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## Long-term modelling of crop yield, nitrogen losses and GHG balance in organic cropping systems

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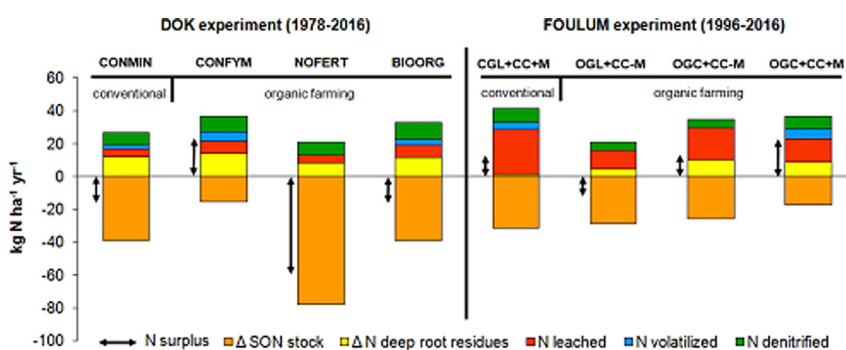
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### HIGHLIGHTS

- The fate of C and N were quantified and modelled in two long term experiments.
- STICS model was improved to simulate organic farming (OF) systems.
- STICS reproduced crop production, N surplus and change in SON stocks.
- OF did not systematically differ from conventional in N surplus, N losses and GHG.
- N losses and GHG was related to N surplus.

### GRAPHICAL ABSTRACT



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### ABSTRACT

Although organic cropping systems are promoted for their environmental benefits, little is known about their long-term impact on nitrogen (N) fate in the soil–plant–atmosphere system. In this paper, we analyze two long-term experiments: DOK in Switzerland (39-yr) and Foulum organic in Denmark (19-yr). Four treatments were considered in each experiment: two conventional treatments with (CONMIN) or without manure (CONFYM), organic with manure (BIOORG) and unfertilized treatment (NOFERT) at DOK; conventional (CGL–CC+IF) and three organic treatments, one with cover crops only (OGL+CC–M) and two including cover crops and grass-clover with (OGC+CC+M) or without manure (OGC+CC–M), at Foulum. STICS model was used to simulate crop production, N surplus, nitrate leaching, gaseous N losses and changes in soil organic N. It was calibrated in the conventional treatments and tested in organic systems. The crop production, N surplus and soil organic N stocks were satisfactorily predicted. The mean N surplus greatly differed between treatments at DOK, from  $-58$  (NOFERT) to  $+21$   $\text{kg N ha}^{-1} \text{yr}^{-1}$  (CONFYM), but only from  $-9$  (OGL+CC–M) to  $+21$   $\text{kg N ha}^{-1} \text{yr}^{-1}$  (OGC+CC+M) in Foulum. Soil N pools declined continuously in both sites and treatments at a rate varying from  $-18$  to  $-78$   $\text{kg N ha}^{-1} \text{yr}^{-1}$ , depending on fertilization and crop rotation. The decline was consistent with the observed N surpluses. Although not all simulations could be tested against field observations and despite of prediction uncertainties, simulations confirm the hypothesis that environmental performances resulting from C and N cycles depend more on specificities of individual than nominal treatments. Significant correlations appeared between long-term N surplus and soil N storage and between total N fertilization and total N gaseous losses. Results showed in both experiments that arable organic systems do not systematically

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have lower N surplus and N losses than conventional ones, providing opportunity for increasing N use efficiency of these systems.

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## 1. Introduction

Given the negative side-effects of conventional agriculture on the environment, the development of organic cropping systems has met a resounding success, with an increase of 74% of the organic agricultural lands in Europe over the last decade (Willer and Lernoud, 2017). Organic farming has been depicted as an opportunity for mitigating climate change by enhancing soil carbon (C) sequestration, protecting the environment by reducing nitrogen (N) losses and avoiding pesticide pollution (Mondelaers et al., 2009; Tuomisto et al., 2012). The impact of organic farming on soil carbon stocks, nitrate leaching or nitrous oxide (N<sub>2</sub>O) emissions has been examined in recent studies (Gattinger et al., 2012; Aguilera et al., 2013; Benoit et al., 2014; Skinner et al., 2014b). Long-term experimental evidence of these impacts requires costly and time consuming field experiments. Coupling experimental data and soil-crop simulation modelling enables assessment of long-term consequences of cropping systems on C and N cycles (Möller, 2009; Constantin et al., 2012). Process-based dynamic models have been developed and assessed for simulating yields and environmental impact of conventional cropping systems (Brisson et al., 1998; Hansen et al., 1991; Jones et al., 2003; Keating et al., 2003; Stöckle et al., 2003), but few studies have considered stockless organic systems (Doltra et al., 2019). Furthermore, crop succession effects are rarely considered (Lorenz et al., 2013) and C and N impacts often treated separately, either for carbon (Leifeld et al., 2009) or nitrogen (Berntsen et al., 2006). Simulating accurately the long-term effect of diversified crop rotations and management practices - as found in organic cropping systems - on C and N fluxes simultaneously remains a scientific challenge, requiring efforts in model parameterization and evaluation (Doltra et al., 2011).

Arable organic farming systems often include diversified crop rotations, cover crops (also called catch crops) (Amossé et al., 2014), intercrops of grain legumes and cereals (Thiessen Martens et al., 2001), or pluri-annual crops like mixed leys, including forage legumes (Teasdale et al., 2004; Stinner et al., 2008). Some of these techniques involve undersowing an auxiliary leguminous crop in an established main crop, resulting in a well-developed cover crop after harvest, able to produce a high biomass and add extra N through symbiotic fixation (De Notaris et al., 2019). The destruction of mixed leys and cover crops releases nutrients in soil, particularly N, available for the subsequent crops (Fustec et al., 2010; Amossé et al., 2014). Another expected benefit of these supplementary crops is the increase in SOC stocks in the tilled layer receiving crop residues (Autret et al., 2016; Blanco-Canqui et al., 2017) and the important root deposition due to herbaceous species (Poorter et al., 2015) which increases with the species diversity in the crop mixture (Lange et al., 2015). However, the mismatch between the release of N through residues N mineralization and the N demand of the next crop may lead to significant nitrate leaching (Olesen et al., 2009; Valkama et al., 2015). Furthermore, cover crops residues, particularly from legumes, tend to promote N<sub>2</sub>O emissions (Rochette and Janzen, 2005; Basche et al., 2014; Plaza-Bonilla et al., 2017). Our first hypothesis (H1) was that the environmental performances for the C–N cycles depend on system management (total and origin of N inputs, cover crop in autumn, ...) and cannot be predicted by a simple nominal approach. We believe that the impact of such systems on C–N cycles over the long-term can be predicted by well tested process oriented models.

Applying deterministic soil-crop models in such complex systems is both a scientific and technical challenge. It involves considering processes such as biological regulation mechanisms, biotic stressors, behaviour of crop mixtures and consequences of frequent legume cropping on soil C–N dynamics. The simulations of such processes require well calibrated models for a wide range of crop species and organic amendments. Experiences of such model applications are scarce (David et al., 2007; Doltra et al., 2011; Smith et al., 2015). Models for such purposes should be applicable in both conventional and organic systems to ensure generality and comparison of performance between these systems. The specification of model requirements may start by extending the use of a current soil-crop model to organic systems through addressing specific hypotheses concerning the behaviour of the cropping systems. Our study relies on two other hypotheses: biomass production and N uptake can be well simulated in organic systems managed with a good weed control (H2) and organic matter turnover formalisms successfully evaluated in conventional farming are valid in organic systems (H3). With these assumptions, the soil-crop model STICS represents a good candidate thanks to its specifications of genericity for crop species, robustness and diversity of model outputs (Brisson et al., 2003).

STICS simulates crop growth and the cycles of N, C and water with their associated environmental impacts (Brisson et al., 1998, 2008). It has been positively evaluated for simulating the impact of agricultural practices on soil C balance (Wattenbach et al., 2010), N mineralization (Gabrielle et al., 2002), nitrate leaching (Poch-Massegú et al., 2014; Constantin et al., 2015; Coucheney et al., 2015; Plaza-Bonilla et al., 2015) and N<sub>2</sub>O emissions (Peyrard et al., 2017; Plaza-Bonilla et al., 2017) across a wide range of cropping and pedo-climatic conditions (Coucheney et al., 2015). STICS can simulate varied agricultural management practices related to organic matter inputs, cover crops (Beaudoin et al., 2008; Constantin et al., 2012) and intercrops (Corre-Hellou et al., 2009). A recent improvement of the model allows simulating perennial crops, including their root turnover, using a “perennial” research version which has been evaluated for Miscanthus (Strullu et al., 2015) and alfalfa (Strullu et al., 2019). This research version has the potential to simulate long-term C–N dynamics in organic cropping systems.

In this work, the scientific strategy consisted in coupling experiments and modelling to compare conventional and organic arable cropping systems varying in rate and form of N inputs. We compiled data from two long-term experiments comparing conventional and organic systems, namely the DOK experiment (39-yr) in Switzerland and the Foulum organic experiment (19-yr) in Denmark. Our objective was to evaluate the ability of STICS for predicting crop biomass, yield, N surplus and changes in soil organic N in organic cropping systems and then investigate the long-term N fate thanks to the model predictions.

## 2. Material and methods

### 2.1. Experimental sites and cropping systems

The two long-term experiments analysed here were the DOK trial, set up in 1978 in Therwil, Switzerland (47°30'N, 7°33'E) and the Foulum experiment, initiated in 1997 at the Foulum Research Centre of Aarhus University, Denmark (56°30'N, 9°34'E). Both

**Table 1**  
Crop rotations<sup>a</sup> and fertilization managements for each treatment from the DOK and Foulum long term experiments.

			DOK (Switzerland)				Foulum (Denmark)			
Treatments			CONMIN	CONFYM	NOFERT	BIOORG	CGL-CC+IF	OGL+CC-M	OGC+CC-M	OGC+CC+M
Duration	yr		39				19			
Crop rotation <sup>a</sup>	1st cycle	1978–1984	PO/WW/cc/CB/WW/WB/CG <sup>b</sup> /CG				1997–2000	SP-SB/O/WW/TR	SP-SB/cc/O/WW/WC	WW/cc/SP-SB/cc/SB/CG <sup>c</sup>
	2nd cycle	1985–1991	PO/cc/WW/cc/B/cc/WW/WB/CG/CG				2001–2004	LU/WW/O/SB	LU/WW/cc/O/cc/SB/cc	WW/cc/LU-SB/cc/SB/CG
	3rd cycle	1992–1998	PO/WW/cc/B/WW/CG/CG/CG				2005–2008	SP-SB/PO/WW/SB	FB/cc/PO/WW/cc/SB/cc	PO/WW/cc/SB/CG
	4th cycle	1999–2005	PO/WW/cc/SO/cc/SM/WW/CG/CG				2009–2012	SP-SB/SW/ PO/SB	SP-SB/cc/SW/cc/PO/SB/cc	PO/cc/SB/AL/AL
	5th cycle	2006–2012	SM/WW/cc/SO/PO/WW/CG/CG				2013–2017	H /SP-SB /SW/O	H/cc/SP-SB/cc/SW/cc/O/cc	SW/cc/PO/cc/SB/CG
	6th cycle	2013–2017	SM/SO/WW/cc/PO/cc/SM/WW/CG/CG							
Catch crops			different mixtures of rye, vetch, oat, rapeseed, sunflower, legumes, grass.				mixtures of ryegrass, chicory, fodder radish, white and red clover, black medic, seradella, birdsfoot-trefoil, subterranean clover, vetch.			
Residues management	main crop	exported	exported	exported	exported	returned	returned	returned	returned	
	catch crop	returned	returned	returned	returned	returned	returned	returned	returned	
	clover-grass cuts	exported	exported	exported	exported			returned	exported <sup>d</sup>	
Mineral N fertilization (kg N ha <sup>-1</sup> yr <sup>-1</sup> )		97	101	-	-	55	-	-	-	
Organic N fertilizer (kg N ha <sup>-1</sup> yr <sup>-1</sup> )		-	54	-	94	-	-	-	50	

AL: alfalfa (*Medicago sativa* L.); B: beetroot (*Bet vulgaris* L.); CB: white cabbage (*Brassica oleracea* L.); CG: clover-grass ley; H: hemp (*Cannabis sativa* L.); LU: lupin (*Lupinus albus* L.); O: oat (*Avena sativa* L.); PO: potato (*Solanum tuberosum* L.); SB: spring barley (*Hordeum vulgare* L.); SM: silage maize (*Zea mays* L.); SO: soybean (*Glycine max* L.); SP: spring pea (*Pisum sativum* L.); SW: spring wheat (*Triticum aestivum* L.); TR: triticale ( $\times$ Triticosecale Wittm. ex A. Camus); WB: winter barley (*Hordeum vulgare* L.); WC: winter cereal; WW: winter wheat (*Triticum aestivum* L.). The “-” stands for associated crops and “cc” for catch crops.

<sup>a</sup> Three different crops of the succession are cultivated each year at the DOK, four at Foulum.

<sup>b</sup> Clover-grass ley composed of a mixture of red clover (*Trifolium pratense* L.); white clover (*Trifolium repens* L.); cock’s-foot (*Dactylis glomerata* L.); fescue (*Festuca rubra* L.); timothy-grass (*Phleum pratense* L.); perennial ryegrass (*Lolium perenne* L.); kentucky bluegrass (*Poa pratensis* L.).

<sup>c</sup> Clover-grass ley composed of a mixture of perennial ryegrass, white clover and red clover.

<sup>d</sup> Returned to soil before 2007.

experiments were set up to evaluate the agronomic and ecological effects of organic cropping systems. Only the main features of these experiments will be presented here, more detail can be found in Mäder et al. (2002) for the DOK experiment, Olesen et al. (2000) and Askegaard et al. (2011) for the Foulum experiment. Both sites allow to compare organic and conventional cropping systems, but differ by their past which was grassland at DOK and arable land at Foulum and by their crop duration, crop species, length of the rotation and fertilization management (Table 1).

