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Insights gained from modeling grain yield, nitrate leaching, and soil nitrogen dynamics in a long-term field experiment with spring cereals on fertilized and unfertilized soil over 35 years

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ABSTRACT

Crop models are useful tools for predicting changes in yield and nitrogen losses in response to changes in agricultural management practices and climate. We used a soil-crop model (CoupModel) to interpret trends in yields, drainage, and nitrate leaching observed for two contrasting treatments (fertilized and unfertilized cereals) in a long-term field experiment (35 years) on a sandy loam in southern Sweden. The model was calibrated using a Monte Carlo-based method, in which the 30 best simulations of 10,000 model runs were identified based on multiple criteria. The posterior distributions differed significantly between the two treatments for 6 of the 16 parameters included. For example, the decomposition rate coefficient of the slow organic matter pool was significantly larger in the unfertilized treatment. The model simulated yearly drainage and nitrate leaching well overall, but did not fully capture between-year variations. Although the simulated mean annual nitrate leaching was 1.4 times greater in the fertilized treatment, N leached per unit of N harvest was twice as large in the unfertilized plot. The model simulated substantial decreases in yield for both treatments in 2018 in response to an extremely hot and dry summer, although not as large as that observed. The range in simulated annual N mineralization due to parameter uncertainty was wider in the fertilized treatment. We conclude that model calibration strategies require careful attention to how different management practices may influence decomposition and long-term N balance components in agroecosystems and that more data on especially belowground biomass would help in reducing uncertainties.

1. Introduction

Indigenous stores of soil nitrogen provide an important resource for N uptake in crops through nitrogen mineralization, in addition to the N applied with fertilizers (Cassman et al., 2002). Nitrogen released by mineralization of organic matter often amounts to more than half of the recovered N in well-fertilized crops (Thomsen et al., 2003). Maintaining soil fertility and a high indigenous N supply is therefore an important management strategy to reduce the need for N fertilizer. Lower input of mineral N provides several benefits, including less addition of reactive N to the ecosystem, which potentially reduces both water and air pollution (Galloway et al., 2003) and provides economic savings for the farmer. However, high mineralization rates in the soil, especially during periods with bare soil, constitute a risk of mineral N accumulation in the soil, which may result in leaching of nitrate (Stenberg et al., 1999) and gaseous losses through denitrification (Mosier et al., 1998). Maintaining and optimizing indigenous soil N supply to the crop as well as reducing the risk of N-losses by management requires an understanding of the system and the long-term storage and change in soil C and N pools.

The mineralization of organic N and immobilization of mineral N are highly dynamic processes that are difficult to measure in the field (Nykänen et al., 2009). Yin et al. (2020) identified four principal ways to estimate N mineralization including (i) laboratory incubation, (ii) using ^{15}N-labeled residues, (iii) in situ N balance methods, and (iv) model simulations. The results of laboratory incubations and isotopic tracer experiments are dependent on experimental conditions. Therefore, models calibrated using such experiments may be poor predictors of N mineralization in field conditions (Cabrera and Kissel, 1988; Johnson et al., 1999). In situ N balance methods such as the 'N-difference' method calculate the difference in N uptake between a crop receiving N

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fertilizer with one that does not. The addition of N may alter the plant's ability to take up N or water, which therefore introduces confounding factors (Cassman et al., 2002). Model simulations may be useful if they correctly capture all components of the N balance (Yin et al., 2020a). Soil-crop models can be used to describe nitrogen dynamics in relation to weather, soil characteristics, crop growth, and management (Kersebaum et al., 2007). Consequently, the long-term effects on soil organic N pools following different fertilization regimes or other management practices can be explored. The knowledge gained by such model applications can be used to assess N leaching risks and mineralization in the short- or long-term for different types of crop and soil management systems.

Agroecosystems include numerous processes and soil-plant interactions. Therefore, soil-crop models are often highly complex with a large number of equations and parameters, which leads to structural and parameter uncertainty. These sources of uncertainty along with uncertainties in the model input data (e.g. weather data, soil data, and data related to observations of crops) lead to uncertainty in model predictions. Furthermore, when a model is run continuously for many years, it must be able to account for carry-over effects between years (Beaudoin et al., 2008). Therefore, long-time series of data are important to evaluate the stability of the model performance over time.

Soil-crop models are seldom universal enough to be directly applied to situations beyond the types of systems and climates for which they were developed and tested. Therefore, crop models generally require some kind of calibration to be useful (Timsina and Humphreys, 2006; Wallach, 2011). It is noteworthy that this is often done by trial and error despite a range of more objective options (Seidel et al., 2018). Moreover, the goal of calibrating crop models has primarily been to find a single acceptable value for each parameter (Alderman and Stanfill, 2017). This approach is problematic, as it neglects the fact that several parameter sets can give equally good fits to the data, a phenomenon referred to as equifinality (Beven, 1993). Following Bayesian theory, a suite of parameter distributions can be used to produce a distribution of outputs instead. In this way, uncertainties in the parameter values are considered (Alderman and Stanfill, 2017). The Generalized Likelihood Uncertainty Estimate method (GLUE) (Beven and Binley, 1992) is an alternative to formal Bayesian methods. It does not rely on statistical assumptions that may not be fulfilled by soil-crop models. Monte Carlo simulation is used to vary the parameters within their "prior" ranges. Then, one or several performance indicators are used to select acceptable parameter sets. A concern with this method is that the choice of performance criteria and the method of combining different criteria introduces subjectivity that influences the results (He et al., 2010). It should be noted that models themselves are to some extent subjective as they are based on a combination of equations, which the developers have chosen to use, not all of which are firmly grounded in proven theory.

CoupModel (Jansson and Karlberg, 2004) is a highly flexible model for soil and vegetation, which was initially especially developed for soil-vegetation ecosystems and prevailing climates in Sweden and Nordic countries. CoupModel takes into account processes related to snow, freezing and thawing, and tile drainage. The latter is estimated to be installed in 49 % of Swedish agricultural land (SCB, 2014). CoupModel and its predecessors (SOIL and SOILN) have been used to study N dynamics in both Sweden and Finland (Aronsson and Torstensson, 1998; Blombäck et al., 2003; Lewan, 1994, 1993; Nykänen et al., 2009; Nylinder et al., 2011; Torstensson and Aronsson, 2000) as well as many contrasting agroecosystems in other climates (e.g. Karlberg et al., 2006; Wu et al., 2019). CoupModel was also applied to study input data resolution effects on crop production in Germany (Constantin et al., 2019; Coucheney et al., 2018; Hoffmann et al., 2015) and recently, to predict future potential yield losses and nitrate leaching for winter wheat (Villa et al., 2022). However, until now the model has only been parameterized and evaluated on field experiments covering limited periods (4–7 years). Long-term predictions and especially climate change impact assessments would benefit from a careful evaluation of soil-vegetation models over periods of at least 20–30 years of field observations related to water and nitrogen flows (Constantin et al., 2012; Yin et al., 2020a). This will help to constrain the model and its parameters, reducing the uncertainty in the predictions and also capturing between-year variations as well as both short-term and long-term feedback under a range of weather conditions.

