer maize double-cropping system (Chem. W/M; a.), optimized winter wheat-summer maize double-cropping system (Opt. W/M; b.), winter wheat-summer maize-fallow-spring maize system (W/M-M; c.), winter wheat-summer soybean-fallow-spring maize system (W/S-M; d.), and spring maize system (M; e.) over the experimental period from June 2009 to June 2013. The  $r^2$  ranged from 0.23 to 0.41 and the overall  $r^2$  is 0.33.

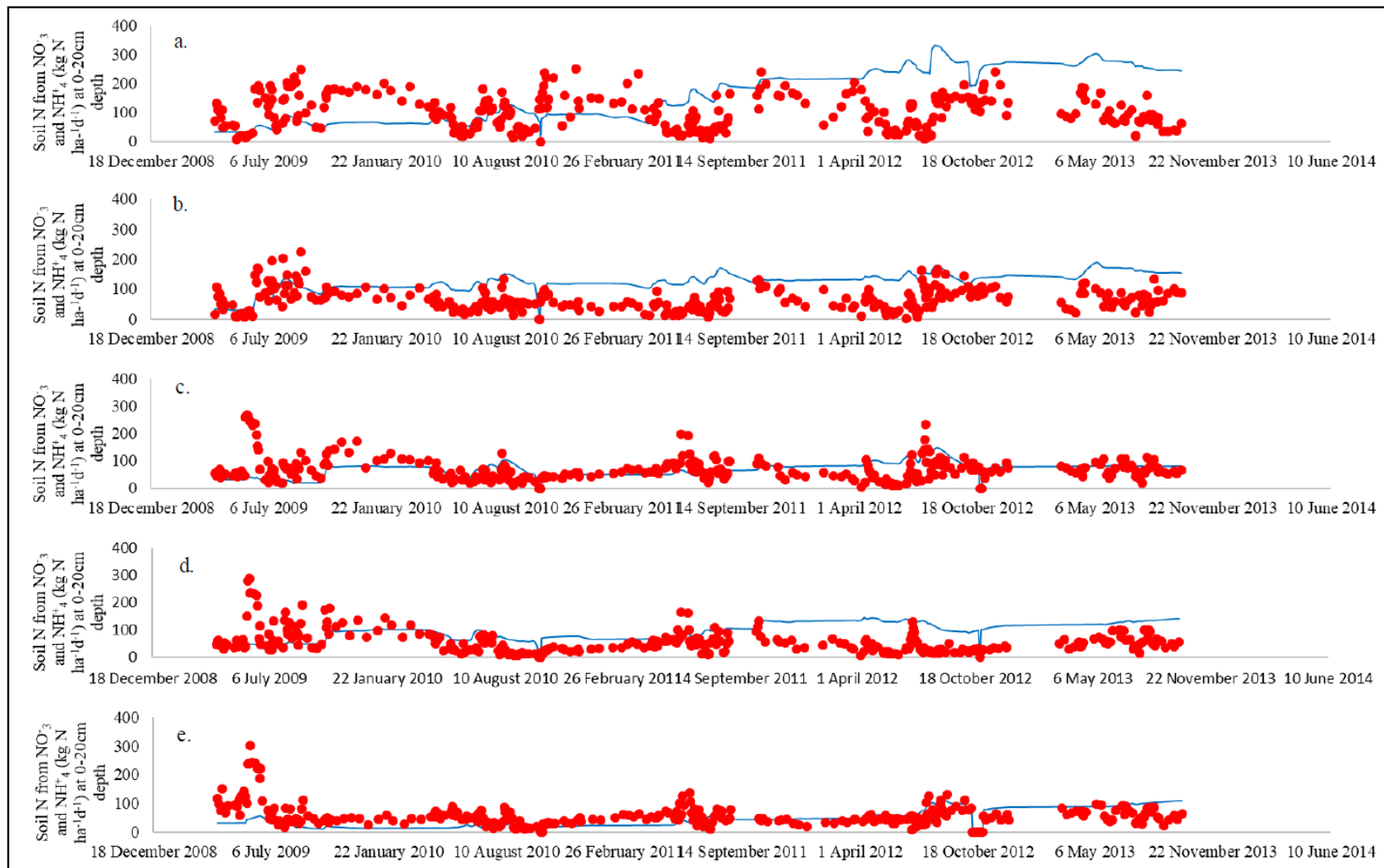
### 3.1.3. Soil Nitrogen (Exchangeable $\text{NH}_4^+$ and $\text{NO}_3^-$ )