Four treatments were selected among the eight treatments available in the DOK trial. This selection represented a total of 48 plots (4 treatments  $\times$  3 crops of the rotation present each year  $\times$  4 replicates) arranged in a split-plot block design. The CONMIN treatment was managed as integrated farming (according to the Swiss national guidelines of integrated plant production), exclusively receiving mineral fertilization (nil between 1978 and 1985). The CONFYM treatment was managed as the CONMIN treatment, but with additional organic fertilizers through stacked manure and slurry (from milk cows) applications. The NOFERT treatment received neither organic nor inorganic fertilizers since the start of the experiment. The organic treatment, BIOORG, received solely organic fertilizers (rotted manure and slurry from milk cows), without addition of mineral fertilizers nor pesticides. The rate of application of organic fertilizer was set at 1.4 livestock unit  $\text{ha}^{-1}$ , which corresponds to average manure application rates of 2.2 and 2.0 t DM  $\text{ha}^{-1} \text{yr}^{-1}$  since 1978 in CONFYM and BIOORG, respectively. The total amount of N applied averaged 0, 95, 154 and 92 kg N  $\text{ha}^{-1} \text{yr}^{-1}$  in NOFERT, CONMIN, CONFYM and BIOORG treatments, respectively. Soil ploughing was done at around 20 cm depth in all treatments before seeding of main crops. Weed pressure was mechanically controlled (mainly by harrowing) in the BIOORG and NOFERT treatments, while herbicides and pesticides were used in CONMIN and CONFYM treatments when the infection threshold was exceeded. Soybean and potatoes were hoed in all treatments.

The Foulum experiment had a factorial design comprising three factors that were i) the presence (GC) or absence (GL) of a grass-clover ley in the crop rotation; ii) the inclusion (+CC) or exclusion (-CC) of cover crops undersown in the main crop in spring and iii) the addition (+M) or the absence (-M) of manure. All crops of rotations GL and GC were represented every year in each of two completely randomized blocks. Among all treatments, we selected three organic (O) treatments: one treatment without manure application and excluding the grass-clover ley (OGL+CC-M), including the grass-clover ley (OGC+CC-M) and one treatment including

application of manure (OGC+CC+M). The average amount of external organic fertilizer applied in OGC+CC+M was of 0.59 t DM  $\text{ha}^{-1} \text{yr}^{-1}$ , as pig slurry, the composition of which varied between years. All organic treatments were managed without pesticides use, according to the European regulation for organic farming. One conventional treatment was also studied (CGL-CC+IF), receiving inorganic fertilizers, but without grass-clover ley and without cover crop. This treatment had been managed without N fertilization (and pesticides) until 2004, prior to conversion into a conventional treatment (Askegaard et al., 2011; Pandey et al., 2018). The amount of total N applied to soil averaged 23 and 51 kg N  $\text{ha}^{-1} \text{yr}^{-1}$  in CGL-CC+IF and OGC+CC+M respectively. All crop residues were returned to soil at harvest for cash crops and during the mechanical destruction for cover crop and grass-clover leys. Prior to 2005, the grass-clover ley cuts were left to decompose on the soil in OGC+CC-M and OGC+CC+M, whereas they were exported from the field in OGC+CC+M thereafter.

## 2.2. Climate and soil characteristics

Prior to the initiation of the experiments, soils were characterized in 1977 for DOK and in 1996 at Foulum (Table 2). DOK soil is classified as Haplic Luvisol and Foulum soil as a Mollic Luvisol (IUSS Working Group WRB, 2006). The two soils have very contrasted textures, with high silt content (71%) and low sand content (12%) at DOK (0–20 cm), and low silt (14%) and high sand content (77%) at Foulum (0–25 cm). Clay content is higher at DOK (16%) than at Foulum (9%). The initial soil organic C content (SOC) was lower at DOK (16.6 vs 22.8 g  $\text{kg}^{-1}$ ), whereas the initial soil organic N content (SON) was similar between sites. In the DOK trial, the initial organic N content was estimated based on the initial SOC content and the final soil C/N ratio measured in 2016. The difference in C/N ratio (8.9 for DOK vs 13.0 for Foulum) could result from the difference in the previous land use: mostly arable crops at Foulum vs grassland at DOK. The experimental sites also differed by climatic conditions, with mean annual precipitation, potential evapotranspiration and air temperature of respectively 860 mm, 684 mm and 10.7 °C at DOK (1977–2016), and 716 mm, 574 mm and 8.2 °C at Foulum (1996–2016).

## 2.3. STICS model

The STICS model is a deterministic soil-crop model simulating crop and soil variables (crop development, biomass production, N uptake, N fixation, ...) and environmental variables (soil water, C

**Table 2**  
Topsoil characteristics used in STICS for initializing DOK and Foulum sites, in 1977 (0–20 cm) and 1996 (0–25 cm) respectively.

Treatment	DOK				Foulum				
	CONMIN	CONFYM	NOFERT	BIOORG	CGL-CC+IF	OGL+CC-M	OGC+CC-M	OGC+CC+M	
Texture class	Haplic Luvisol				Mollic Luvisol				
Clay	g $\text{kg}^{-1}$	167	145	162	151	85	101	90	88
Silt	g $\text{kg}^{-1}$	700	709	707	714	129	150	138	149
Sand	g $\text{kg}^{-1}$	113	126	114	114	785	749	772	763
Organic C	g $\text{kg}^{-1}$	16.2	15.2	18.1	16.7	21.4	24.2	21.5	23.9
Total N <sup>d</sup>	g $\text{kg}^{-1}$	1.81	1.70	2.03	1.86	1.66	1.81	1.71	1.79
C:N ratio <sup>d</sup>		8.9	8.9	8.9	9.0	12.9	13.3	12.5	13.4
CaCO <sub>3</sub>	g $\text{kg}^{-1}$	2.2	2.2	2.5	2.3	0	0	0	0
pH <sub>H2O</sub>		6.18	6.29	6.21	6.30	6.45	6.43	6.59	6.50
Bulk density	g $\text{cm}^{-3}$	1.32	1.32	1.32	1.31	1.42	1.42	1.42	1.42
WFC <sup>a</sup>	g $\text{kg}^{-1}$	296	301	306	305	192	192	192	192
WPWP <sup>b</sup>	g $\text{kg}^{-1}$	133	135	138	137	82	82	82	82
PAW <sup>c</sup>	mm	322	327	332	330	234	234	234	234

<sup>a</sup> Water content at field capacity.

<sup>b</sup> Water content at permanent wilting point.

<sup>c</sup> Plant available water on 150 cm.

<sup>d</sup> Total N calculated at the DOK with the organic C content in 1977 and C/N ratio of 2016.

and N fluxes). Initial soil characteristics (N content, C/N ratio, clay content, ...), daily weather data, crop characteristics and agricultural practices must be given as input data. Potential crop development and growth are simulated using specific plant parameters, and abiotic stress factors (related to temperature, water or nitrogen) are applied to calculate effective growth rates. The soil is divided into layers, characterized by their water content at field capacity, permanent wilting point and bulk density. Organic matter decomposition in soil is simulated with three compartments: fresh organic matter, microbial biomass and humified organic matter, the latter being composed of an active and a stable fraction (Fig. 1). Carbon and nitrogen fluxes between these pools depend on their C/N ratio, soil temperature, water content and mineral N content, and potential mineralization parameters: decomposition rate of residues, C decomposition rate into microbial biomass, decay rate of microbial biomass and humification rate (Nicolardot et al., 2001). The parameters for decomposition of crop residues and organic fertilizers were calibrated on large datasets of laboratory incubations (Justes et al., 2009). The N mineralized from humified organic matter depends on a potential mineralization rate, related to clay, CaCO<sub>3</sub> and SON contents, and the temperature and moisture conditions of the biologically active soil layer. The vertical transport of nitrate in soil is described with the mixing cell concept, simulating solute dispersion. Gaseous N losses (NH<sub>3</sub>, N<sub>2</sub> and N<sub>2</sub>O) are simulated either empirically (fraction of fertilizer lost) or more mechanistically (Peyrard et al., 2017).

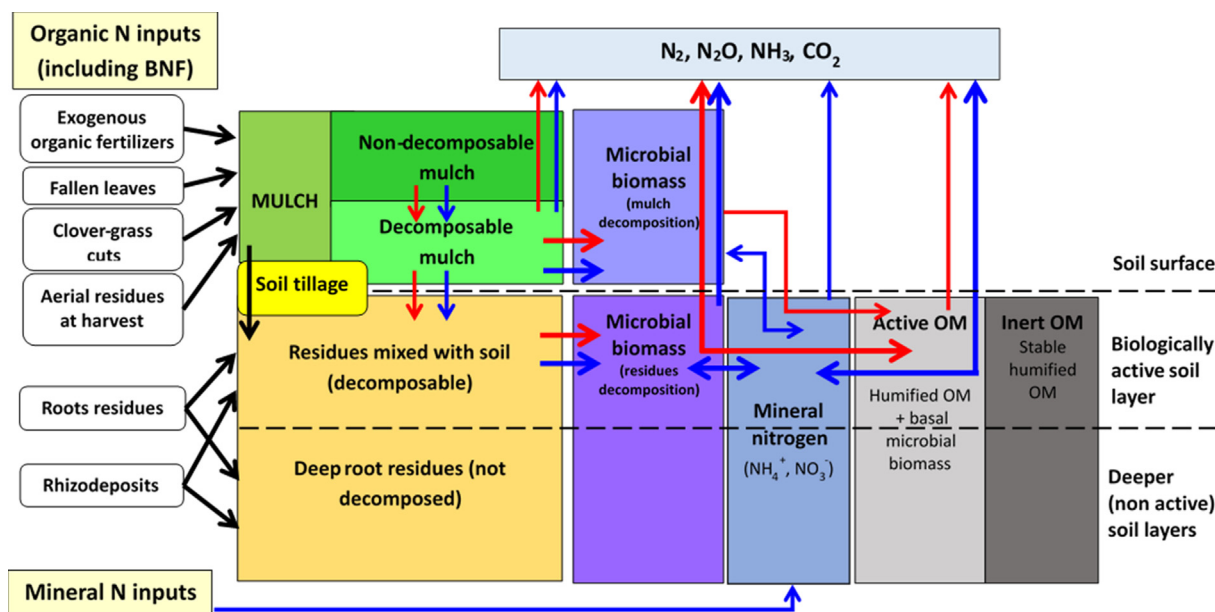
A research version of STICS (v1610) was used in this study to widen the range of possibilities offered by the currently available standard version (v8.4). We improved the version evaluated by Strullu et al. (2015) in order to i) run successive simulations including intercrops; ii) run simulations of grass-clover over successive years; iii) simulate a cover crop undersown in an already established crop and simulate its subsequent growth after harvest of the main crop; iv) account for partial return to soil of grassland cuttings, and v) simulate the enhanced C–N mineralization rates during the year following grassland destruction. The latter process was mimicked by an artificial input of organic matter, from 2.5 to 5.0 t DM ha<sup>-1</sup> yr<sup>-1</sup> according to the grassland age, with a low C/N ratio (12). This add-on is justified by observations made in grassland soils, such as fast release of N after grassland destruction,

accumulation of particulate organic matter under grassland (Vertès et al., 2002) and deposition of N-rich legume nodules as proposed by Christensen et al. (2009), not simulated by STICS model. This research version is expected to become the standard version in 2020 since it successfully passed the non-regression tests on the dataset described by Coucheny et al. (2015).

Crop parameterization was met in three steps. At first, a method for calibrating the new root parameters in the research version of the model was independently tested for winter wheat, spring and winter barley, triticale and winter fababeans using independent datasets obtained in other organic farming experiments (Chlebowski et al., 2017). Secondly, the new root parameters were defined for all crop species, while the other crop parameters remained the same than for the standard version (Appendix A). Thirdly, some orphan crop species, like beetroot and hemp, which appeared scarcely in the trials, were briefly calibrated starting from an already calibrated reference crop having a close ecophysiology (Appendix B); the mixed grassland, consisting in a mixture of grass and legume, was simulated using the existing fescue plant file, in which biological N fixation (BNF) was activated and calibrated. All these crop calibrations were done against data from conventional treatments. Soil parameters were either fixed independently, according to literature or measurements, or optimized using the conventional treatments dataset. They concerned the depth of the mineralisation layer, the maximal rooting depth and the ratio of stable to total SON. Thereafter, the organic treatments were used for an independent test of the model and for testing the hypotheses H2 and H3.

#### 2.4. Experimental data used for modelling

Data collected throughout the 39 or 19-yr experiments were used for model evaluation. They concerned the aboveground biomass and N content measured during the crop growth and/or at harvest, along with soil organic C (SOC) and N (SON) contents, soil water content (SWC) and soil mineral N (SMN, nitrate and ammonium) contents at different dates and frequencies. Details about measurement methodologies are given in previous studies for DOK (Mäder et al., 2007; Leifeld et al., 2009; Mayer et al., 2015) and Foulum (Askegaard et al., 2011; Doltra et al., 2011; Petersen et al., 2013). Complementary measurements of SWC and SMN were



**Fig. 1.** Soil C and N compartments and incoming and outgoing C–N fluxes in the STICS model. Blue arrows show C fluxes and red arrows N fluxes. BNF: biological nitrogen fixation; OM: organic matter. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

realized three times per year between 2015 and 2017 in the DOK experiment, in order to evaluate the predictions of soil water content and SMN evolution over three successive drainage seasons.

We calculated the N surplus (or soil surface N balance) both at annual and long-term scales for two purposes: at annual scale, it allows to check the model prediction across crops and years; at the long-term, it is a proxy of the N enrichment of the cropping system, which is a necessary but not sufficient intermediate variable for investigating the N fate (Autret et al., 2019). The estimated N inputs and outputs allowed calculation of N surplus ( $N_{sur}$ ), as follows:

$$N_{sur} = N_{fert} + N_{fix} + N_{atm} - N_{exp} \quad (1)$$

where  $N_{fert}$  is the N fertilization (mineral+organic),  $N_{fix}$  the N input deriving from symbiotic fixation,  $N_{atm}$  the atmospheric N deposition and  $N_{exp}$  the N exported from the field at harvest, all values in  $\text{kg N ha}^{-1} \text{ yr}^{-1}$ .  $N_{atm}$  was estimated based on the European Monitoring and Evaluation Program (<http://www.emep.int/>), providing an annual deposition of 17 and 14  $\text{kg ha}^{-1} \text{ yr}^{-1}$  in Switzerland and Denmark, respectively, for the 1980–2015 period. The values of  $N_{fert}$  and  $N_{exp}$  were annual data provided by experimenters, and  $N_{fix}$  was calculated for the leguminous crops with the equation proposed by (Anglade et al., 2015a):

$$Ndfa = \alpha \cdot N_y + \beta \quad (2)$$

where  $\alpha$  and  $\beta$  are the slope and intercept coefficients, specific of each crop (Appendix C),  $N_y$  is the N yield, defined as the total N accumulated in the aboveground biomass, and calculated as follows:

$$N_y = Y \cdot N_c / NHI \quad (3)$$

where  $Y$  is the harvested crop yield ( $\text{Mg DM ha}^{-1}$ ),  $N_c$  is the N content in the dry matter ( $\text{g kg}^{-1}$ ), and  $NHI$  is the N harvest index defined as the ratio of N contained in the harvested material to the total N in the aboveground biomass. Nitrogen yield was determined using the measured grain yield for pulses (fababean, lupin, pea and soybean), the estimates of aboveground biomass for the other legumes (alfalfa, vetch and clover), an average value of measured N content for pea, and standard values of N content for the other leguminous species (Anglade et al., 2015a; CORPEN, 1988; Parr et al., 2011). The biological N fixation in legumes was calculated as the product of  $N_y$  and a factor accounting for belowground contributions (BGN-F), which varied between legume species (Anglade et al., 2015a).