The aim of this study was to test and evaluate the robustness of a frequently used soil-crop model, CoupModel, from a long-term perspective with a focus on its ability to reproduce harvest, water, and N dynamics in agroecosystems over several decades, based on data and field observations covering 35 years. In particular, we explored between-year variations and potential trends in observed and simulated yields and nitrate leaching. We used the model to simulate and compare the long-term temporal dynamics in nitrogen pools and mineralization in two contrasting treatments, fertilized and unfertilized spring cereals on a sandy loam soil in southern Sweden. Each treatment was calibrated separately to compare potential differences between the systems in terms of posterior distributions of key parameters. The uncertainty in the simulated mineralization of organic N caused by parameter uncertainty was highlighted. Finally, we established and compared the average annual budgets of internal and external N-fluxes for each treatment.

2. Material and methods

2.1. Field site and management

The Mellby field trial (R0–8403) is a part of the Swedish University of Agricultural Sciences program for long-term field experiments (Bergkvist and Öborn, 2011). The field site is located in the southwest of Sweden (lat. 56° 29' N, long. 13° 00' E, alt. 10 m). The climate of the region is cold temperate and semi-humid with a mean annual temperature at the field site of 8.2°C and an annual precipitation of 812 mm (1984–2020 SMHIGridClim (Andersson et al., 2021)). The field site consists of 14 big experimental plots that are 40 × 40 m in size. The treatments were started in 1983 with the main purpose to gain insight into effects of different management practices, including mineral and organic fertilizers and cover crops on nutrient leaching, e.g. for the development of national legislation for agriculture. The topsoil is a sandy loam with a clay content of 5–10 % (Table 1) and an organic matter content of around 5 % at the start of the experiment (Lewan, 1994). The sand deposits (90–130 cm) are underlain by glacio-fluvial clay (Johnsson, 1991) which is more or less impermeable. Each plot is drained individually through tile drainage, with the tiles positioned at 0.9 m depth and spaced 7 m apart. Discard drainage pipes prevent lateral inflow from the surroundings.

Table 1
Soil characteristics and general management at Mellby.

Soil properties					
	Particle size distribution (%)				
	Clay (< 2 μm)	Silt (2–60 μm)	Sand (60 μm-2 mm)	Organic matter content (%)	pH
Topsoil (0–23 cm)	10.4	10.2	79.4	5.9	6.2
Subsoil (23–45 cm)	2.9	2.3	94.9	0.4	5.7
Management					
	Sowing	Fertilization	Harvest	Surface cultivation	Tillage
	April-May	~90 kg N ha^{-1} in spring	Aug-Sep, straw removed	Disc cultivator after harvest	20 cm Nov 4th- Dec 13th

Before the start of the experiment, the field received manure following agricultural praxis in Sweden, estimated at around 10–15 t ha^{-1} (fresh matter) every second to fourth year (Swedish Board of Agriculture, 2001). In this study, treatments supplied with or without mineral N fertilizer were used (not replicated). Spring cereals (wheat, barley, or oats) were grown in most years, with occasional crops of potatoes (3 years), spring oilseed rape (3 years), and triticale (1 year, sown in autumn) (Table S1). The fertilized treatment received 90–110 kg of mineral N ha^{-1} yr^{-1}, while both treatments received 20 kg P and 64 kg K ha^{-1} yr^{-1} until 2009. Thereafter, the unfertilized treatment no longer received P. The crops were sown in April and harvested in August (Table S1). The straw (cereals) was removed, whereas the potato haulm was chemically terminated two weeks before harvest and left in the field. Rapeseed straw was left in the field. The soil was surface cultivated (10–15 cm depth) with a disc cultivator shortly after harvest and plowed between November 4th and December 13th to 20 cm depth. Thereafter the soil was left bare over winter.

2.2. Field measurements and analyses

The drainage water from each plot was directed into an underground measuring station. The flow rate was measured with tipping bucket flow gauges, made of stainless steel with a volume of 4 L. The tips were registered by a pulse generator connected to a data logger, with continuous registration. Total N was measured by grab sampling every two weeks during 1984–1998. Thereafter, flow-proportional water sampling was used. For every 0.2 mm of drainage water entering the measuring station, 15 ml subsamples were pumped into plot-specific bottles. Every two weeks, when there was drainage, the bottles were emptied and water samples were taken and sent for analysis to accredited laboratories at the Swedish University of Agricultural sciences (at the Department of Soil and Environment until 2014 and thereafter to the Department of Aquatic Sciences and Assessment). Unfiltered water samples were used for the determination of total N and NO_3-N (also including NO_2-N) according to European standards (for total N: SIS 028131 until 2009, EN 12260–1 during 2010–2014 and SS-EN 12260–2 from 2014 and for NO_3-N + NO_2-N: SIS 028133–2 until 1997, SS-EN ISO 13395 during 1997–2014 and ISO 15923–1:2013 from 2014). Both total N and NO_3-N were analyzed colorimetrically, total N after oxidization to NO_3-N.

At the beginning of the experiment, both total N and nitrate-N (NO_3-N) were analyzed in the drainage water. Since 2012, only total N was measured. Therefore, a relationship between NO_3-N and total N was established for the data prior to 2012 with linear regression (intercept locked to zero, R^2 0.992, p-value <2.2e-16), to estimate NO_3-N concentrations. NO_3-N was found to be 90 % of the total N in solution. For the period with grab sampling, daily concentrations of total N and NO_3-N were obtained by linear interpolation between sampling events. However, for periods without drainage, e.g. during summer periods, the concentrations of the last sample before drainage ceased were used until the day when drainage stopped. For the period with flow-proportional water sampling, the measured concentration for each sampling period of two weeks was used every day during that period. NO_3-N load was calculated by the daily discharge multiplied by the daily concentration. Mean annual concentrations of NO_3-N were calculated by dividing annual accumulated leached NO_3-N by the annual drainage.