The DNDC model over/underestimated the magnitude of daily observed total soil mineral N (exchangeable  $\text{NH}_4^+$  and  $\text{NO}_3^-$ ). The correlations between observed and simulated values for the different cropping systems were poor, and the overall correlation ( $r^2$ ) was 0.10. The average of the observed soil N was  $68 \text{ kg N ha}^{-1}$  and RMSE ranged from 48 to  $124 \text{ kg N ha}^{-1}$ . nRMSE ranged from 72% to 128%, and d ranged from  $-0.13$  to 0.27 (Figure 3). The difficulties in correctly estimating daily soil N were due to the presence of multiple N sources, including synthetic fertilisers, N deposition and N turnover from different added crop residues in these long-term multi-cropping systems. However, the model reasonably estimated cumulative soil N with RD values ranging from  $-2$  to 86% and an overall RD of 39% (Table 1). The correlation ( $r^2$ ) between cumulative observed and simulated soil N was 0.58. Similar variations were already shown by [56] for a reduced tillage-cover crop experiment and by [35] for a summer maize-winter wheat double cropping system. In order to improve the performance of DNDC to simulate daily soil N, [20] suggested upgrading the present algorithms for multiple cropping systems in the model.

### 3.2. Evaluation of the DNDC Model to Estimate Crop Yield

The DNDC model effectively estimated the observed grain yield for all grown crops across all cropping systems (summer maize, winter wheat, spring maize and summer soybean) with average RD values of 0.2,  $-30$ , 12 and  $-17\%$ , respectively. Here, the DNDC simulated summer maize perfectly compared to the other grown crops. The overall  $r^2$  of observed and simulated grain yields of all crops was 0.56 (Table 2; Figure S1). The DNDC showed a good agreement between observed and simulated yield of winter wheat-summer maize cropping system [57]. The model simulates plant growth and yield using a group of physiological parameters to define the plant growth curve based on weather condition, field management and soil. Simulating grain yield correctly by the DNDC is essential for a satisfactory prediction of  $\text{N}_2\text{O}$  emissions by this process-based model. With the exception of the control treatment (zero N), the DNDC model correctly simulated grain yield for all fertilised winter wheat-summer maize double cropping systems [35]. Both observed and simulated results showed that the Opt. W/M cropping system increased summer maize and winter wheat grain yields by 8 and 6% and 37 and 16%, respectively, compared to the Chem. W/M cropping system. These higher grain yields by the Opt. W/M took place in spite of fewer N fertiliser (total of  $1330 \text{ kg N ha}^{-1}$ ) applied to this cropping system compared to that (total of  $2200 \text{ kg N ha}^{-1}$ ) applied to Chem. W/M (Table S2). The production of each cropping system was influenced by the dynamics of the crop rotation such as soil properties and water and nutrient status due to differences in crop root structures and residue inputs [58,59]. Similar findings of high productivity and less N use were reported by [38].





**Figure 3.** Field observed (●) and DNDC simulated (line) daily soil N (kg N ha<sup>-1</sup>d<sup>-1</sup>) for the conventional winter wheat-summer maize double-cropping system (Chem. W/M; a.), optimized winter wheat-summer maize double-cropping system (Opt. W/M; b.), winter wheat-summer maize-fallow-spring maize system (W/M-M; c.), winter wheat-summer soybean-fallow-spring maize system (W/S-M; d.), and spring maize system (M; e.) over the experimental period from June 2009 to June 2013.