### 2.5. Model parameterization and simulation strategy

Most model inputs were derived from measurements in the experiments. The initialization of the SOC and SON pools are based on initial measurements of soil organic matter. Soil water content at field capacity (FC) and permanent wilting point (WP) were determined differently between sites. For the DOK trial, in situ gravimetric measurements were done so that FC was set as the median of the highest values of SWC measured in mid-winter; WP was set at 45% FC, which is the mean value of the WP/FC ratio given by pedotransfer functions of Wösten et al. (2001) and Al Majou et al. (2008) for this texture. For Foulum, soil water retention curves (Djurhuus and Olesen, 2000) enabled to define FC ( $pF = 2.5$ ) and WP ( $pF = 4.2$ ). The bulk density, which is fixed in the current version of the model, was set at  $1.32 \text{ g cm}^{-3}$  in the 0–20 cm soil layer at DOK (Leifeld et al., 2009) and  $1.42 \text{ g cm}^{-3}$  in the 0–30 cm soil layer at Foulum (Djurhuus and Olesen, 2000). The depth of the biologically active layer (“mineralization depth”) was assumed to be 25 cm in both experiments, corresponding to the ploughing depth plus 10% (Brisson et al., 2008).

Some soil and crop parameters were calibrated against data from the conventional treatments (CONMIN and CGL-CC+IF). The target was the best compromise in the quality of fit for crop production, N uptake, SWC and SMN contents. During the calibration process, several plant parameters were changed to reach a good simulation of crop growth and N uptake, particularly involving calibration of radiation use efficiency and root traits of beetroot, hemp and silage maize.

Considering the spatial scale, the model was run at the treatment scale by averaging replicates (4 replicates at DOK, 2 at Foulum), assuming that the soil spatial variability of model inputs is very low. With regard to the time scale, continuous simulations relied on the assumption that there is no drift in the model, according to the two hypotheses and following Beaudoin et al. (2008) and Constantin et al. (2012). Resetting the model every year, which would have more forced the predictions of N losses, was impossible due to lack of annual data (soil water, mineral N and organic N contents). Continuous simulations allowed to determine the initial size of the active fraction of soil organic matter by fitting model outputs to the measurements of soil organic N made in the conventional treatments, using a trial–error procedure. Above all, they allowed to account for the possible carry over effects affecting C and N dynamics.

### 2.6. Model evaluation

The model was evaluated both for the conventional treatments used for calibration and the organic treatments used for independent testing, against SWC, SMN, crop biomass (above and below-ground), crop N content and yield, N surplus and soil organic N. A good prediction of these variables is required for having confidence in the C and N fluxes simulated by the model, particularly C and N deposition by crop residues, C and N mineralization, N leaching and gaseous N emissions.

We characterized the model performance by calculating complementary statistical criteria based on the comparison of observed and simulated data. They allowed us to estimate the magnitude of model errors and model ability to reproduce observed data variability for each output variable. They include the mean difference (MD) and the root mean square error (RMSE) calculated as follows:

$$MD = \frac{1}{n} \sum_{i=1}^n (S_i - O_i) \quad (4)$$

$$RMSE = \sqrt{\frac{1}{n} \cdot \sum_{i=1}^n (S_i - O_i)^2} \quad (5)$$

where  $O$  and  $S$  are the observed and the simulated values, respectively, and  $n$  is the number of observation–simulation pairs.  $MD$  gives the bias of the model, whereas  $RMSE$  gives an estimate of the magnitude of the model error. It can be decomposed into two components describing the systematic error ( $RMSEs$ ) and the unsystematic error ( $RMSEu$ ), calculated as follows (Willmott, 1981):

$$RMSEs = \sqrt{\frac{1}{n} \cdot \sum_{i=1}^n (\bar{S}_i - O_i)^2} \quad (6)$$

$$RMSEu = \sqrt{\frac{1}{n} \cdot \sum_{i=1}^n (S_i - \bar{S}_i)^2} \quad (7)$$

with  $\bar{S}_i$  deriving from the following linear regression of predicted vs. observed values:  $\hat{S}_i = a + bO_i$ ,  $a$  and  $b$  being the slope and intercept of the regression, respectively.  $RMSEs$  gives the systematic bias of

the model, while *RMSEu* reveals the dispersion of the simulated values. A prevalence of systematic error means that there was an error during model parameterization or that the model misses important process(es) needed to accurately simulate the behaviour of the soil-crop system. Unsystematic error is linked to i) uncertainties in inputs or measurements, or ii) effect of exceptional environmental conditions or biotic stresses not accounted for by the model.

We considered that model predictions were satisfactory (acceptance criterion) if two conditions are fulfilled: i) the relative mean difference and systematic bias (*MD* and *RMSEs*) are lower than 10% (Beaudoin et al., 2008) in long-term simulations; ii) the unsystematic root mean square error (*RMSEu*) is equal or lower than the data variability in measurements (standard deviation) (Willmott, 1982).

### 2.7. Greenhouse gas balance

The total greenhouse gas (GHG) emissions of the DOK and Foulum experiments were calculated considering treatment specificity and expressed in CO<sub>2</sub>-equivalents, with a standard 100-year global warming potential of 296 for N<sub>2</sub>O. The boundaries of the analysis are defined by the primary and secondary sources of GHG at the field scale due to the C–N cycles. They do not include the secondary sources due other inputs (pesticides or PK fertilizers) nor the tertiary sources (Ceschia et al., 2010). The annual GHG balance (*GHG<sub>b</sub>*, in kg CO<sub>2</sub>eq ha<sup>-1</sup> yr<sup>-1</sup>) was calculated similarly to that defined by Autret et al. (2019):

$$GHG_b = F + M + 296 \frac{44}{28} (directN_2O + indirectN_2O) - \frac{44}{12} SOC_{storage} \quad (8)$$

where *F* is the amount of CO<sub>2</sub> emitted during the N fertilizer synthesis (kg CO<sub>2</sub> ha<sup>-1</sup> yr<sup>-1</sup>), *M* is the amount of CO<sub>2</sub> from fossil fuels emitted during agricultural management practices (kg CO<sub>2</sub> ha<sup>-1</sup> yr<sup>-1</sup>), *direct N<sub>2</sub>O* the amount of N<sub>2</sub>O emitted from the soil (kg N<sub>2</sub>O-N ha<sup>-1</sup> yr<sup>-1</sup>), *indirect N<sub>2</sub>O* the amount of N<sub>2</sub>O emitted throughout the N cascade (kg N<sub>2</sub>O-N ha<sup>-1</sup> yr<sup>-1</sup>) and *SOC<sub>storage</sub>* the amount of carbon yearly stored in the soil (kg C ha<sup>-1</sup> yr<sup>-1</sup>). Let us remind that a positive balance corresponds to a net emission of CO<sub>2</sub> in the atmosphere. *F* was calculated as the product of the amount of fertilizer applied per hectare and the corresponding emission factors which were 6.17 kg CO<sub>2</sub>eq kg<sup>-1</sup> N for ammonium-nitrate (Gac et al., 2011). The amount of fuel (diesel) consumed per hectare for soil and crop management were the following: 27.6 l ha<sup>-1</sup> for soil ploughing, 5.6 l ha<sup>-1</sup> for soil surface tillage and 20.5 l ha<sup>-1</sup> for the combine harvester. This consumption was multiplied by the emission factor of 0.81 kg C per liter of fuel consumed (Lorin, 2010) and by a conversion factor of 3.67 kg CO<sub>2</sub> per kg C to get an estimate of the equivalent CO<sub>2</sub> emitted. The *direct N<sub>2</sub>O* emissions and the *SOC<sub>storage</sub>* were simulated by STICS model for each cropping system, while the *indirect N<sub>2</sub>O* emissions were estimated with the emission factor defined by IPCC (2006), namely 0.75% of the leached N and 0.10% of the N fertilizer applied being transformed into N<sub>2</sub>O along the N cascade. *GHG<sub>b</sub>* was expressed either in kg CO<sub>2</sub>eq ha<sup>-1</sup> yr<sup>-1</sup> or kg CO<sub>2</sub>eq Mg<sup>-1</sup> of wheat grain.

### 2.8. Statistical analysis

The mean annual variables related to C and N balances were analysed statistically for each treatment, i.e. NOFERT, CONMIN, CONFYM and BIOORG for the DOK experiment and OGL+CC-M, OGC+CC-M, OGC+CC+M and CGL+CC+IF for Foulum, using a repeated measures mixed model with cropping system as fixed effect. An analysis of variance (ANOVA) was realized, when possible, to identify the effects of the treatments when considering

the factors crop species and year within the residual variability. It was performed to test the effect of cropping system on the previous C and N fluxes affected. The normal distribution of model residues was verified by the Shapiro-Wilk and Levene tests. When needed, a BoxCox transformation was used to normalize the data. When significant differences among treatments were identified, a LSD test was applied at the 5% probability level of significance. If the hypotheses of variance homogeneity and normality were not fulfilled, the non-parametric test of Kruskal-Wallis was used, followed by means comparison with the *kruskal.test* from the *agricolae* package of R (De Mendiburu, 2014). Finally, analysis of crossed correlation was done using the non-parametric test of Spearman, between the main N inputs and N outputs of treatments, according to the model, with the following inference: highly significant if *p*-value < 0.01; significant for if *p*-value < 0.05 using the *cormat* test from the *pgirmess* (v 1.6.9) package of R.

## 3. Results

### 3.1. Evaluation of STICS for biomass production and N uptake

The global evaluation of the STICS model for the aerial biomass and the crop N content is shown at Table 3 and Fig. 2. The model performances after calibration and validation are analysed separately. In the conventional treatments, the simulations with calibration gave a slight overestimation of the exported biomass with an average *RMSE* of 2.5 and 2.4 Mg DM ha<sup>-1</sup> at DOK and Foulum, respectively. The bias was slightly higher in the validation treatments (average *MD* = 1.8 and 1.1 Mg DM ha<sup>-1</sup> at DOK and Foulum, respectively). The *RMSEs* was always lower or equal to the *RMSEu*, indicating that model bias was low but with limited ability to simulate variability. Conversely, the model could satisfactorily reproduce the dispersion of yields among crops, reaching highest values for potato (16.2 Mg DM ha<sup>-1</sup>) and lowest for white cabbage (0.3 Mg DM ha<sup>-1</sup>). The exported biomass was overestimated in the unfertilized treatments (NOFERT and OGC+CC-M).

In spite of the calibration, the exported N in harvested biomass was slightly underestimated in the conventional treatments for both experiments (*MD* = -10 for DOK and -18 kg N ha<sup>-1</sup> for Foulum). In the DOK trial, the model error mainly came from dispersion (*RMSEu* = 40 kg N ha<sup>-1</sup>) rather than from a bias (*RMSEs* = 18 kg N ha<sup>-1</sup>). In the Foulum experiment, the difference between *RMSEu* and *RMSEs* was lower: 28 and 31 kg N ha<sup>-1</sup> respectively. The validation gave better results. For DOK, N content in exported biomass was well simulated in the BIOORG treatment, with a low *RMSE* (43 kg N ha<sup>-1</sup>), underestimated in CONFYM and overestimated in NOFERT. At Foulum, the exported N in biomass was well simulated in the organic treatments of rotation OGC (*MD* = 5 kg N ha<sup>-1</sup>), and slightly underestimated in the OGL+CC-M treatment (*MD* = -10 kg N ha<sup>-1</sup> on average).

The exported biomass in grass-clover cuts was well predicted in the conventional treatments, with a mean difference of 0.3 Mg DM ha<sup>-1</sup> in CONMIN. The corresponding N exported was slightly overestimated (+12 kg N ha<sup>-1</sup>) with a high *RMSEs* (31 kg N ha<sup>-1</sup>). The evaluation phase showed an overestimation of the exported biomass of grass-clover (including OGC+CC+M, the only treatment in which grass-clover cuts were exported at Foulum). The corresponding N exports were overestimated by 15 kg N ha<sup>-1</sup> on average, the mean *RMSEs* (29 kg N ha<sup>-1</sup>) being close to that of calibration.

The model simulated correctly the aerial crop biomass after calibration, with a small mean difference of 0.6 Mg DM ha<sup>-1</sup> at DOK and -0.1 Mg DM ha<sup>-1</sup> at Foulum. Their respective *RMSEu* were 1.8 and 2.4 Mg DM ha<sup>-1</sup>. The N accumulated in aerial biomass

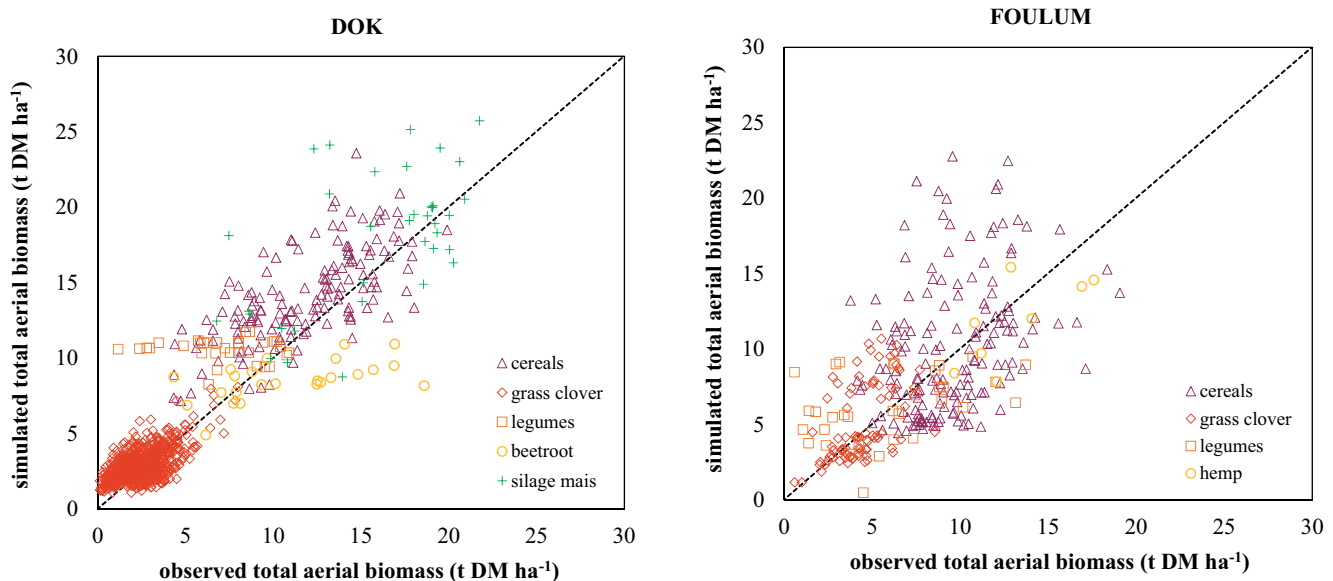
**Table 3**  
Performances of STICS model for the dataset used for the calibration (bold) and the evaluation of aboveground biomass and N content. Values in brackets are standard deviations.