Grain, potato, straw, and haulm (not removed) yields were determined for three replicate samples in each plot with a known harvest area. Samples were dried at 60 °C and total N content was measured with an elemental analyzer (NA 1500 or LECO CNS-2000). We assumed that measured dry biomass consisted of 40 % C (Kröbel et al., 2011).

2.3. Climate data

Model driving data (daily air temperature, precipitation, and air humidity) was retrieved from a gridded database, SMHIGridClim (Andersson et al., 2021), provided by the Swedish Meteorological and Hydrological Institute, with a horizontal resolution of 2.5 km. For wind speed and global radiation, we used ERA5 (Hersbach et al., 2018), which has a horizontal resolution of 0.25° x 0.25° (~28 km). A Mann-Kendall test was performed to check for trends in each variable.

2.4. Model description and model setup

CoupModel version 6.2.5 was used in this study (Jansson and Karlberg, 2004; Jansson, 2012; He et al., 2021). The core of the model is the coupling of two differential equations for heat and water, derived from Fourier's and Darcy's law, respectively. The model structure can be adjusted by the user to suit specific needs through a series of options. Water retention was expressed using the function of Brooks and Corey (Brooks and Corey, 1964) and unsaturated hydraulic conductivity following Mualem (Mualem, 1976). The soil profile was described by 12 layers with thicknesses of 5, 10, 15, 20, and 30 cm at depths of 0–5, 5–15, 15–90, 90–110 and 110–230 cm, respectively. Water flow through the drainage pipes was expressed by the Hooghoudt drainage equation (Hooghoudt, 1940). The bottom layer, which was nearly impermeable, due to the glacio-fluvial clay layer, was represented by a seepage equation (Table S2) where the outflow is given as a function of water table depth and the depth of a theoretical drain depth and spacing. The Penman-Monteith equation (Monteith, 1965) was used to simulate transpiration from the plant cover and for soil evaporation. Partitioning of net radiation between the leaf canopy and soil followed Beer's law. The water and heat flows drive the carbon and nitrogen at every time step. The abiotic environment interacts dynamically with plant growth, which was modeled with an "explicit big leaf" approach. Plant growth is divided into four growth stage indices (GSI), starting with emergence followed by grain filling, maturation, and finally harvest. GSI is either estimated as a function of temperature sums or is given as Julian days by the user. In this study, the sowing, emergence and harvest dates were specified as Julian days. N allocation is controlled by the N demand of the leaf, root, and stem (Table S2). C allocation fractions to roots and leaf were set to constant values. The remaining fraction was allocated to stems. When grain filling starts, C and N is allocated to the grain from all plant compartments.

Harvest of potatoes was simulated in the same way as grains, but the potato haulm was left on the field and plowed down, to account for the green manuring by plant residues. The soil organic C and N were represented by a slow pool (called humus pool in the model), a litter pool, and an inert pool. The litter pool represents fresh organic material and has a higher turnover rate than the slow pool. The soil organic matter (SOM) in the slow pool has a slower turnover rate due to both physical protection and chemical stability of the material. Decomposition is modeled assuming first-order kinetics.

2.5. Parameterization, initialization, and model calibration

Since a predecessor of the CoupModel (SOIL-SOILN, Lewan, 1993; Lewan, 1994 and Blombäck et al., 2003) was applied to the same field site (but for limited periods <7 years and on other plots), we could make use of previous calibrations to set some parameters (Table 2). Values for the Brooks-Corey-Mualem hydraulic parameters in each layer were taken from Lewan (1993) based on Johnsson (1991). Soil samples for C and N measurements were taken in 1988 at 0–30, 30–60, and 60–90 cm depths. We used the average values for each depth, from 10 different plots with different treatments as initial values and used interpolation to make the data compatible with the soil layers used in the model (Table S3). The C/N ratio was 19.2 in the topsoil (0–30 cm), 25.4 at 30–60 cm depth, and 24.2 at 60–90 cm depth. Before the end of the 19th century, the site was most likely a heathland that was grazed and subjected to burning (Frisk and Larsson, 1999), which would explain the unusually high C/N ratio (a value of around 10 is more common in agricultural soils in Sweden; Eriksson et al., 2010). Springob and

Table 2
Key parameters with fixed values during the calibration.

Parameter	Value	Unit	Explanation	References
			1. Crop parameters	
CN LOpt	8.9	-	Optimum C-N ratio in leaves for photosynthesis.	Wu et al., (1998)
CN ratio min Leaf	8	-	CN ratio to calculate N demand	Blombäck et al., (2003)
CN ratio min roots	25	-	CN ratio to calculate N demand	Default
CN ratio min stem	25	-	CN ratio to calculate N demand	Default
Root Mass c1	0.4	-	Fraction of the mobile carbon assimilates allocated to the roots in the response function for nitrogen concentration in leaves.	Salo et al., (2016)
CondRis	5×10^6	J m^{-2} day^{-1}	The global radiation intensity that represents half-light saturation in the light response.	Default
CondVPD	1100	Pa	The vapour pressure deficit that corresponds to a 50 % reduction of stomata conductance	Blombäck et al., (2003)
RespTemQ10Bas	20	°C	Base temperature for the plant respiration at which the response is 1	Johnsson et al., (1987)
WaterCapacityPerLAI	0.2	mm	Interception storage capacity per LAI unit.	Lewan, (1993)
RntLAI	0.5	-	Extinction coefficient	Johnsson and Jansson, (1991)
			2.Litter and respiration	
Eff humus	0.5	-	Efficiency of the decay of humus	Johnsson et al., (1987)
Eff litter	0.5	-	Efficiency of the decay of litter	Johnsson et al., (1987)
RateCoefLitter	0.035	day^{-1}	Rate coefficient for the decay of litter	Default
RateCoefInert	10^{-7}	day^{-1}	Rate coefficient for the inert pool	
			3. Soil parameters	
AlbedoDry,	25	%	Albedo of a dry soil	Lewan, (1993)
AlbedoLeaf	25	%	Albedo of leaf	Lewan, (1993)
DenitNitrateHalfSat	10	mg N L^{-1}	Half saturation constant in function for nitrate concentration effect on denitrification.	Johnsson et al., (1987)
DenitPotentialRate	0.4	g N m^{-2} day^{-1}	The potential rate of denitrification.	Default

Table 2 (*continued*)