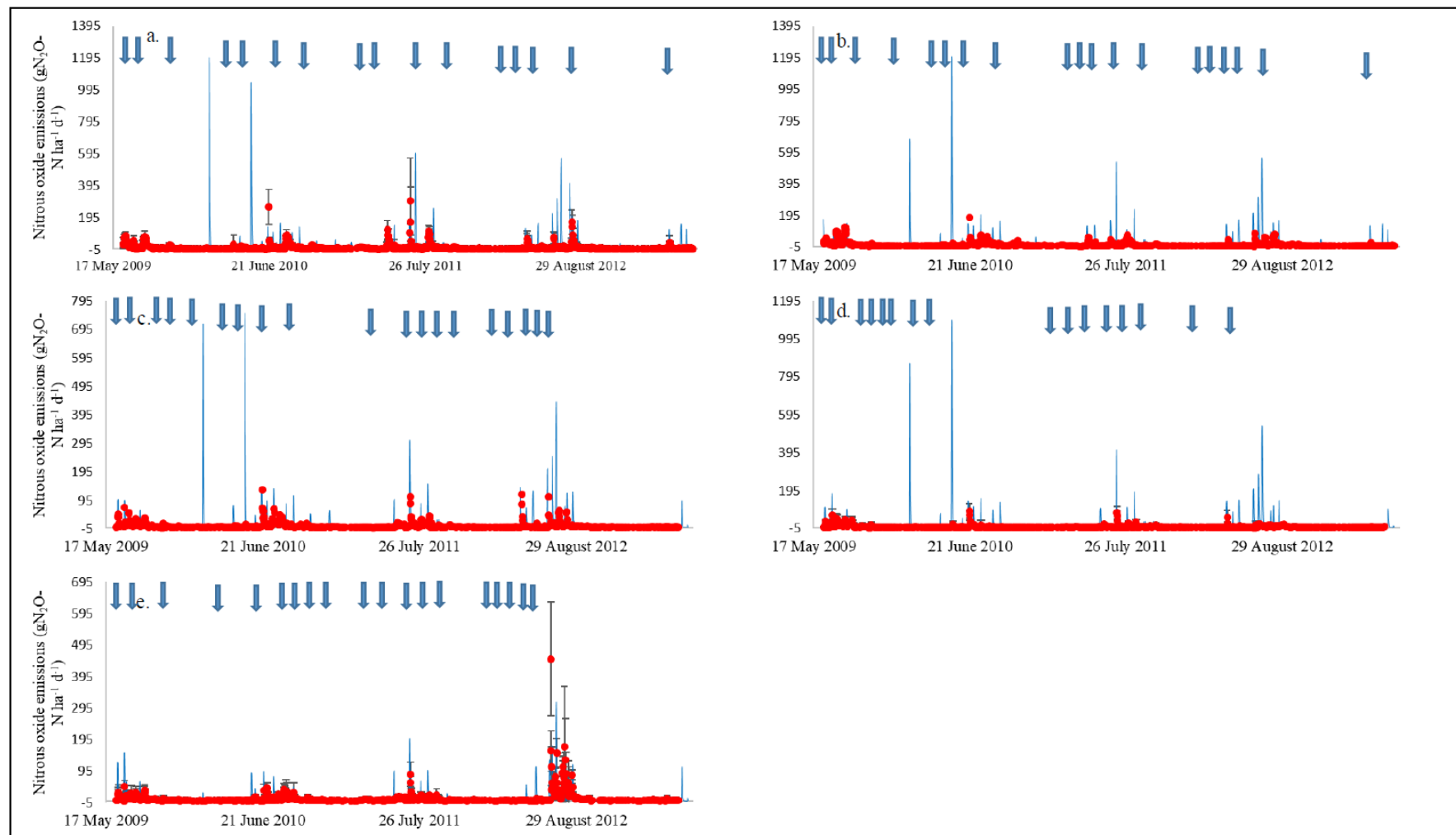
**Table 2.** Comparisons between the DNDC- simulated and observed annual grain yields for each crop (i.e., summer maize, winter wheat, spring maize and summer soybean) and cumulative N<sub>2</sub>O fluxes for the different cropping systems for 2009–2013.