		DOK				Foulum			
		CONMIN	CONFYM	NOFERT	BIOORG	CGL-CC+IF	OGL+CC-M	OGC+CC-M	OGC+CC+M
Exported biomass <sup>a</sup> (Mg DM ha <sup>-1</sup> )	n	<b>64</b>	64	64	63	<b>86</b>	86	64	64
	X obs	<b>5.4 (2.8)</b>	5.8 (3.0)	2.5 (1.0)	4.5 (2.2)	<b>4.1 (2.3)</b>	3.1 (1.3)	3.6 (1.3)	4.1 (1.5)
	X sim	<b>6.7 (3.5)</b>	7.1 (3.8)	4.9 (2.5)	6.1 (3.2)	<b>5.0 (3.3)</b>	3.8 (2.4)	5.0 (3.5)	5.4 (3.6)
	RMSE	<b>2.5</b>	2.5	3.5	3.0	<b>2.4</b>	2.3	3.3	3.3
	RMSEs	<b>1.3</b>	1.4	2.5	1.5	<b>1.0</b>	0.7	1.6	1.4
Exported N at harvest <sup>a</sup> (kg N ha <sup>-1</sup> )	n	<b>69</b>	69	69	69	<b>83</b>	83	63	63
	X obs	<b>126 (41)</b>	139 (43)	66 (30)	104 (41)	<b>88 (49)</b>	66 (39)	68 (27)	80 (28)
	X sim	<b>116 (48)</b>	126 (51)	83 (49)	103 (44)	<b>70 (37)</b>	56 (35)	74 (53)	84 (55)
	RMSE	<b>43</b>	57	41	43	<b>42</b>	39	47	48
	RMSEs	<b>18</b>	31	18	20	<b>31</b>	24	6	4
Exported grass-clover cuts (Mg DM ha <sup>-1</sup> )	n	<b>182</b>	182	182	182	<b>28</b>	30	47	48
	X obs	<b>2.6 (1.3)</b>	2.9 (1.2)	1.6 (0.9)	2.5 (1.2)				3.4 (1.9)
	X sim	<b>2.9 (1.0)</b>	3.2 (1.0)	2.4 (0.9)	2.9 (1.0)				4.0 (2.8)
	RMSE	<b>1.1</b>	1.0	1.3	1.1				2.4
	RMSEs	<b>0.7</b>	0.6	1.0	0.7				0.7
Exported N in grass-clover cuts (kg N ha <sup>-1</sup> )	n	<b>177</b>	177	177	177				56
	X obs	<b>69 (35)</b>	78 (35)	46 (27)	69 (35)				73 (40)
	X sim	<b>81 (25)</b>	92 (26)	57 (17)	79 (22)				100 (58)
	RMSE	<b>39</b>	40	30	35				62
	RMSEs	<b>31</b>	32	25	29				32
Total aerial biomass <sup>b</sup> (Mg DM ha <sup>-1</sup> )	n	<b>241</b>	241	241	241	<b>62</b>	89	123	119
	X obs	<b>5.1 (5.0)</b>	5.6 (5.3)	3.1 (3.1)	4.8 (4.6)	<b>10.6 (3.9)</b>	6.9 (3.8)	5.3 (3.4)	5.8 (4.1)
	X sim	<b>5.7 (5.4)</b>	6.1 (5.8)	4.5 (4.0)	5.5 (4.9)	<b>10.7 (3.0)</b>	6.6 (4.0)	5.9 (4.7)	6.5 (5.4)
	RMSE	<b>1.9</b>	2.2	2.4	1.7	<b>3.2</b>	2.9	3.4	3.8
	RMSEs	<b>0.6</b>	0.5	1.5	0.7	<b>2.1</b>	1.0	0.6	0.7
Total aerial N uptake <sup>b</sup> (kg N ha <sup>-1</sup> )	n	<b>240</b>	240	240	240	<b>58</b>	85	111	107
	X obs	<b>96 (61)</b>	107 (65)	61 (39)	89 (54)	<b>138 (66)</b>	93 (60)	88 (41)	91 (45)
	X sim	<b>104 (52)</b>	116 (55)	74 (44)	99 (46)	<b>106 (43)</b>	68 (33)	99 (57)	107 (69)
	RMSE	<b>43</b>	49	39	41	<b>61</b>	56	58	76
	RMSEs	<b>25</b>	28	18	24	<b>51</b>	49	23	35
	RMSEu	<b>36</b>	40	34	33	<b>33</b>	28	53	67

n = number of observed/simulated data pairs, X obs = mean of measured values, X sim = mean of simulated values  
RMSE = root mean square error, RMSEs = systematic RMSE, RMSEu = unsystematic RMSE

<sup>a</sup> Except clover-grass cuts.

<sup>b</sup> Grain, stubble and straw.



**Fig. 2.** Comparison of simulated and observed total aerial biomass. Each dot refers to the total annual aerial biomass for different crop groups, for each treatment at the DOK and Foulum experiments.



was well simulated in the DOK calibration treatment ( $MD = 8 \text{ kg N ha}^{-1}$ ), but underestimated at Foulum ( $MD = -32 \text{ kg N ha}^{-1}$ ). The evaluation showed small differences between observed and simulated aboveground biomass:  $MD = 0.9$  and  $0.3 \text{ t DM ha}^{-1}$  at DOK and Foulum, respectively. The corresponding N content simulated in aerial biomass varied according to treatments, with a general overestimation for all treatments at DOK and in organic treatments of rotation OGC at Foulum, and an underestimation in OGL.

In summary, on the basis of the acceptance criterion, we conclude that the model satisfactorily predicted crop biomass, both harvested yield and total aboveground biomass. This validated the hypothesis H2 possibly because the experiments were well managed with generally low pressure from weeds, pests and diseases (Shah et al., 2017). The discrepancies in yield prediction may have affected the prediction of crop residue quantity and their C/N ratio since the N accumulated in aboveground biomass was not always well captured ( $RMSEu$  equal or greater than the standard deviations of measurements). This error appears in some treatments and is likely to be related with a poor simulation of soil mineral N content which concerned all the treatments.

### 3.2. Evaluation of STICS for soil water and mineral N

The results of simulation of soil water and nitrate contents are presented in Table 4, for the 0–90 cm soil layer for DOK and 0–25 cm soil layer for Foulum, which was the single layer for which data were available. Soil water content was well simulated in conventional treatments, model residuals being low in both experiments with a  $RMSE$  of 24 and 16 mm for DOK and Foulum, respectively. The  $RMSEs$  was lower than  $RMSEu$  at DOK (13 vs 21 mm, respectively) whereas the opposite result was found at Foulum (15 vs 6 mm, respectively), indicating a bias in simulating soil water content in the sandy soil at Foulum. Similar results were found in the organic treatments, with an average  $RMSE$  of 24 and 18 mm for DOK and Foulum, respectively. The  $RMSEs$  was also lower than the  $RMSEu$  at DOK (15 vs 19 mm) and *vice versa* at Foulum (16 vs 6 mm). Soil water was therefore satisfactorily simulated at DOK and slightly under-estimated at Foulum.

Soil mineral N was under-estimated by the model in all treatments at both sites. The mean difference was  $-20 \text{ kg N ha}^{-1}$  in the CONMIN at DOK and in the CGL-CC+IF treatment at Foulum. This poor agreement was reflected in a greater  $RMSEs$  than  $RMSEu$  for both experiments. The model predicted SMN more satisfactorily at Foulum than at DOK, with a mean difference of  $-6 \text{ kg N ha}^{-1}$ . However, the  $RMSEs$  was always greater than the

$RMSEu$  in the evaluation phase. Hence, the model simulated SMN variability better than its mean.

### 3.3. Soil organic C and N stocks

The temporal evolution of observed and simulated SON stocks is shown in Fig. 3. SON stocks were very well simulated in both experiments: the  $MD$  were  $-0.12 \text{ Mg N ha}^{-1}$  at DOK and  $+0.21 \text{ Mg N ha}^{-1}$  at Foulum. SON stocks decreased markedly in all treatments of the DOK experiment and this decrease was well captured by the model, possibly with a slight underestimation in the last years. The root mean square error ( $RMSE = 0.38 \text{ Mg N ha}^{-1}$ ) was much lower than the measurement error (mean standard deviation =  $0.63 \text{ Mg N ha}^{-1}$ ). In the Foulum experiment, the observed SON stocks slightly decreased throughout time. The model succeeded in simulating this slow decrease in all treatments. The model error ( $RMSE = 0.38 \text{ Mg N ha}^{-1}$ ) was also much lower than the measurement error (mean SD =  $0.71 \text{ Mg N ha}^{-1}$ ), confirming the satisfactory quality of prediction.

The simulated annual rates of change of soil organic C and N are summarized in Table 5, along with the components of the C and N balance over the whole soil profile. These estimates include the entire experimental period, *i.e.* 39 years for DOK and 19 years for Foulum. In the DOK experiment, the rate of SON change ranged as follows:  $\text{NOFERT} < \text{CONMIN} = \text{BIOORG} < \text{CONFYM}$ . Similar trends were observed for changes in SOC stocks. N contained in deep root residues (dead roots below the ploughed layer) increased with time, at the rate of  $9\text{--}14 \text{ kg N ha}^{-1} \text{ yr}^{-1}$ , since their decomposition was not simulated by the model.

The C and N input fluxes derived from organic fertilizer, crop residues and total dead roots (over the whole soil profile) were highest in CONFYM and smallest in NOFERT. The N mineralization rate varied from 145 (NOFERT) to 192 (BIOORG)  $\text{kg N ha}^{-1} \text{ yr}^{-1}$ .

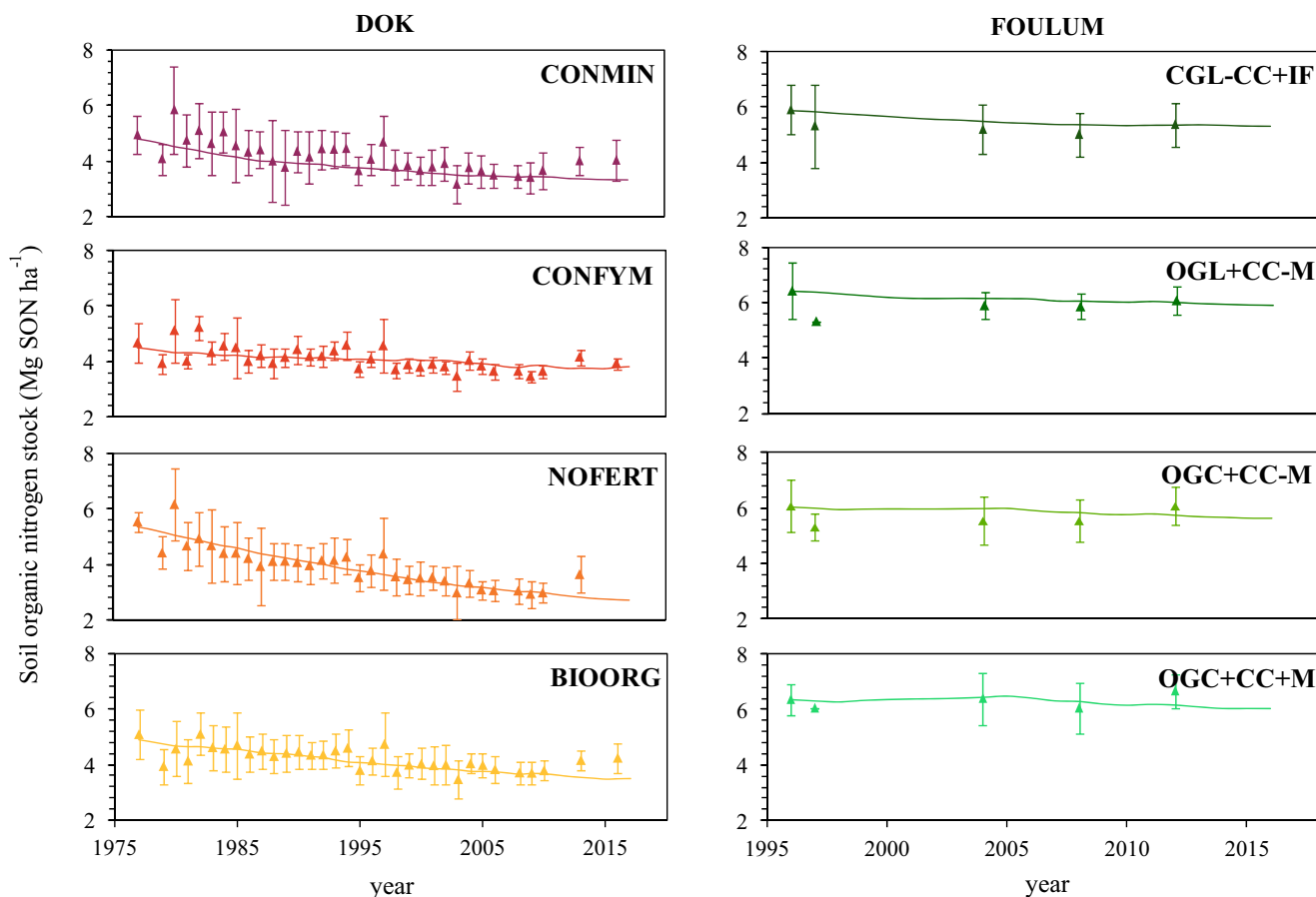
In the Foulum experiment, the rate of SON change was highest in OGC+CC+M ( $-17 \text{ kg N ha}^{-1} \text{ yr}^{-1}$ ) and similar in the three other treatments ( $-27 \text{ kg N ha}^{-1} \text{ yr}^{-1}$  on average). Changes in SOC stocks were also negative but did not differ significantly between treatments. N contained in deep root residues increased at a small rate in rotation OGL ( $5 \text{ kg N ha}^{-1} \text{ yr}^{-1}$ ) and faster in rotation OGC with grass-clover ley ( $8\text{--}10 \text{ kg N ha}^{-1} \text{ yr}^{-1}$ ). The N inputs derived from crop residues and total dead roots were smaller in rotation OGL than in rotation OGC, due to the inclusion of grass-clover in the latter rotation. Hence, the main factor determining N fate was the type of crop rotation and not the treatment. The annual N mineralization rate also varied widely between rotations:  $115 \text{ kg N ha}^{-1} \text{ yr}^{-1}$  in rotation OGL and  $183\text{--}198 \text{ kg N ha}^{-1} \text{ yr}^{-1}$  in rotation OGC.