Parameter	Value	Unit	Explanation	References
NitrificSpecificRate	0.2	day^{-1}	Nitrification rate under optimal moisture and temperature conditions	Johnsson et al., (1987)
RoughLBareSoilMom	0.01	m	Minimum value of roughness length, valid when the soil is bare	Assumed
Saturation activity	0.6	-	Saturation activity in soil moisture response function.	Johnsson et al., (1987)
T Lmin	5	°C	Threshold temperature for the microbial activity, mineralisation-immobilisation, nitrification and denitrification below which the response is more strong than above and ceases at 0 °C.	Bergström and Johnsson, (1988)

Kirchmann (2002) found that 74.8 % of the SOC at Mellby was HCl-resistant, suggesting that it is highly recalcitrant. They found similar results across a range of soils in northern Europe, which have been under similar historical land management ("plaggen" or heath-land). To account for the fraction of inert SOM, we followed the advice given by Springob and Kirchmann (2010) and considered the active pool to have a C/N ratio of 10 and the inert pool a C/N ratio of 35 (Table S3). The decomposition rate constant for the inert pool, accounting for 71 % of the total SOC and 41 % of the total SON was set to such a low value (10^{-7} day^{-1}) that decomposition was near zero.

To allow the litter pool to stabilize, the first simulated year (1984) was run twice. We supplied the model with all available field management records, including dates of tillage, fertilizer application, sowing, emergence, and harvest (Table S1).

To calibrate the model and to account for parameter uncertainty we selected 16 parameters representing different parts of the agroecosystem that were considered important for this study based on expert knowledge and former model applications (Table 3). The model was run 10,000 times with the parameter values randomly sampled from uniform prior distributions (Table 3). Among the available measurements that we could use to constrain the model, we identified annual total N leaching (g NO_3-N m^{-2}), tile drainage (mm), N content in grain and dry grain yield (g m^{-2}), and total aboveground biomass (dry matter) and N at harvest (g m^{-2}) to be the most important for satisfactory simulations of the two treatments. Calculated leaching of NO_3-N was preferred over measured concentrations due to the method used for water sampling (flow-proportional from 1998) where the NO_3-N concentrations were integrated over sampling periods to get the best possible estimates of the total leaching losses.

The prior ranges of the parameters in the calibration were adjusted until the mean error of the validation variables was as centered around zero as possible. This was to minimize bias in the prior distribution. Bias in the posterior distributions are therefore primarily a result of trade-offs between the different output variables used in the calibration. RMSE was used as an objective function to constrain N transport and drainage based on yearly accumulated data (Table 4). Using RMSE (Eq. 1) on accumulated values has the benefit that daily values are down-weighted while seasonal patterns are still considered. It was not considered important that the model captured the exact timing (day) of N leaching, but rather the cumulative yearly amount. We then used R^2 and ME (Eq. 2) to further improve the fit of grain yield, and aboveground harvest and their respective N content. To evaluate the model performance, the

Table 3
Parameters which were included and varied in the Monte-Carlo calibration procedure.

Parameter	Min/max	unit	Symbol	Function
CLeaftoGrain	0.01/0.04	-	$a_{C,lg}$	Fraction of carbon in leaves reallocated to grains during grain development
CStemtoGrain	0.01/0.04	-	$a_{C,sg}$	Fraction of carbon in stem reallocated to grains during grain development
CNLTh	60/100	-	$p_{CN,Th}$	Threshold above which no photosynthesis occurs
ConductMax	0.01/0.04	$m\ s^{-1}$	g_{max}	The maximal conductance of a fully open stomata
CritThresholdDry	50/200	cm water	Ψ_c	Critical pressure head for reduction of potential water uptake
DrainSpacingLowerB	10/15	m	d_{p2}	Distance between assumed drainage system for calculation of deep percolation.
FlexibilityDegree	0.02/0.6	-	f_{umov}	A compensatory uptake of water will be calculated if a deficiency occurs because of too high water tensions at some layers in the soil profile simultaneously as the water tension is below the critical threshold at other layers
Leafc1	0.3/0.4	-	l_{c1}	Fraction of the mobile carbon assimilates allocated to the new shoots
NLeaftoGrain	0.02/0.05	-	$a_{N,lg}$	Fraction of nitrogen in leaves reallocated to grains during grain development
NStemtoGrain	0.02/0.05	-	$a_{N,sg}$	Nitrogen flux from stem to grain.
NUptFlexibilityDeg	0.2/0.6	-	$n_{Uptflex}$	Compensatory N uptake from layers with excess of N.
RadEfficiency	1.5/3	gDw MJ^{-1}	ε_L	Radiation use efficiency for photosynthesis at optimum temperature, moisture and C-N ratio.
RateCoefHumus	5×10^{-5} /4×10^{-4}	day^{-1}	K_h	Rate coefficient for the decay of humus (slow pool).
LeafMassPerArea	10/20	gC m^{-2}	$P_{l,sp}$	Parameter to convert leaf C mass into leaf area
ThetaLowerRange	5/13	vol%	$P_{\theta Low}$	Water content interval in the soil moisture response function for microbial activity, mineralisation-immobilisation, nitrification and denitrification.
Humfraclitter	0.1/0.3	gC gC^{-1}	$f_{h,l}$	Fraction of carbon and nitrogen contained in the litter pool of the soil that will enter the humus pool

Nash-Sutcliffe model efficiency coefficient (NSE) was used (Eq. 3).

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(yi - \hat{y}i)^2} \quad (1)$$

$$ME = \frac{1}{n}\sum_{i=1}^{n}(\hat{y}i - yi) \quad (2)$$

$$NSE = 1 - \frac{\sum_{i=1}^{n}(yi - \hat{y}i)^2}{\sum_{i=1}^{n}(yi - \bar{y})^2} \quad (3)$$

where n is the total number of measurements, y_i is the measured value for the i^{th} measurement,

$\bar{y}$ is the average of the measured value, and $\hat{y}i$ is the simulated value for the i^{th} measurement.

The 30 best ("accepted") model runs obtained for each treatment were used to compare the mineralization dynamics between treatments and their average annual N budgets. N budgets were calculated based on the mean values of the 30 accepted simulations. A Mann-Kendall test was performed on the mean annual values of the 30 accepted simulations and for the measurements, to test for trends in annual discharge, NO_3-N concentration, NO_3-N leaching, N mineralization, and yield.

3. Results

3.1. Trends in climate data

The Mann-Kendall test was significant ($P < 0.05$) for the average annual temperature, with an increase of 0.06 °C yr^{-1} (Table 5). While all the other climate variables also had positive slopes, none of them were significant.