Cropping System	Grown Crop	Season/Year	Observed Yield (t ha <sup>-1</sup> )	Simulated Yield (t ha <sup>-1</sup> )	RD (%)	Observed Cumulative N <sub>2</sub> O(kg N <sub>2</sub> O-N ha <sup>-1</sup> )	Simulated Cumulative N <sub>2</sub> O(kg N <sub>2</sub> O-N ha <sup>-1</sup> )	RD (%)
Chem. W/M	Summer maize	2009	7.2	8.4	17	7.9	8.3	6
	Winter wheat	2009–2010	4.4	2.9	−34			
	Summer maize	2010	6.9	5.7	−17			
	Winter wheat	2010–2011	4.1	2.8	−32			
	Summer maize	2011	6.7	6.4	−4			
	Winter wheat	2011–2012	5.9	5.0	−15			
	Summer maize	2012	8.9	9.5	7			
Opt. W/M	Winter wheat	2012–2013	3.9	5.4	38	7.4	7.9	7
	Summer maize	2009	7.1	8.4	18			
	Winter wheat	2009–2010	6.0	3.2	−47			
	Summer maize	2010	7.4	6.1	−18			
	Winter wheat	2010–2011	5.8	5.3	−9			
	Summer maize	2011	7.5	7.9	5			
	Winter wheat	2011–2012	6.5	4.6	−29			
W/M-M	Summer maize	2012	10.2	9.4	−8	5.5	5.4	−1
	Winter wheat	2012–2013	6.7	5.6	−16			
	Spring maize	2009	7.1	9.6	35			
	Winter wheat	2009–2010	6.8	2.9	−57			
	Summer maize	2010	7.5	8.6	15			
	Spring maize	2011	9.1	7.7	−15			
	Winter wheat	2011–2012	6.7	4.5	−33			
W/S-M	Summer maize	2012	10.4	9.6	−8	4.0	6.2	56
	Spring maize	2009	7.3	9.6	32			
	Winter wheat	2009–2010	6.8	2.9	−57			
	Summer soybean	2010	3.1	2.2	−29			
	Spring maize	2011	9.8	9.0	−8			
	Winter wheat	2011–2012	6.7	4.3	−36			
	Summer soybean	2012	3.3	3.1	−6			
M	Spring maize	2009	7.2	9.7	35	6.2	4.5	−27
	Spring maize	2010	6.6	9.6	45			
	Spring maize	2011	8.9	9.6	8			
	Spring maize	2012	10.6	9.6	−9			

Chem. W/M = conventional winter wheat-summer maize double-cropping system using the local N fertilisation rates; Opt. W/M = optimized winter wheat-summer maize double-cropping system; W/M-M = winter wheat-summer maize-fallow-spring maize system; W/S-M = winter wheat-summer soybean-fallow-spring maize system; and M = a single spring maize system with one crop per year.