**Table 4**

Performances of STICS for predicting soil water and nitrate contents (0–90 cm at DOK and 0–25 cm at Foulum). Treatments used for the calibration are in bold, other treatments were used for the evaluation.

		DOK				Foulum			
		<b>CONMIN</b>	CONFYM	NOFERT	BIOORG	<b>CGL-CC+IF</b>	OGL+CC-M	OGC+CC-M	OGC+CC+M
Soil water content (mm)	n	<b>73</b>	73	28	76	<b>34</b>	31	27	34
	X obs	<b>322 (39)</b>	322 (37)	334 (34)	322 (40)	<b>87 (19)</b>	98 (16)	88 (16)	95 (21)
	X sim	<b>322 (34)</b>	318 (34)	339 (26)	323 (33)	<b>86 (7)</b>	85 (8)	84 (9)	86 (8)
	RMSE	<b>24</b>	15	31	26	<b>16</b>	18	14	21
	RMSEs	<b>13</b>	7	21	15	<b>15</b>	17	12	20
	RMSEu	<b>21</b>	13	22	21	<b>6</b>	7	8	2
Soil nitrate content ( $\text{kg N ha}^{-1}$ )	n	<b>116</b>	119	42	118	<b>74</b>	17	53	57
	X obs	<b>47 (36)</b>	56 (40)	56 (45)	50 (37)	<b>42 (51)</b>	9 (9)	16 (27)	23 (6)
	X sim	<b>27 (28)</b>	34 (33)	29 (29)	31 (37)	<b>22 (25)</b>	6 (3)	10 (12)	13 (2)
	RMSE	<b>36</b>	39	47	40	<b>50</b>	9	32	43
	RMSEs	<b>28</b>	29	40	29	<b>44</b>	9	30	41
	RMSEu	<b>23</b>	25	24	27	<b>22</b>	3	11	14

n = number of observed/simulated data pairs, X obs = mean of measured values, X sim = mean of simulated values. RMSE = root mean square error, RMSEs = systematic RMSE, RMSEu = unsystematic RMSE.



**Fig. 3.** Temporal evolution of soil organic N stocks, over 0–20 cm and 0–25 cm for the DOK and Foulum experiments, respectively. Symbols (▲) display the observed soil organic N stocks for sampling dates,  $\pm$ SD. Lines are mean values of simulation for single plots ( $n = 3$  for the DOK,  $n = 4$  for the Foulum).

### 3.4. N Surplus at annual and long-term scale

The simulated annual N surplus was compared to the ‘observed’ surplus, calculated for each treatment and each crop cycle (Fig. 4). For DOK, the observed surplus varied between  $-103$  and  $+135$   $\text{kg N ha}^{-1} \text{yr}^{-1}$  and the simulated surplus between  $-96$  and  $+96$   $\text{kg N ha}^{-1} \text{yr}^{-1}$ . Both variables were well correlated ( $R = 0.81$ ), but the model slightly overestimated the N surplus, by  $5$   $\text{kg N ha}^{-1} \text{yr}^{-1}$  on average. The correlation was smaller in Foulum experiment ( $R = 0.58$ ), the surplus being overestimated by  $9$   $\text{kg N ha}^{-1} \text{yr}^{-1}$  on average in the CGL treatment and underestimated by  $8$   $\text{kg N ha}^{-1} \text{yr}^{-1}$  in the OGC treatments.

The simulated long-term N surplus varied among experiments and treatments (Table 6). In the DOK trial, the N surplus varied between treatments and ranked as follows:  $\text{NOFERT} < \text{BIOORG} = \text{CONMIN} < \text{CONFYM}$ . It was positive only in the CONFYM treatment. Less contrasted N surpluses were found at Foulum: only the OGL+CC-M treatment had a negative N surplus, significantly lower than the other treatments. The differences in N surpluses resulted from differences in quality and quantity of inputs and outputs.

In the DOK trial, total N inputs were highest in the CONFYM treatment, 62% deriving from fertilization and 31% from BNF. N inputs were similar in the CONMIN and BIOORG treatments ( $183$ – $189$   $\text{kg N ha}^{-1} \text{yr}^{-1}$ ), 51% coming from fertilization and 40% from BNF. BNF contributed to 79% of total N inputs in NOFERT. Total N exportations were highest in CONFYM and lowest in NOFERT.

At Foulum, the OGC+CC+M treatment had the highest N inputs, 39% deriving from fertilization and 49% from the BNF. Total N

inputs did not differ significantly between CGL-CC+IF and OGC+CC-M, but had different origins, particularly in OGC+CC-M treatment where 81% of N inputs came from BNF. The total N outputs followed the same ranking as N inputs between treatments, the highest N exportations occurring in OGC+CC+M ( $121$   $\text{kg N ha}^{-1} \text{yr}^{-1}$ ), in which grass-clover cuts were exported. Overall the study, the long-term N surplus appeared highly significantly correlated only with N storage and volatilized N (Appendix D). It was neither correlated with N inputs nor with N exported.

### 3.5. Nitrogen fate

The components of the simulated N surplus in each treatment are presented in Fig. 5. A positive surplus implies N losses in the environment and/or positive soil N storage whereas a negative surplus implies a decline in soil organic N. The model predicted large differences in gaseous losses and nitrate losses between the two experimental sites. In the DOK experiment, the N surplus varied widely between treatments, and most of its variation resulted in changes in soil N pools. Changes in deep root residues (below the plough layer) did not differ between treatments. N losses were small and did not differ significantly between treatments, whether by leaching ( $7$   $\text{kg N ha}^{-1} \text{yr}^{-1}$ ), denitrification ( $2$   $\text{kg N ha}^{-1} \text{yr}^{-1}$ ) or volatilization ( $3$   $\text{kg N ha}^{-1} \text{yr}^{-1}$ ).

In the Foulum experiment, the N surplus varied little between treatments whereas its fate differed significantly. Changes in SON stocks and deep root residues were mainly affected by the rotation, whereas N losses varied with treatments. N leaching was smallest in treatment OGL+CC-M ( $12$   $\text{kg N ha}^{-1} \text{yr}^{-1}$ ) and highest in the conventional treatment ( $29$   $\text{kg N ha}^{-1} \text{yr}^{-1}$ ). The volatilization losses

**Table 5** Simulated balance of soil organic C and N at 25 cm depth. Values are the mean of 39 years and three replicates for DOK, 19 years and four replicates for Foulum. Letters indicate significant differences between cropping systems for each field experiment ( $p < 0.05$ ).

	DOK					Foulum										
	CONMIN	CONFYM	NOFERT	BIOORG	CGL-CC+IF	OGL+CC-M	OGC+CC-M	OGC+CC+M	OGC+CC+M	OGC+CC+M						
Soil organic C (kg C ha <sup>-1</sup> yr <sup>-1</sup> )	-481	c	-173	a	-711	d	-360	b	-322	a	-305	a	-454	a	-377	a
changes of humified C stocks <sup>a</sup>	343	a	372	a	282	a	333	a	84	c	147	b	227	a	192	ab
changes of deep root C stocks <sup>a</sup>	0	c	1107	a	0	c	1010	b	0	b	1	ab	-226	c	31	a
input fluxes	1490	ab	1578	a	1229	c	1423	b	2049	d	2377	c	3443	a	2979	b
organic fertilizer <sup>b</sup>	1281	ab	1389	a	1022	c	1258	b	749	b	662	b	1086	a	1160	a
crop residues <sup>a</sup>	2908	c	3874	a	2681	d	3717	b	3036	b	3198	b	4530	a	4355	a
dead roots <sup>a</sup>	-40	b	-16	a	-78	c	-39	b	-29	b	-28	b	-25	b	-17	a
mineralization <sup>a</sup>	12	a	14	a	9	a	12	a	1	c	5	b	10	a	8	a
Soil organic N (kg N ha <sup>-1</sup> yr <sup>-1</sup> )	0	c	54	b	0	c	64	a	0	c	0	b	1	b	20	a
changes of deep root N stocks <sup>a</sup>	71	b	67	a	40	c	49	b	43	d	75	c	141	a	108	b
input fluxes	52	ab	61	a	35	c	51	b	12	b	16	b	41	a	46	a
organic fertilizer <sup>b</sup>	152	b	184	a	145	c	192	a	84	c	115	b	198	a	183	a
crop residues <sup>a</sup>																
dead roots <sup>a</sup>																
mineralization <sup>a</sup>																

<sup>a</sup> Simulated data.

<sup>b</sup> Observed data.

were similar in CGL-CC+IF and OGC+CC+M (5 kg N ha<sup>-1</sup> yr<sup>-1</sup> on average) and nil under the OGL+CC-M and OGC+CC-M treatments. Only denitrification losses were similar between treatments, and averaged 1 kg N ha<sup>-1</sup> yr<sup>-1</sup>.

Overall the study, some N outputs were correlated with N inputs: The N contained in deep root residues was highly significantly correlated with BNF and significantly correlated with total N inputs and N exportation (Appendix D). Leached N was correlated neither with N inputs nor with BNF. Gaseous N losses were significantly correlated with total N fertilization.

### 3.6. N Mineralization

The temporal evolution of the simulated annual mineralization of N derived from humified organic matter (SON) and organic residues and the total N mineralization is shown in Fig. 6. In the DOK trial, the annual average mineralization from SON pool was 149 kg N ha<sup>-1</sup> yr<sup>-1</sup>. It was higher in CONFYM and BIOORG (average 172 kg N ha<sup>-1</sup> yr<sup>-1</sup>) than in CONMIN and NOFERT (average 127 kg N ha<sup>-1</sup> yr<sup>-1</sup>). The mineralization deriving from crop residues was almost similar in all treatments, averaging 21 kg N ha<sup>-1</sup> yr<sup>-1</sup>. Annual variations were linked to manure application and grass-clover destruction. The total N mineralization was higher in CONFYM and BIOORG (189 kg N ha<sup>-1</sup> yr<sup>-1</sup>) than in NOFERT and CONMIN (148 kg N ha<sup>-1</sup> yr<sup>-1</sup>) and the differences between treatments increased after 1990.

At Foulum, the SON mineralization was less variable across years, while the net mineralization rate of crop residues varied widely between treatments and years. The latter was high in rotation OGC (95 kg N ha<sup>-1</sup> yr<sup>-1</sup>), low in OGL+CC-M (28 kg N ha<sup>-1</sup> yr<sup>-1</sup>) and very low in CGL-CC+IF (-5 kg N ha<sup>-1</sup> yr<sup>-1</sup>). In addition, a temporal shift was observed in OGC after 2006, with a net decline in residue-derived mineralization. The total N mineralization exacerbated the differences in humus and residue N mineralization between treatments, with differences appearing early after the start of the experiment. Over the 19 yr period, the mean amount of N mineralized was 99 kg N ha<sup>-1</sup> yr<sup>-1</sup> in rotation OGL and 188 kg N ha<sup>-1</sup> yr<sup>-1</sup> in rotation OGC.

Hence, significant differences between treatments originated from humus mineralization at DOK, while they originated from mineralization of residues at Foulum. This result highlights the variation in N resource between organic systems, according to their design and management. Overall the study, N mineralization was significantly correlated with BNF. It was neither correlated with total N input nor with N surplus (Appendix D).

### 3.7. GHG balance due to C-N cycles

The GHG balance calculated for each cropping system is presented in Table 7. It was estimated on the 1978–2016 period at DOK and the 1998–2016 period at Foulum. The direct N<sub>2</sub>O emissions and CO<sub>2</sub> emissions coming from soil were the main sources of variability in the GHG balance. Emissions deriving from the synthesis of fertilizers were highest in conventional treatments, receiving mineral fertilizer, with 521 and 338 kg CO<sub>2</sub>eq ha<sup>-1</sup> yr<sup>-1</sup> in CONMIN and CGL-CC+IF, respectively. The CO<sub>2</sub> emissions related to soil and crop management were equivalent between systems and averaged 125 kg CO<sub>2</sub>eq ha<sup>-1</sup> yr<sup>-1</sup> for DOK and 91 kg CO<sub>2</sub>eq ha<sup>-1</sup> yr<sup>-1</sup> for Foulum. The indirect N<sub>2</sub>O emissions occurring during the N cascade were positively correlated to the rate of fertilization in each treatment; these losses varied from 18 kg CO<sub>2</sub>eq ha<sup>-1</sup> yr<sup>-1</sup> in NOFERT to 128 kg CO<sub>2</sub>eq ha<sup>-1</sup> yr<sup>-1</sup> in CGL-CC+IF treatment.