3.2. Model calibration and model performance

3.2.1. Constrained parameter ranges

The criteria used in the calibration substantially reduced the prior parameter ranges for most parameters (Fig. 1). There were significant differences in parameter ranges between the fertilized and unfertilized treatments for 6 of the 16 parameters. The unfertilized treatment had a higher mean value of the *RateCoefHumus* parameter (K_h) (rate coefficient in the degradation function for organic matter in the slow pool, eq 9 in Table S2), *LeafMassPerArea* ($P_{l,sp}$) (parameter to convert leaf C mass into leaf area, eq 8 in Table S2) as well as *NUptFlexibilityDeg* ($n_{Uptflex}$) (compensatory N uptake from layers with excess of N, eq 7 in Table S2) and *CritThresholdDry* (Ψc) (critical pressure head for reduction of potential water uptake, eq 12 in Table S2). However, *CLeaftoGrain* ($a_{C,lg}$) and *CStemtoGrain* ($a_{C,sg}$) (fraction of carbon in leaves and stem reallocated to grains during grain development, Eq. 1 in Table S2) were higher in the fertilized treatment.

There were some trade-offs in the calibration, which led to certain biases in the posterior distributions (Table 6). In the fertilized treatment, ME was above zero for N total harvest for all the accepted simulations although some candidates in the prior were below zero. In the unfertilized treatment, N total harvest showed less bias. However, ME for N grain was below zero for the vast majority of accepted runs. At the same time, ME for NO_3-N leaching was above zero for all accepted runs. There

Table 4
Threshold limits used in the calibration and their removal efficiency on the total number of simulations (10,000).

Measured variable	Unit	Data points	RMSE max	R^2 min	ME min	max	No. of remaining runs	Efficiency of rejection (%)
Fertilized treatment								
NO_3-N leaching	mg L^{-1}	13134	2	-	−0.0014	0.0014	2907	71
Drainage	mm	13134	50	-	−0.12	0.12	9550	4
Grain yield	g C m^{-2}	36	-	0.4	−100	100	965	90
Aboveground harvest	g C m^{-2}	19	-	-	−125	125	4984	50
N grain harvest	g N m^{-2}	36	-	0.43	−1.2	1.2	2176	78
N total harvest	g N m^{-2}	19	-	-	−2	2	3934	61
Unfertilized treatment								
NO_3-N leaching	mg L^{-1}	13134	0.8		−0.0014	0.0014	3741	63
Drainage	mm	13134	50		−0.12	0.12	9412	6
Grain yield	g C m^{-2}	36	-	0.2	−75	75	3820	62
Aboveground harvest	g C m^{-2}	19	-	-	−100	100	7137	29
N grain harvest	g N m^{-2}	36	-	0.08	−0.4	0.4	199	98
N total harvest	g N m^{-2}	19	-	-	−2	2	9855	1

Table 5
Mann-Kendall trend test of the weather variables for the period 1984–2020. A tau value of one ($\tau = 1$) means that the trend is perfectly monotonous and increasing. Theil Sen's slope represents the trend. Only temperature showed a significant trend ($P < 0.05$).

	Tau (τ)	Theil Sen's slope	P value
Temperature (°C yr^{-1})	0.45	0.06	9.20E−05
Humidity (% day^{-1})	0.192	0.05	0.1
Windspeed (m s^{-1} day^{-1})	0.129	0.003	0.3
Global radiation (J m^{-2} day^{-1})	0.195	10564	0.1
Precipitation (mm yr^{-1})	0.0661	1.3	0.6

were no clear trade-offs between the variables in terms of temporal dynamics, and R^2 generally increased or remained largely unchanged in the posterior distributions except for NO_3-N leaching in the fertilized treatment and N total harvest in the unfertilized treatment.

3.2.2. Discharge, NO_3-N concentration and NO_3-N leaching in drainage water

The model reproduced yearly drainage rather well for both treatments (NSE was 0.67 ± 0.04 and 0.65 ± 0.04 in the fertilized and unfertilized, respectively). However, the model failed to reproduce the unusually high drainage in a few individual years, e.g. in 1988 and 2002 (Fig. 2A).