### 3.3. Evaluation of the DNDC Model to Estimate N<sub>2</sub>O Emissions

The DNDC model was able to predict trends of the observed daily N<sub>2</sub>O fluxes for all cropping systems, with the exception of some higher peaks as well. However, the model over/underestimated the magnitude of the daily values (Figure 4). These over/underestimated peaks by DNDC resulted in a poor fit between observed and simulated daily values (RMSE ranged from 33.4 to 54.6 g N<sub>2</sub>O-N ha<sup>-1</sup> d<sup>-1</sup>) (Table 1). One of the reasons causing this discrepancy was the imperfect estimations of the daily total soil available N by the DNDC. Another reason for this poor fit is the underestimation of simulated WFPS (%), which is one of the key factors that regulate N<sub>2</sub>O emissions [60]. It was also not possible to validate some of the parameters included in the DNDC model (e.g., soil microbial biomass) [61]. Additionally, as N<sub>2</sub>O flux measurements were not continuous, it is possible that these peaks were missed, especially the two higher peaks simulated, from all four multi-cropping systems on 19 January and 6 May 2010 [62]. N<sub>2</sub>O is normally released to the atmosphere in the form of pulses [63], which disappear in less than a few weeks [64]. Higher peaks relate to the application of N fertiliser, higher rainfall and irrigation [35,47,56]. These parameters influence soil nitrification and denitrification processes and, thereby, stimulate both observed and simulated N<sub>2</sub>O emissions [65]. However, the model effectively estimated cumulative N<sub>2</sub>O fluxes from each of the investigated cropping systems. The overall RD between simulated and observed values for Chem. W/M; Opt. W/M; W/M-M; W/S-M; and M cropping systems were 6, 7, -1, 56 and -27%, respectively, (Table 2). The overall r<sup>2</sup> between observed and simulated flux was 0.3 (Figure S2). This indicates that although the DNDC model was not perfect for estimating the daily N<sub>2</sub>O emissions from these long-term multi-cropping systems, it could still be used to predict cumulative N<sub>2</sub>O emissions. Both observed and simulated results showed that the optimized and alternative cropping systems (Opt. W/M; W/M-M; W/S-M and M) decreased N<sub>2</sub>O cumulative fluxes by 6, 30, 50 and 21% (observed) and by 5, 35, 26 and 46% (simulated), compared to the Chem. W/M. Here, both optimized and alternative cropping systems (Opt. W/M; W/M-M; W/S-M and M) received significantly less N fertiliser compared to Chem. W/M. According to [66], fertiliser optimisation management can significantly reduce N loss from soils. A two-year study on the same site by [37] showed that Opt. W/M increased grain yields and decreased fertiliser used and N<sub>2</sub>O emissions but increased total net greenhouse gas emissions (from N<sub>2</sub>O and CH<sub>4</sub>) and irrigation water required, compared to Chem. W/M. However, the alternative cropping systems W/M-M, W/S-M and M decreased net greenhouse gas emissions, N fertiliser and irrigation water required but decreased grain yield (except in the W/M-M).



**Figure 4.** Field observed (●) and DNDC simulated (line) daily N<sub>2</sub>O fluxes (gN<sub>2</sub>O-N ha<sup>-1</sup>d<sup>-1</sup>) for the conventional winter wheat-summer maize double-cropping system (Chem. W/M; a.), optimized winter wheat-summer maize double-cropping system (Opt. W/M; b.), winter wheat-summer maize-fallow-spring maize system (W/M-M; c.), winter wheat-summer soybean-fallow-spring maize system (W/S-M; d.), and spring maize system (M; e.) over the experimental period from June 2009 to June 2013. Blue arrows show time of application of N fertiliser.

#### 4. Conclusions

The DNDC model effectively simulated daily soil temperature and crop yields for long-term multiple cropping systems. However, the model underestimated water filled pore space and had difficulties in correctly estimating daily soil nitrogen (N) (exchangeable  $\text{NH}_4^+$  and  $\text{NO}_3^-$ ) but reasonably estimated their cumulative values. This was due to the multiple N sources in these types of cropping systems. The model predicted the trends of the observed daily  $\text{N}_2\text{O}$  emissions well and overestimated some of the higher peaks but performed satisfactorily in estimating cumulative  $\text{N}_2\text{O}$  emissions. We found that although the DNDC model (v. 9.5) is not perfect in estimating daily  $\text{N}_2\text{O}$  emissions, for these long-term multi-cropping systems, it could still be used to effectively predict cumulative emissions. The optimized and alternative cropping systems used less N fertiliser, increased grain yield and decreased emissions compared to the conventional cropping system.

**Supplementary Materials:** The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/agronomy12010109/s1>, Table S1: The crop within each season in the five cropping systems over the four-year study period. Table S2: Detailed field management practices in the five different treatments over the four-year study period. Table S3 Detailed field management practices in the five different treatments over the four-year study period. Table S4: Chem.W/M, Opt.W/M, W/M-M, W/S-M and M represent conventional chemical fertilization and optimized winter wheat – summer maize with two harvests in one year, winter wheat – summer maize (or summer soybean) – spring maize with three harvests in two years and single spring maize per year, respectively.

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