In the DOK experiment, the global GHG balance per unit of area was highest in CONMIN and NOFERT (average 3438 kg CO<sub>2</sub>eq ha<sup>-1</sup> yr<sup>-1</sup>) and smaller in CONFYM and BIOORG (2472 kg CO<sub>2</sub>eq ha<sup>-1</sup> yr<sup>-1</sup>). When the GHG balance was expressed per unit of wheat

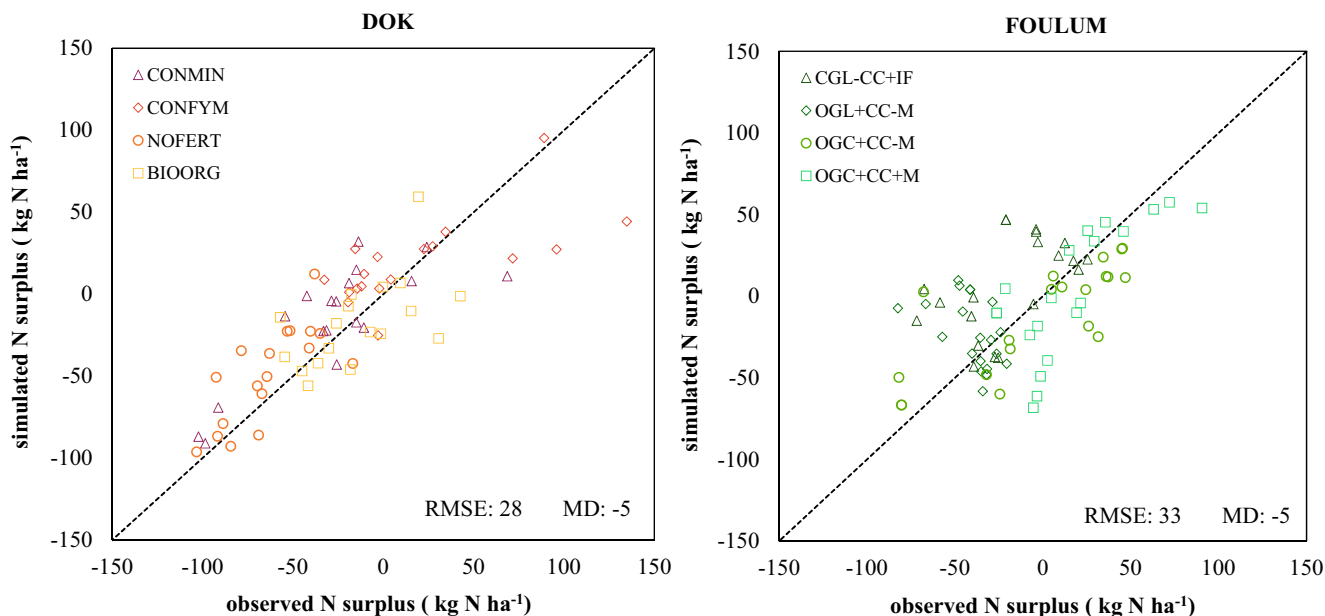


Fig. 4. Comparison of simulated and observed (calculated from measurements) N surplus. Each dot refers to the average N surplus for a given crop cycle (Table 1), for each treatment at the DOK and Foulum experiments.

Table 6  
Mean values of N inputs, N exported and N surplus (kg N ha<sup>-1</sup> yr<sup>-1</sup>) between the start of the experiments and 2016. Total N input is the sum of mineral and organic N fertilization, BNF and atmospheric N deposition. Letters indicate significant differences between cropping systems for each field experiment (p < 0.05).

	DOK				Foulum											
	CONMIN	CONFYM	NOFERT	BIOORG	CGL-CC+IF	OGL+CC-M	OGC+CC-M	OGC+CC+M								
N fertilization <sup>b</sup>	97	b	155	a	0	c	94	b	56	a	1	b	1	b	54	a
BNF <sup>a</sup>	75	a	77	a	65	a	72	a	16	c	35	b	72	a	67	a
Atmospheric N deposition <sup>a</sup>	17		17		17		17		15		16		16		16	
Total N input <sup>a</sup>	189	b	249	a	81	c	183	b	87	b	52	c	89	b	137	a
Total N exported <sup>a</sup>	209	b	235	a	145	c	197	b	81	b	62	c	81	b	121	a
N surplus <sup>a</sup>	-20	b	14	a	-64	c	-14	b	6	a	-11	b	9	a	16	a

<sup>a</sup> Simulated data.  
<sup>b</sup> Observed data.

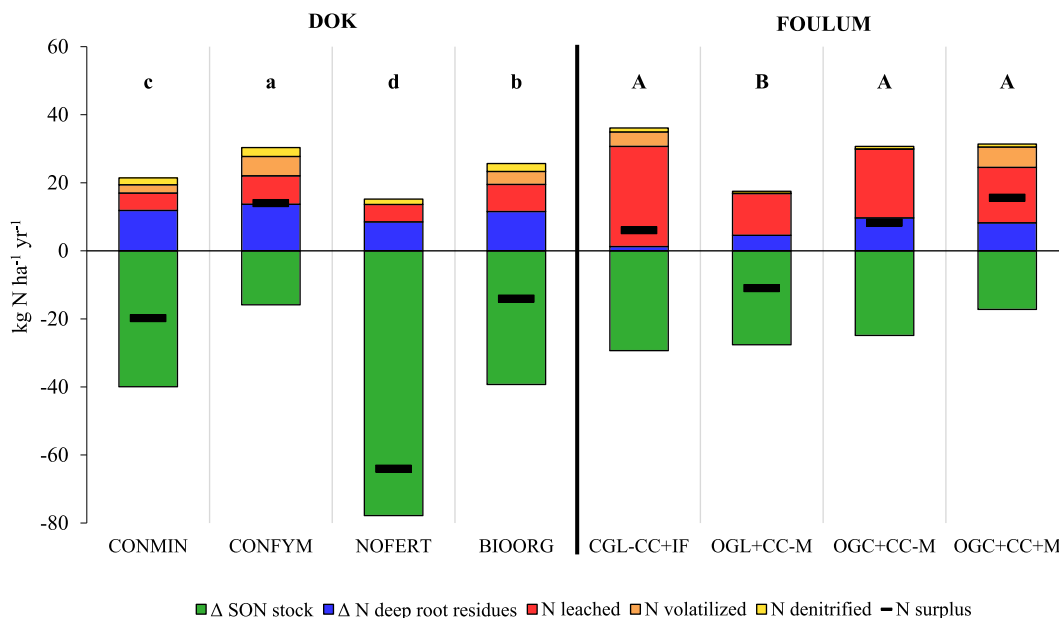
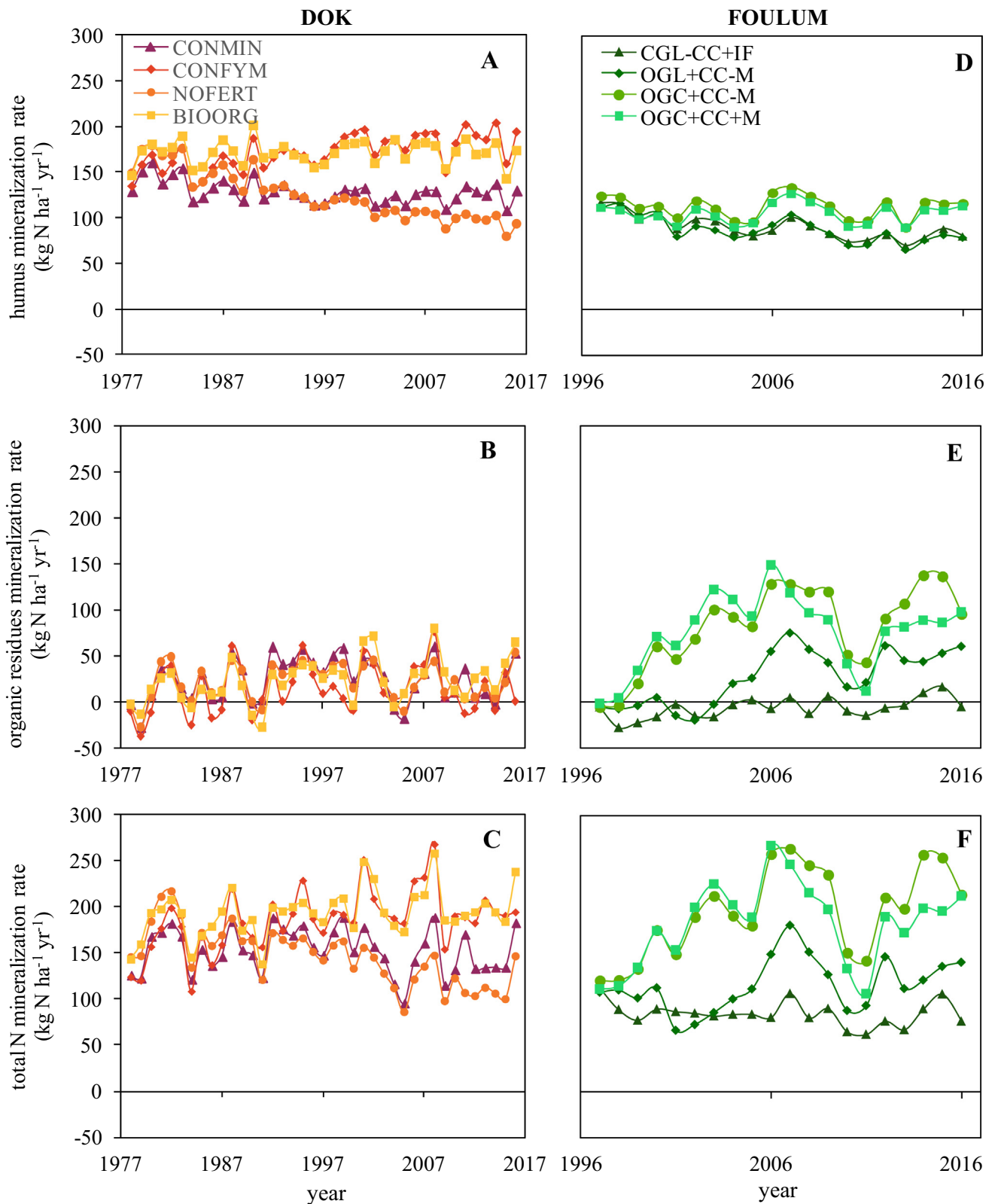


Fig. 5. Decomposition of the simulated annual N surplus between changes in SON stocks, N leaching and gaseous N emissions. Letters indicate significant differences in N surplus between cropping systems for each field experiment (p < 0.05).



**Fig. 6.** Simulated annual mineralization rate of humified N, organic residue and total N of the DOK (A, B and C) and Foulum (D, E, and F) experiments, respectively.

grain exported ( $\text{kg CO}_2\text{eq Mg}^{-1}$  wheat grain), the following ranking was obtained: CONFYM (4 9 5) < BIOORG (6 6 9) = CONMIN (7 1 7) < NOFERT (1351). In the Foulum experiment, the global GHG balance was smaller and varied less between treatments, from  $1541 \text{ kg CO}_2\text{eq ha}^{-1} \text{ yr}^{-1}$  in OGL+CC-M up to  $2282 \text{ kg CO}_2\text{-}$

$\text{eq ha}^{-1} \text{ yr}^{-1}$  in CGL-CC+IF. When expressed per unit of wheat grain exported, the unfertilized treatment had the highest GHG emissions with  $602 \text{ kg CO}_2\text{eq Mg}^{-1}$  wheat grain on average for OGL+CC-M and OGC+CC-M against  $413 \text{ kg CO}_2\text{eq Mg}^{-1}$  wheat grain for CGL-CC+IF and OGC+CC+M.

**Table 7**  
GHG balance and components estimated for the DOK and Foulum experiments for the 1978–2016 and 1998–2016 periods, respectively. Letters indicate significant differences between cropping systems for each field experiment ( $p < 0.05$ ).

		DOK				Foulum				
		CONMIN	CONFYM	NOFERT	BIOORG	CGL-CC+IF	OGL+CC-M	OGC+CC-M	OGC+CC+M	
Fertilizer <sup>a</sup>	kg CO <sub>2eq</sub> ha <sup>-1</sup> yr <sup>-1</sup>	521	a 298	b 0	c 12	c 338	a 0	b 0	b 13	b
Fuel combustion <sup>b</sup>		124	a 124	a 127	a 127	a 95	a 94	a 88	b 88	b
Direct N <sub>2</sub> O emissions		934	c 1216	a 719	d 1086	b 541	a 284	c 339	bc 409	b
Indirect N <sub>2</sub> O emissions		63	b 101	a 18	c 28	b 128	a 43	b 71	b 57	b
SOC storage rate		-1762	c -633	a -2608	d -1318	b -1180	a -1120	a -1666	a -1381	a
GHG balance	kg CO <sub>2eq</sub> ha <sup>-1</sup> yr <sup>-1</sup>	<b>3404</b>	<b>a 2373</b>	<b>b 3471</b>	<b>a 2571</b>	<b>b 2282</b>	<b>a 1541</b>	<b>b 2164</b>	<b>a 1949</b>	<b>ab</b>
	kg CO <sub>2eq</sub> t <sup>-1</sup> wheat grain	<b>717</b>	<b>b 495</b>	<b>c 1351</b>	<b>a 669</b>	<b>b 435</b>	<b>b 624</b>	<b>a 580</b>	<b>a 391</b>	<b>b</b>

Direct and indirect N<sub>2</sub>O emissions are the N<sub>2</sub>O fluxes directly emitted by the soil-crop system and throughout the N cascade, respectively. SOC storage rates are estimated with STICS model.

<sup>a</sup> Equivalent amount of CO<sub>2</sub> emitted during fertilizer synthesis and application.

<sup>b</sup> Equivalent amount of CO<sub>2</sub> emitted by tractors during crops and soil management.

## 4. Discussion

### 4.1. Performance of the STICS model

The model satisfactorily simulated crop biomass, both exported biomass (grains, tuber, grass-clover cuts) and total aboveground biomass. The quality of predictions was similar for organic and conventional systems, validating our hypothesis H3 that the model could predict both systems. The *RMSE* range for biomass prediction (1.6–3.7 Mg DM ha<sup>-1</sup>) was close to that (1.7–4.3 Mg DM ha<sup>-1</sup>) obtained in three long-term experiments with conventional systems (Constantin et al., 2012). The relative *RMSE* was greater for the harvested biomass than the total biomass, both in our results and the latter reference, indicating a poor prediction of the harvest index. The prediction of aboveground N content, with a *RMSE* of 37–72 kg N ha<sup>-1</sup>, was not as good as that obtained by Constantin et al. (2012), with a *RMSE* range of 24–48 kg N ha<sup>-1</sup>, but was consistent with Coucheney et al. (2015) who obtained a mean *RMSE* of 48 kg N ha<sup>-1</sup> for fifteen crops. Harvested N contents were less well simulated, with a *RMSE* range close to those of Constantin et al. (2012). This difficulty can be attributed to: i) the occurrence of yield gaps in organic systems, due to biotic factors (weeds, pests and diseases) which are not accounted for in STICS (Rakotovololona et al., 2018); ii) the better ability to simulate aerial N uptake than its repartition between exported organs and residues returned to soil, as already observed in conventional cropping systems (Beaudoin et al., 2008).