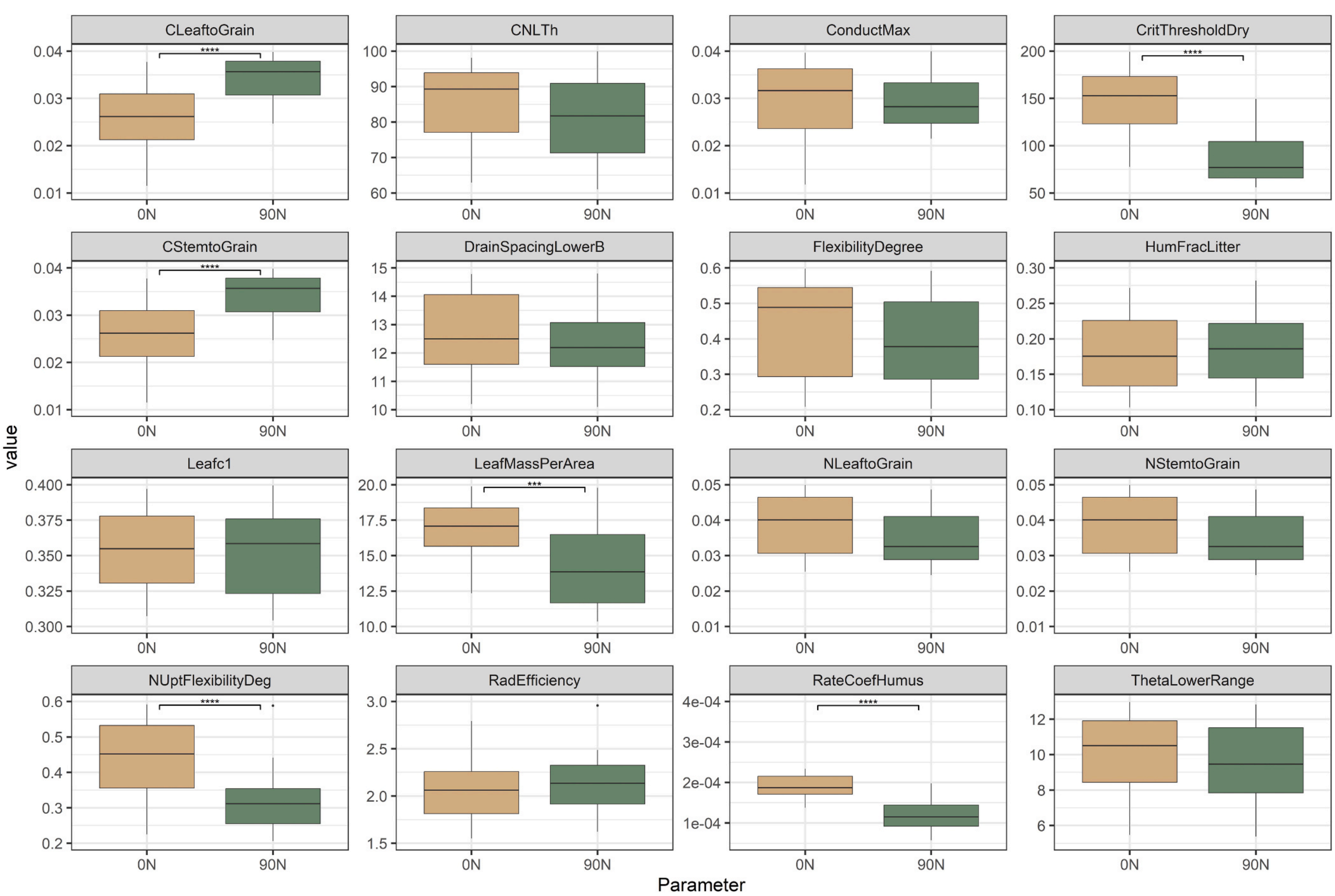

Fig. 1. Posterior ranges and medians of the accepted parameter values included in the Monte-Carlo calibration procedure, for the fertilized (0 N) and unfertilized (90 N) treatments. Vertical lines show the min./max. values of the prior ranges. Significant differences between treatments are represented by stars (****=$p < 10^{-4}$).

Table 6
Model performance based on yearly cumulative values, before and after calibration, for selected output variables.

		Fertilized (90 N)		Unfertilized (0 N)	
Performance index	**Variable**	**Prior**	**Posterior**	**Prior**	**Posterior**
ME	NO_3-N leaching	0.002 ± 0.006	−0.0003 ± 0.001	0.002 ± 0.002	0.001 ± 0.0004
	Drainage	−0.01 ± 0.06	0.02 ± 0.06	−0.003 ± 0.07	−0.03 ± 0.04
	Grain yield	−12.28 ± 143.68	−35.73 ± 41.01	7.03 ± 65.63	7.23 ± 35.18
	Aboveground harvest	50.43 ± 179.85	−39.73 ± 52.95	1.13 ± 90.45	−0.78 ± 34.38
	N grain harvest	−0.03 ± 1.72	−0.39 ± 0.47	−0.44 ± 0.7	−0.25 ± 0.14
	N total harvest	2.36 ± 1.48	1.66 ± 0.26	0.00 ± 0.99	0.12 ± 0.19
R^2	NO_3-N leaching	0.46 ± 0.05	0.42 ± 0.04	0.38 ± 0.05	0.37 ± 0.03
	Drainage	0.82 ± 0.01	0.83 ± 0.01	0.82 ± 0.01	0.81 ± 0.01
	Grain yield	0.34 ± 0.09	0.44 ± 0.02	0.20 ± 0.06	0.24 ± 0.03
	Aboveground harvest	0.09 ± 0.07	0.19 ± 0.05	0.04 ± 0.07	0.04 ± 0.03
	N grain harvest	0.40 ± 0.07	0.46 ± 0.02	0.06 ± 0.02	0.08 ± 0
	N total harvest	0.03 ± 0.03	0.02 ± 0.02	0.06 ± 0.06	0.01 ± 0.02
RMSE	NO_3-N leaching	1.55 ± 0.72	1.25 ± 0.07	0.90 ± 0.27	0.72 ± 0.03
	Drainage	41.55 ± 1.84	40.5 ± 1.31	41.96 ± 2.14	41.83 ± 1.38
	Grain yield	179.8 ± 59.85	123.18 ± 10.65	113.28 ± 23.98	98.58 ± 6.78
	Aboveground harvest	231.50 ± 83.18	160.18 ± 11.6	148.4 ± 31.63	122.45 ± 5.18
	N grain harvest	2.17 ± 0.71	1.52 ± 0.11	1.31 ± 0.26	1.06 ± 0.03
	N total harvest	3.05 ± 1.1	2.18 ± 0.21	1.68 ± 0.3	1.35 ± 0.03

The ensemble mean of simulated annual NO_3-N -concentrations in drainage water from the fertilized treatment was generally below the annual average of observed concentrations (10.81 ± 1.2 compared to 13.1 mg L^{-1}). On the contrary, the ensemble mean concentration for the unfertilized treatment was systematically higher than the observed mean (7.69 ± 0.73 compared to 6.53 mg L^{-1}). The between-year variations in annual mean NO_3-N concentrations were not very well reproduced by the model and NSE was negative for both treatments (-0.36 ± 0.24 and −0.08 ± 0.25 in the fertilized and unfertilized treatments respectively), see also Fig. 2B.

The observed annual NO_3-N leaching was on average more than twice as high in the fertilized treatment compared to the unfertilized over the whole period (3.7 compared to 1.8 g NO_3-N m^{-2} yr^{-1}). The corresponding ensemble mean of the simulated annual NO_3-N leaching for the fertilized and unfertilized treatments were 2.7 ± 0.3 and 1.9 ± 0.1 g NO_3-N m^{-2} yr^{-1}, respectively). The between-year variation in average annual nitrate concentrations was better captured for the unfertilized treatment compared to the fertilized (NSE was 0.12 ± 0.07 and-0.03 ± 0.12, respectively), Fig. 2C.

The summer of 2018 was exceptionally dry, with only 9.5 mm of rainfall in May, 25.7 mm in June, and 6.8 mm in July. Interestingly, all accepted model runs reproduced the annual NO_3-N leaching well in both 2018 and the following year in both treatments. This indicates that the model captured a carry-over effect in terms of high NO_3-N concentrations and leaching early in 2019, in response to the extremely dry summer and thus poor N uptake by the crop in 2018.

3.2.3. Trends in NO_3-N leaching, drainage and NO_3-N concentration

No significant trend in drainage was detected in the measurements or simulations for any of the treatments. The measured NO_3-N leaching showed a small, yet significant, decrease in both treatments and Sen's slope was −0.09 and −0.05 g NO_3-N m^{-2} yr^{-1} in the fertilized and unfertilized treatments, respectively. In the simulations, there were no significant trends for NO_3-N leaching. All simulations and measurements showed a significant decrease in mean annual NO_3-N concentration in both treatments. In the fertilized treatment, Sen's slope was −0.24 mg L^{-1} yr^{-1} for the measurements and on average −0.12 ± 0.04 mg L^{-1} yr^{-1} for the simulations. In the unfertilized treatment, Sen's slope was −0.23 mg L^{-1} yr^{-1} for the measurements and on average −0.1 ± 0.02 mg L^{-1} yr^{-1} for the simulations.

3.2.4. Grain yield and N grain

The measured grain yield was on average 2.2 times larger in the fertilized treatment (408 compared to 188 g m^{-2}). Similarly, the N in the harvested grain (N grain) was 2.6 times larger in the fertilized treatment (6.6 compared to 2.5 g N m^{-2}) (Fig. 3). The mean simulated grain yield was slightly overestimated for both treatments (455 ± 70 and 200 ± 35 g m^{-2} in the fertilized and unfertilized, respectively). The mean simulated N grain was slightly overestimated for the fertilized and slightly underestimated for the unfertilized (6.8 ± 0.6 and 2.3 ± 0.15 g N m^{-2} for the fertilized and unfertilized, respectively). The between-year variations in grain yield and N grain were better captured for the fertilized treatment (Table 6). In 2005, when triticale was grown, the observed harvest was surprisingly high in the unfertilized treatment but remained at a normal level in the fertilized treatment. In 1995 when rapeseed was grown, the observed harvest was exceptionally low in the unfertilized treatment. Observed N grain showed a small but significant downward trend (Sen's slope was −0.07 g N m^{-2} yr^{-1}) for the fertilized treatment. Only four of the model runs showed a significant trend (Sen's slope was −0.03 g N m^{-2} yr^{-1}). The simulations also indicated a weak but significant trend in N grain for the unfertilized treatment (Sen's slope −0.01 g N m^{-2} yr^{-1}). Grain yield showed a decreasing trend only in two simulations for the fertilized treatment (Sen's slope −2.25 g m^{-2} yr^{-1}). For the unfertilized treatment, all simulations showed a significant downward trend (Sen's slope was −2.1 g m^{-2} yr^{-1}).

3.2.5. Below-ground allocation of dry matter and N

The simulated dry matter and N allocated below-ground were slightly higher in the unfertilized treatment compared to the fertilized treatment. The percentage of total dry matter found in the roots at the time of harvest was 27 ± 2 % in the fertilized treatment and 29 ± 1 % in the unfertilized treatment. The corresponding values for N were 30 ± 3 % and 33.3 ± 3 % for the fertilized and unfertilized treatments, respectively.

3.3. Evolution of soil organic N and annual N mineralization

Soil organic N (SON) declined in all simulations for the unfertilized and in 23 of 30 model runs for the fertilized treatment (Fig. 4). According to the simulations, the change in SON by mineralization during the whole period was −8.8 ± 14.7 and −121.4 ± 11.3 g N m^{-2} in the fertilized and unfertilized treatment respectively.

The fertilized treatment showed a higher uncertainty in the simulated annual N mineralization. The difference between the minimum and maximum values varied between 2.5 and 5.6 g N m^{-2} yr^{-1} compared to 1.7–3.4 g N m^{-2} yr^{-1} in the unfertilized treatment (Fig. 5). There was a substantial overlap with the range obtained for the unfertilized treatment. Nevertheless, the fertilized treatment showed