The SWC was accurately simulated at both sites. However, the measurements at Foulum were only available for the upper layer, so that it is difficult to ensure that water content was well simulated in the whole profile. The *RMSE* range (15–31 mm) remains lower than the range of 23 to 39 mm obtained in similar soil by Constantin et al. (2012) and close to the 19 mm average obtained by Coucheney et al. (2015). The SMN was systematically underestimated (by 45–48%) in all treatments of DOK and in the conventional treatment at Foulum, but a better prediction was obtained in the organic treatments of Foulum (relative MD = -19% to +13%). For comparison, a positive bias between 14 and 26% was obtained in long-term simulations of Constantin et al. (2012). This older model version could have underestimated the dead root residues, the decomposition of which results in N immobilization. However, SMN measurements were too scarce to confirm a systematic underestimation in the experiments. For example, the small amounts of SMN measured under the grass-clover ley were well reproduced by the model. The evolution of SMN contents after grass-clover destruction was partly, but not fully, mimicked. This may be due to the root turnover of the grass-clover ley, with clover having a higher net N mineralization rates than grasses, therefore

leading to higher SMN following grass-clover leys (Rasmussen et al., 2008), while we considered a single root turnover rate for the mixture.

Unsatisfactory parametrization of crop parameters could decrease the quality of simulations, showing a need for improving particular crops, such as beetroot, hemp, fababean, especially for organic cultivation. In addition, biotic stresses such as diseases, pests and competition with weeds for nutrients are not considered by the STICS model, e.g. fungal diseases in organic wheat (Gunst et al., 2006) at DOK, potato late blight (Zihlmann et al., 2004, Shah et al., 2017) at DOK and Foulum, or weed pressure at Foulum (Olesen et al., 2007). Finally, the overestimation of crop yield for some years can be explained by the fact that the model did not take into account possible stresses linked with potassium and phosphorus shortage. Oehl et al. (2002) reported a significant decrease in soil P content in the NOFERT treatment from 1978 to 2002 at DOK, potentially leading to low yields compared to the simulations.

### 4.2. Observed and simulated N surplus, at annual or long-term scale

The model could correctly reproduce the large variability in N surplus among treatments and years, varying from -276 to +331 kg N ha<sup>-1</sup> yr<sup>-1</sup> (observed) and -235 to +348 kg N ha<sup>-1</sup> yr<sup>-1</sup> (simulated). This performance was obtained in spite of the high frequency of legumes which increased the uncertainty of the N surplus estimates due to the empirical nature of the BNF estimations.

Concerning the long-term simulated N surplus, we found that organic systems receiving as much N input as conventional ones can have equal (OGC+CC+M vs CGL-CC+IF) or higher N surplus (BIOORG vs CONMIN). This was also observed by Reganold and Wachter (2016). Conversely, Anglade et al. (2015b) found a N surplus 26% lower in organic than in conventional cropping systems, related to the smaller inputs (-12%) in organic systems. Thus, the difference between conventional and organic treatments may not appear in the N surplus, but may consist in contrasted N losses. The N surplus has been promoted as an environmental indicator revealing the potential N losses from cultivated lands (OECD, 2001). According to Oenema et al. (2005), a reduction of the N surplus should decrease the risk of N losses. However, no relationship was found between N surplus and N leaching in a three year study in arable organic cropping systems (Rakotovololona et al., 2018). The long-term N surplus seemed more useful to predict the GHG balance if it is coupled with a N storage assessment (Autret et al., 2019). It should be noted that a positive N surplus may also correspond to small N losses and high storage in soil organic nitrogen pool (Poudel et al., 2001; Watson et al., 2002; Anglade et al., 2015b). At Foulum, De Notaris et al. (2018) and Pandey et al.

(2018) also found weak relationships between long-term N surplus and N leaching losses.

#### 4.3. Drivers of N leaching in organic systems

The soils at the two sites are freely draining and their textures allow to use the tipping bucket modelling approach to assess the water balance and the mixing cell concept to simulate the solute convection and dispersion (Mary et al., 1999). Nitrate leaching has been shown to be well simulated by STICS over multi-year continuous runs whatever the soil type (Beaudoin et al., 2008; Jegu et al., 2012; Constantin et al., 2012). We simulated a low N leaching in the DOK trial (7 kg N ha<sup>-1</sup> yr<sup>-1</sup> on average) with similar values among the different treatments. In this trial, the underestimation of SMN contents might have led to underestimate N leaching but only in wet winters, as shown by Rakotovololona et al. (2018) in deep loamy soils. Only one paper reported measurements of SMN under potato crop from 1999 to 2002 at DOK, after destruction of the previous grass-clover ley (Zihlmann et al., 2004). The authors found that SMN contents were slightly higher in manured treatments than in CONMIN, increasing the risk of leaching in the following autumn–winter period. The higher, although not significant, N leaching simulated in CONFYM and BIOORG (8 kg N ha<sup>-1</sup> yr<sup>-1</sup>) compared to CONMIN and NOFERT (5 kg N ha<sup>-1</sup> yr<sup>-1</sup>) is consistent with this conclusion. The simulation outputs showed that N leaching was mainly regulated by the type of soil cover rather than the amount of N inputs (CONMIN vs CONFYM) or type of fertilizer used (mineral fertilizer vs manure and slurry).

In the Foulum experiment, the climate and soil type promote the risk of N leaching and enhance the differences between treatments. The model indicated that the organic treatments significantly impacted nitrate leaching. Compared to the conventional treatment, which had the highest leaching (28 kg N ha<sup>-1</sup> yr<sup>-1</sup>), the N leaching was significantly reduced by 60% in the OGL+CC-M treatment, in which no manure was applied and a cover crop was grown during autumn and winter. Askegaard et al. (2011) found in the same experiment that the use of cover crops could reduce nitrate leaching by 7 to 63%, indicating that the establishment of cover crops must contribute to reduce nitrate leaching in organic systems. STICS simulated a 24% reduction in the two organic treatments (rotation OGC) compared to the conventional (rotation CGL). Conversely, the inclusion of a grass-clover ley in rotation OGC had no significant effect on leaching compared to the organic rotation OGL (Askegaard et al., 2011) or to the conventional rotation CGL (Pugesgaard et al., 2017). Mondelaers et al. (2009) reported no correlation between the proportion of grass in the rotation and N leaching in simulation studies.

Our simulations corroborate the finding that N leaching is rather insensitive to the amount of N applied in fertilizers or manure (Stopes et al., 2002; Stark et al., 2006; Brozyna et al., 2013), up to levels of fertilization close to the economic optimum. Benoit et al. (2014) explored the differences among sources of N inputs and found increased N concentrations when poultry manure is applied, and decreased concentrations for compost. In fact, the date of application of organic fertilizer seems to be crucial, unless a cover crop can capture and retain excess soil mineral N after harvest of the main crop.

#### 4.4. Gaseous N losses affected by the fertilization

Besides N leaching, the model simulated gaseous N losses by volatilisation and denitrification. The predicted values can hardly be compared to observations since measurements are difficult, scarce and made on the short term (Chirinda et al., 2010; Skinner et al., 2014a; Li et al., 2015; Pugesgaard et al., 2017). In the DOK

trial, STICS predicted the highest denitrification rate (N<sub>2</sub> + N<sub>2</sub>O) and highest N<sub>2</sub>O emissions in the CONFYM treatment. The highest N<sub>2</sub>O emissions measured in 2013 by Skinner et al. (2014a) were also found in this treatment. However, these authors found no differences in N<sub>2</sub>O emissions between CONMIN and BIOORG and NOFERT, while simulations gave the following ranking: NOFERT < CONMIN < BIOORG.

At Foulum, we simulated small losses through denitrification, which were 33% higher in fertilized than unfertilized treatments. Volatilization losses occurred in the conventional and OGC+CC+M treatments only. Pugesgaard et al. (2017) estimated annual denitrification and volatilization at Foulum for the 2006–2009 period. Their estimates of denitrification were higher than our simulations: 12 vs 8 kg N ha<sup>-1</sup> yr<sup>-1</sup> in the conventional treatment, and 16 vs 8 kg N ha<sup>-1</sup> yr<sup>-1</sup> in OGC+CC+M. Their estimate of volatilization in the conventional treatment was close to ours (3 vs 4 kg N ha<sup>-1</sup> yr<sup>-1</sup>), but 2 to 4 times higher than ours in the organic treatments.

Soil N<sub>2</sub>O production and emission involves several complex processes and is influenced by numerous factors such as available nitrate, soil water content, temperature, pH, mineral N and readily available C. All these factors may be modified by agricultural practices such as the supply of N fertilizers and the incorporation of crop residues. In our study, higher denitrification was simulated at DOK than at Foulum, which may be mainly linked with differences in water-filled pore space (WFPS) since the small differences in soil pH must have had a limited effect on N<sub>2</sub>O emissions. High N<sub>2</sub> and N<sub>2</sub>O emissions were simulated at the Danish experiment in the conventional and the OGC+CC+M treatments, while they were lower in OGC+CC-M and OGL+CC-M; they were mainly driven by the amount of N fertilizer applied. In the DOK trial, higher denitrification was found in systems receiving external organic N inputs (manure and slurry), i.e. BIOORG and CONFYM.

#### 4.5. Long-term evolution of soil organic N pools

Besides N losses, variations in soil organic N pools can represent a source or a sink of N component in the long-term N surplus. Our hypothesis H3 was validated, since SON dynamics was equally well simulated in conventional and organic systems with the same formalism. Contrasted changes in SON content were simulated in the DOK experiment. The evolution of SON stocks was correctly modelled after increasing the initial proportion of active soil organic matter from 35% to 55%. This change is consistent with the previous history of the experiment, since grassland is known to increase carbon storage and therefore the proportion of active fraction, compared to arable cropping. Leifeld et al. (2009) modelled satisfactorily the SOC stocks evolution for DOK from 1978 to 2006 with RothC model. They justified their slight underestimation of SOC stocks in CONFYM by the N input rate, three times higher than in other treatments, which could have accelerated the decomposition of SOM, thus decreasing the SOC stock. Such a hypothesis was not necessary in our modelling which predicted satisfactorily both SON and SOC in the CONFYM treatment.

In the Foulum experiment, which had a previous history of mostly arable cropping, the proportion of active fraction was maintained to its default value, 35%. Changes in SON stocks were also well simulated, with an average decrease of -34 and -4 kg N ha<sup>-1</sup> yr<sup>-1</sup> in rotation OGL and OGC, respectively over 19 years. Pugesgaard et al. (2017) estimated the variation of SON stocks in the same experiment by subtracting N losses from the long-term N surplus calculated for the 2006–2009 period. Their results were very close to ours, -30 and +2 kg N ha<sup>-1</sup> yr<sup>-1</sup>, in rotations OGL and OGC, respectively.

The evolution of SON stocks was well simulated in the DOK experiment. A high SON decrease rate was observed and simulated in NOFERT ( $-78 \text{ kg N ha}^{-1} \text{ yr}^{-1}$ ), a lower decrease was simulated in CONMIN and BIOORG ( $-39 \text{ kg N ha}^{-1} \text{ yr}^{-1}$ ) and in CONFYM ( $-15 \text{ kg N ha}^{-1} \text{ yr}^{-1}$ ). The SON evolution was also satisfactorily simulated in the Foulum experiment, with an average decrease rate of  $-34$  and  $-4 \text{ kg N ha}^{-1} \text{ yr}^{-1}$  in rotations OGL and OGC, respectively, over 19 years.

The sensitivity of SOC and SON predictions to the size of the initial stable pool was tested. Increasing the size of this pool would have enhanced the rate of decrease of the SOC or SON pool and *vice versa* (and degraded the quality of fit in both cases), but would result in minor changes on the differences between treatments, even on the very long-term (100 years).

In both experiments, we observed a marked decrease in SOC and SON stocks. This trend, surprising at the first glance, may be representative of old mixed farming systems which were dominant in Europe in the past, before the farms evolved towards specialized systems (Mignolet et al., 2007). Hence, a significant part of the current arable lands has originated from ancient grasslands or highly manured arable fields. The SOM content of these fields has decreased with declining livestock. Changes in organic N pool were affected by crop management in both experiments, affecting the amount and type of organic residues (0–25 cm) and in deep root deposits (25–100 cm). Organic residues were crop residues (straw, stubble and root localized in the 0–25 cm soil layer), grass-clover cuts, cover crop residues and organic fertilizers (manure and slurry), mineralized according to specific model parameters. Among all crops, grass-clover contributed to a large part of the root inputs, like at Foulum where we simulated four times more root N inputs in organic treatments of rotation OGC (including grass-clover) compared to the conventional treatment. These root inputs represented from 4 to  $175 \text{ kg N ha}^{-1}$  according to the duration of the simulation unit, with an average C/N ratio of 20. Similar root N inputs were reported previously, with up to  $156 \text{ kg N ha}^{-1}$  in the top 20 cm of soil at the destruction of a three year old grass-clover ley whose C/N ratio was close to 20 (Eriksen and Jensen, 2001). However, studies often report the root C and N inputs recovered at harvest, not reflecting the previous turnover simulated by the model. Conversely, a low amount of aboveground crop residues was returned to soil in rotation OGL at Foulum, with straw and stubble having a mean C/N ratio of 33 and 60, respectively. These elevated ratios explain the lower N mineralization from residue and even N immobilisation simulated in treatments OGL+CC+M and CGL+CC+IF. The limited availability of mineral N may have induced a priming effect and lead to SOM mining as shown by Fontaine et al. (2011).

The last component of the organic N balance is the deep root residues. Its evolution is linked with the root dynamics simulated in the subsoil (25–150 cm). This pool increased with time in the STICS model since no decomposition was considered in this soil layer. The turn-over rate of the deep root N is known to be slow and decreasing with depth (Balesdent et al., 2018). STICS simulated important root biomass inputs below the soil mineralization layer, especially for DOK where it increased from  $8$  to  $14 \text{ kg N ha}^{-1} \text{ yr}^{-1}$ . Simulating the decomposition of these root residues would lead on the long-term to higher mineral N release, either absorbed by crops or leached or to soil organic N accumulation. Jenkinson and Coleman (2008) intended the modelling of subsoil root residues with the dynamical model RothC-26.3, by adding parameters to consider downward C flows and the slower decomposition of deep root residues. However, the approach is very simplified since the model considered uniform conditions of temperature and moisture in soil over 1 m depth. Hence, further data would be required to parametrize the mineralization of deep root residues in the long-

term (Rumpel and Kögel-Knabner, 2011), with accurate measurements of deep soil characteristics, deep C and N inputs and C and N losses.

#### 4.6. The GHG balance

We estimated the GHG balance (*i.e.* the net GHG emissions) in the DOK and Foulum experiments. It took into account the major sources of  $\text{CO}_2$  emissions, *i.e.* mineral fertilizer synthesis, fuel combustion from crop and soil management, direct and indirect  $\text{N}_2\text{O}$  emissions and net variation of SOC stock. The GHG balance differed between the two experimental sites mainly because of the variation in  $\text{N}_2\text{O}$  emissions and SOC stocks. The marked decrease in SOC stocks over time, particularly in the DOK experiment, lead to a very positive GHG balance. In the DOK experiment, the rate of decrease of SOC stocks was lower in treatments CONFYM and BIOORG, explaining their improved GHG balance compared to the conventional treatment. However, when considering the GHG balance per unit of wheat produced, we found that the CONFYM treatment had the more favourable (smallest) GHG balance, followed by BIOORG and CONMIN treatments which did not significantly differ from each other despite differences in wheat yields. At Foulum, the GHG balance of the conventional treatment ( $2282 \text{ kg CO}_{2\text{eq}} \text{ ha}^{-1} \text{ yr}^{-1}$ ) was close to that found by Knudsen et al. (2014) with  $2558 \text{ kg CO}_{2\text{eq}} \text{ ha}^{-1} \text{ yr}^{-1}$ . The conventional system showed higher GHG balance than the organic ones, due to higher N inputs originating from fertilizers. However, it did not differ significantly from the organic treatment OGC+CC+M, which shows that organic treatments can produce as much GHG emissions than conventional treatments; this conclusion would be strengthened when considering the GHG emitted per unit of production of the system. Hence, reducing the yield gap in organic systems is expected to improve their final GHG balance.

## 5. Conclusions

We simulated crop production and the related C and N fluxes of conventional and organic cropping systems in the long-term experiments of DOK (Switzerland) and Foulum (Denmark) with the agro-environmental model STICS. The two sites differed by pedoclimatic conditions as well as crop rotation. However, both were affected by a long-term decline of the SON stock, which could have impacted the N losses and the associated GHG budget as compared to other case-studies. The model should be able to simulate other scenarios of initial SON stock, in order to predict the variability of the GHG budget of the studied treatments. The STICS model was found to well reproduce the aboveground biomass both in conventional and organic treatments. It predicted crop N uptake with less accuracy, so that some of the predicted N fluxes, *i.e.* soil N storage, nitrate leaching, volatilization, denitrification and  $\text{N}_2\text{O}$  emissions, may be biased. However, we satisfactorily simulated the long-term N surplus, as an indicator of the potential losses from cropping systems. We found that the contrasted N surplus observed among DOK treatments can correspond to similar levels of N losses, whereas the Foulum treatments had similar N surpluses but contrasted N losses. We found highly significant correlations between i) N surplus and N storage and ii) total N fertilization and total N gaseous losses. Simulations showed that the N related environmental impacts depended on cropping system and management: leaching was more affected by crop rotation, gaseous losses mainly by fertilization rate, and soil N decay rate was sensitive to both factors. Agro-environmental models can contribute to the understanding and quantification of long-term changes of C and N fluxes in cropping systems under contrasted pedo-climatic situations and crop management.



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## Appendix A

Values of the new parameters added in the STICS v1610, relatively to the standard version, for every crop

Process	Parameter	Description	O/SB/SW/TR/ WB/WC/WW	SM	SP	AL	B	H	CG	PO	LU	CB
Root growth	repracpermax	Maximum root biomass relative to total biomass	0.85	0.63	0.85	0.10	0.30	0.50	0.65	0.40	0.80	0.40
	repracpermin	Minimum root biomass relative to total biomass	0.09	0.05	0.09	0.10	0.10	0.10	0.25	0.10	0.03	0.20
	krepracperm	Parameter of biomass root partitioning : evolution of the ratio root/total	1.79	1.48	1.79	1.27	1.27	1.79	1.27	1.27	1.00	1.27
Root N demand	parazorac	C:N ratio of roots for an NNI equal to 1	26	32	18	15	26	26	25	25	25	25

AL: alfalfa (*Medicago sativa* L.); B: beetroot (*Bet vulgaris* L.); CB: white cabbage (*Brassica oleracea* L.); H: hemp (*Cannabis sativa* L.); LU: lupin (*Lupinus albus* L.); O: oat (*Avena sativa* L.); PO: potato (*Solanum tuberosum* L.); SB: spring barley (*Hordeum vulgare* L.); SM: silage maize (*Zea mays* L.); SO: soybean (*Glycine max* L.); SP: spring pea (*Pisum sativum* L.); SW: spring wheat (*Triticum aestivum* L.); TR: triticale (*Triticosecale Wittm. ex A. Camus*); WB: winter barley (*Hordeum vulgare* L.); WC: winter cereal; WW: winter wheat (*Triticum aestivum* L.).

## Appendix B

Values of the parameters fixed for orphan crops. The “reference crop” is the crop with a close ecophysiology, from which the most part of the parameters are derived, in reference from Couchney et al. (2015).

Crop name				Triticale	Beetroot	Hemp	Grassfix
Reference crop for default values				Winter wheat	Sugar beet	Winter wheat	Grass
Process	Acronym	Description	Unit	Value	Value	Value	Value
Development	stressdev	Maximum phasic delay allowed due to stresses	SD		0.9		
	tdmin	Minimum temperature below which development stops	degreeC			1	
	tdmax	Maximum temperature above which development stops	degreeC			40	
	phosat	Aaturating photoperiod	hours			13.8	
	codebfroid	Option of chilling requirements	code 1/2/3			NO	
	tfroid	Optimal temperature for vernalisation	degreeC	4.5			
	ampfroid	Semi thermal amplitude for vernalising effect	degreeC	9			
	stpltger	Cumulative thermal time allowing germination	degree-d			24.1	
	potgermi	Soil water potential under which seed imbibition is impeded	MPa			-3.2	

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## Appendix B (continued)

Crop name				Triticale	Beetroot	Hemp	Grassfix
Leaf expansion	hautmax	Maximum height of crop	m	1.4			
	tcxstop	Temperature beyond which foliar growth stops	degreeC		30		
	parazofmorte	Parameter relating the C/N of dead leaves and the INN	SD		13		
	tcmin	Minimum temperature at which growth ceases	degreeC			1	
	tcmax	Maximum temperature at which growth ceases	degreeC	37			
	dlaimin	Accelerating parameter for the lai growth rate	SD			0.1	
	vlaimax	ulai at the inflexion point of the function DELTAI = f(ULAI)	SD			2.2	
	dlaimaxbrut	Maximum rate of the setting up of LAI	m <sup>2</sup> leaf.plant-1.degree-d-1	0.00041	0.00075	0.00065	
	innturgmin	Parameter of the N stress function active on leaf expansion (INNLAI)	SD		0	-0.8	
	innsen	Parameter of the N stress function active on senescence (INNsenes)	SD	0.17			
Shoot growth	extin	Extinction coefficient of photosynthetic active radiation in the canopy	SD			0.96	
	temin	Minimum temperature for development	degreeC			1	
	temax	Maximal temperature above which plant growth stops	degreeC	37		45	
	teopt	Optimal temperature (1/2) for plant growth	degreeC			15	
	efcroijuv	maximum radiation use efficiency during the juvenile phase	g.MJ-1	1.9	2.0	1.75	1.0
	efcroiveg	Maximum radiation use efficiency during the vegetative stage	g.MJ-1	3.8	4.0	3.5	2.0
	efcroirepro	Maximum radiation use efficiency during the grain filling phase	g.MJ-1	3.8	3.5	3.5	2.0
	tigefuille	Ratio stem (structural part)/leaf on the cutting day	SD		0.45	4	
	spfrmin	Minimal sources/sinks value allowing the trophic stress calc. for fruit onset	SD		0.1		
	spfrmax	Maximal sources/sinks value allowing the trophic stress calc. for fruit onset	SD		1		
Yield formation	vitircarb	Rate of increase of the N harvest index vs time	g grain.g-1.d-1	0.0107			
	vitirazo	Rate of increase of the N harvest index vs time	g grain.g-1.d-1	0.0165	0.035	0.0165	
root expansion	stoprac	Stage when root growth stops	SD			lax	lax
	lvfront	Root density at the root apex	cm.cm-3		0.25	0.4	
	draclong	Maximum rate of root length production per plant	cm.plant-1.degree-d-1				400
	sensrsec	Index of root sensitivity to drought (1 = insensitive)	SD				0.05
	sensanox	Index of anoxia sensitivity (0 = insensitive)	SD				1
	Debsensrac	Sum of degrees.days defining the beginning of root senescence (root life time)	degree-d		10		1200

## Appendix B (continued)

Crop name				Triticale	Beetroot	Hemp	Grassfix
Longsperac parazorac	Specific root length	cm.g-1					9000
	Parameter relating the C/N of dead leaves and the INN	SD					15
rapdia	Aerodynamic resistance (for volatilization module when we use ETP approach)	s.m-1					1.91
RTD propracfmax	Minimal stomatal resistance of leaves	s.m-1					0.147
	Ratio of root mass to aerial mass at harvest	g.g-1					0.72
Frost threshold	tgelle10	temperature resulting in 10% of frost damages on plantlet	degreeC	-4.5			
	tgelle90	Temperature resulting in 90% of frost damages on plantlet	degreeC	-23			
	tgeljuv10	Temperature resulting in 10% of frost damage on LAI (juvenile stage)	degreeC	-11.5			
	tgeljuv90	Temperature resulting in 90% of frost damage on LAI (juvenile stage)	degreeC	-23			
	tgelve10	Temperature resulting in 10% of frost damage on LAI (adult stage)	degreeC	-5			
	tgelve90	Temperature resulting in 90% of frost damage on LAI (adult stage)	degreeC	-11.5			
	tgelflo10	Temperature resulting in 10% of frost damages on flowers and fruits	degreeC	-5			
	tgelflo90	Temperature resulting in 90% of frost damages on flowers and fruits	degreeC	-7.5			
Water use	kmax	Maximum crop coefficient for water requirements (=MET/PET)	SD	1.08	1.4		
	psisto	Potential of stomatal closing (absolute value)	bars		10		
N fixation	codelegume	is the crop a legume fixing N ? (1 = yes, 2 = no)	code 1/2				YES
	vitno	Rate of nodule onset expressed as a proportion of fixmax per degree day	degree-d-1				0.03
	profnod	Maximum depth of N2 fixation by legume crops	cm				40
	concNnodseuil	Maximal concentration of mineral N in soil for nodule onset	kg.ha-1.mm-1				1
	concNrac0	Nitrate-N concentration above which N fixation is totally inhibited	kg.ha-1.mm-1 or kg.ha-1.cm-1				1
	concNrac100	Nitrate-N concentration below which N fixation is maximum	kg.ha-1.mm-1 or kg.ha-1.cm-2				0.5
	tempnod1	Temperature parameter (1/4) used to calculate N fixation by legumes	degreeC				0
	tempnod2	temperature parameter (2/4) used to calculate N fixation by legumes	degreeC				30
	tempnod3	Temperature parameter (3/4) used to calculate N fixation by legumes	degreeC				36
	tempnod4	Temperature parameter (4/4) used to calculate N fixation by legumes	degreeC				50
	fixmaxveg	Maximal N symbiotic fixation rate per unit of vegetative growth rate	kg.t-1				30
	fixmaxgr	Maximal N symbiotic fixation rate per unit of grain growth rate	kg.t-1				6

(continued on next page)

## Appendix B (continued)

Crop name				Triticale	Beetroot	Hemp	Grassfix
Nitrogen uptake	Vmax1	Maximum specific N uptake rate with the low affinity transport system	$\mu\text{mole.cm}^{-1} \text{ h}^{-1}$	0.0012	0.0025	0.005	
	Vmax2	Maximum specific N uptake rate with the high affinity transport system	$\mu\text{mole.cm}^{-1} \text{ h}^{-1}$	0.032	0.05		
	adilmax	Parameter of the maximum dilution curve [Nplante] = adilmax MS <sup>(-bdilmax)</sup>	% DM	7.3	7.2	7.5	5.8
	bdilmax	Parameter of the maximum dilution curve [Nplante] = adilmax MS <sup>(-bdilmax)</sup>	SD	0.41			
	adil	Parameter of the critical dilution curve [Nplante] = adil MS <sup>(-bdil)</sup>	% DM	5.22			
	bdil	Parameter of the critical dilution curve [Nplante] = adil MS <sup>(-bdil)</sup>	SD	0.41			
	INNmin	Minimum value of INN possible for the crop	SD		0.1		
	codeINN	Option to compute INN (1 = cumulative, 2 = instantaneous)	code 1/2	0.41	1		

## Appendix C

Parameters of the regression model and belowground nitrogen factor for the estimation of biological nitrogen fixation (Anglade et al., 2015a).

Crop species	$\alpha$	$\beta$	BGN
Alfalfa	0.81	-13.9	1.70
Clover	0.78	3.06	1.60
Faba bean	0.73	5.45	1.53
Lentil	0.64	3.32	1.40
Pea	0.66	4.32	1.33
Soybean	0.66	4.32	1.50
Lupin	0.64	5.45	1.50

## Appendix D

Table of crossed Spearman correlation coefficients. \*\*\* = very highly significant (p-value  $\leq 0.001$ ); \*\* = highly significant (p-value  $\leq 0.01$ ); \* = significant (p-value  $\leq 0.05$ ).

r Spearman correlation	Total N inputs	BNF	N fertilisation	total N exportation	N surplus	N mineralization	$\Delta$ humus	$\Delta$ deep root residues	N leached	N denitrified	N volatilized	Gaseous N losses
Total N inputs	1											
BNF	0.89 **	1										
N fertilisation	0.87 **	0.64	1									
total N exportation	0.85 **	0.8 *	0.7	1								
N surplus	0.43	0.2	0.46	0.08	1							
N mineralization	0.57	0.73 *	0.22	0.37	0.29	1						
$\Delta$ humus	0.29	0.25	0.25	-0.07	0.88 **	0.36	1					
$\Delta$ deep root residues	0.81 *	0.93 ***	0.59	0.89 **	0.02	0.65	0.02	1				
N leached	-0.3	-0.47	-0.17	-0.69	0.59	-0.05	0.53	-0.66	1			
N denitrified	0.7	0.47	0.66	0.8 *	0.28	0.32	-0.05	0.63	-0.36	1		
N volatilized	0.67	0.32	0.71 *	0.49	0.78 *	0.16	0.52	0.24	0.14	0.68	1	
Gaseous N losses	0.75 *	0.45	0.73 *	0.69	0.66	0.29	0.36	0.47	-0.07	0.87 **	0.94 ***	1

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