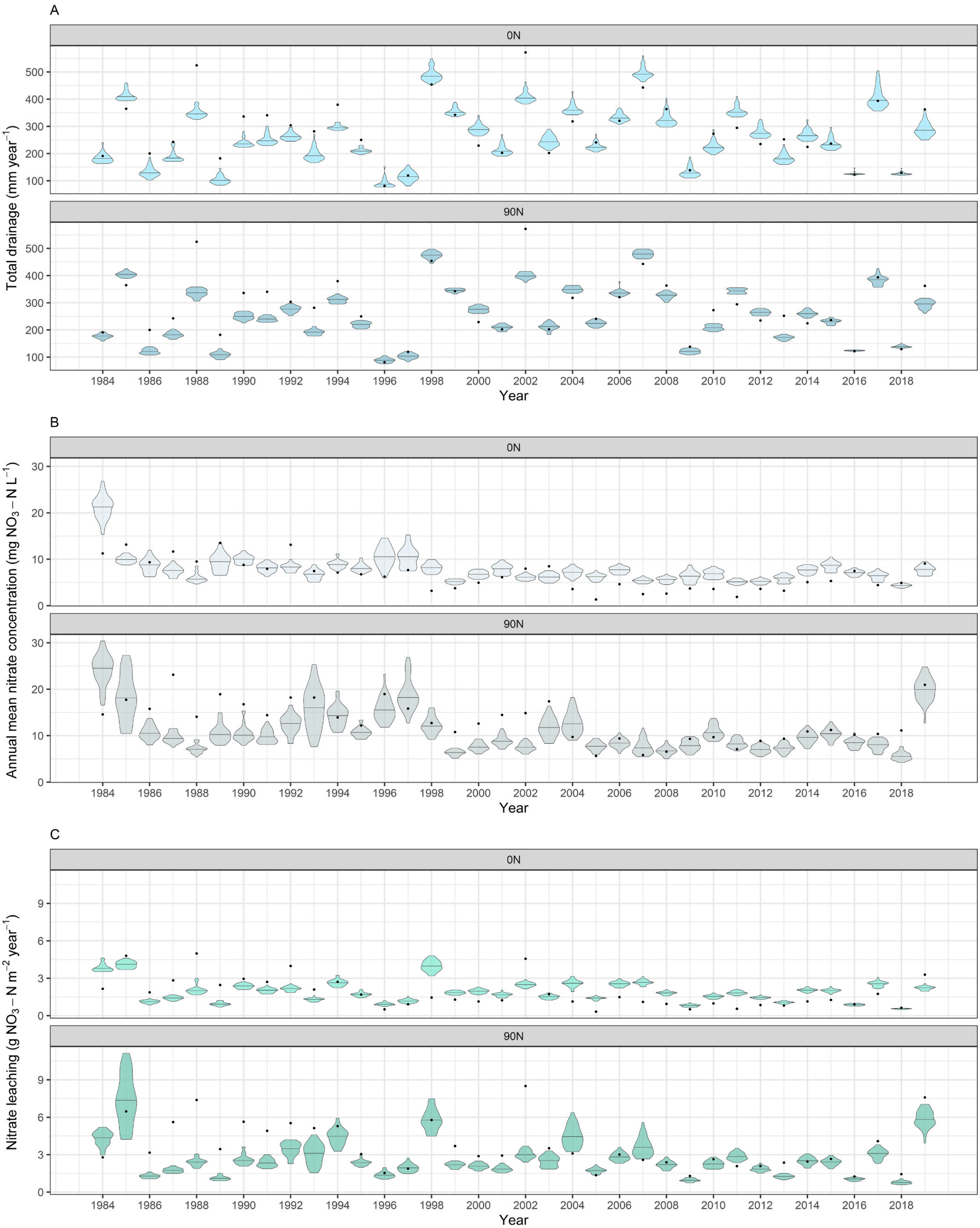

Fig. 2. Annual total drainage (mm yr^{-1}) (A), annual mean nitrate concentration (mg NO_3-N L^{-1}) (B), and annual nitrate leaching in the drainage water (g NO_3-N m^{-2}) (C) for the fertilized (90 N) and unfertilized (0N) treatments , 1984–2019. Dots represent values based on observations and the violin plots represent the results from the 30 best/accepted model-runs for each treatment. The horizontal line is the median value.

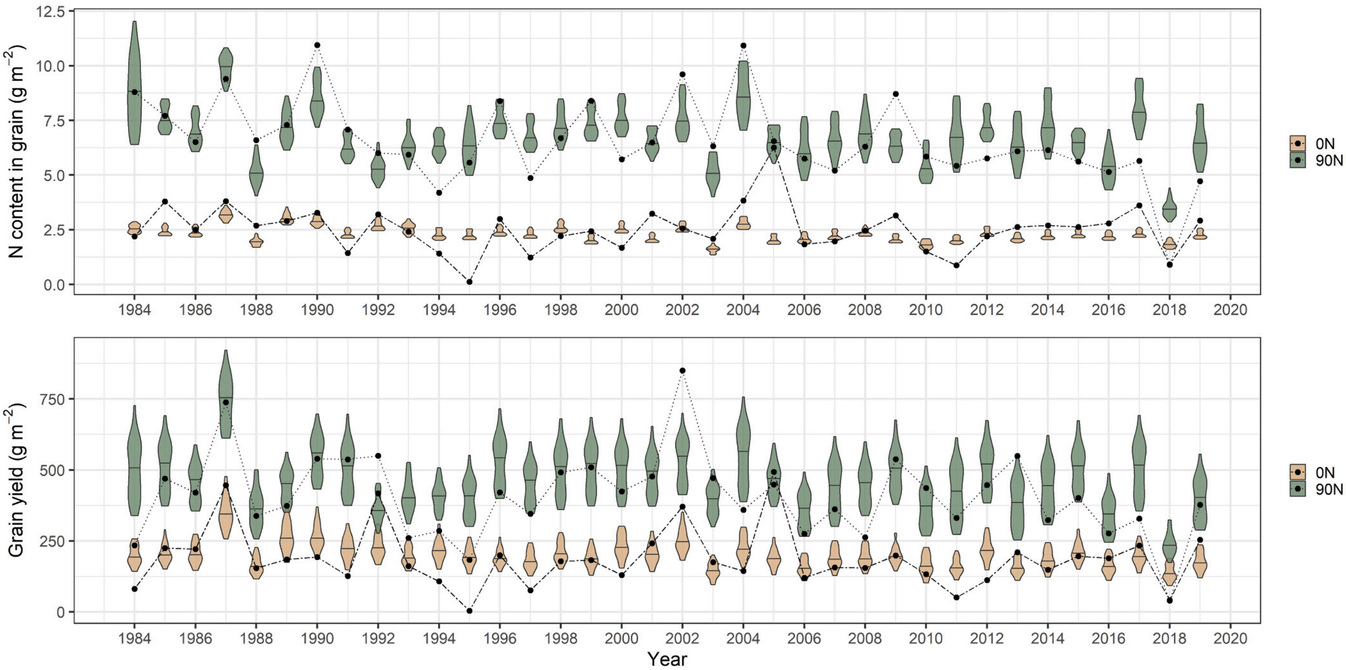

Fig. 3. Yield (g m^{-2}) and nitrogen content (g N m^{-2}) in the harvested grains/tubers/seeds for the fertilized (90 N) and unfertilized (0 N) treatments. Dots represent observations and violin plots represent the results from the 30 best/accepted model-runs for each treatment. The horizontal line is the median value.

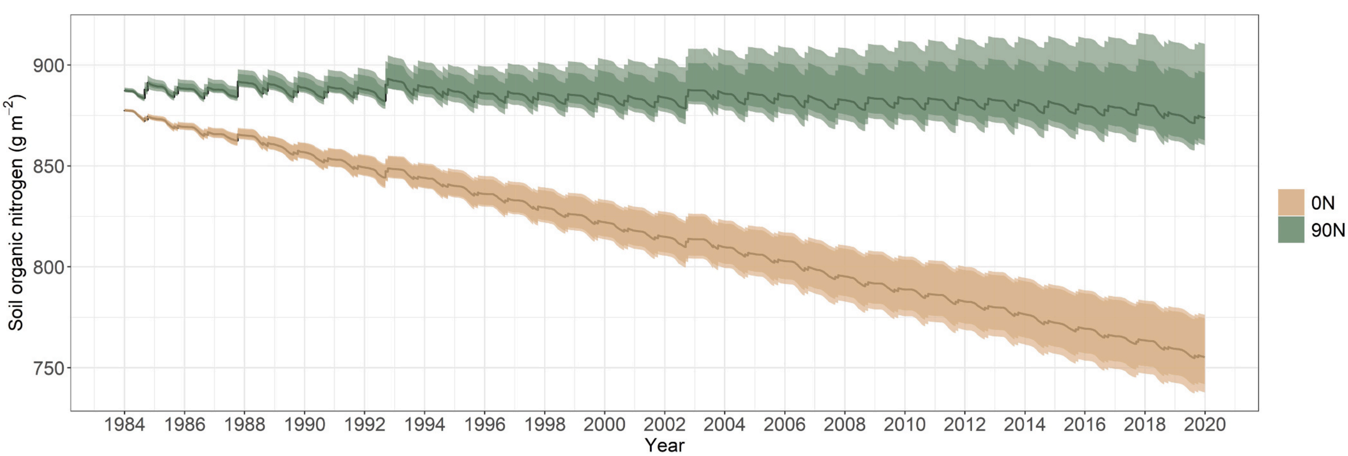

Fig. 4. Simulated soil organic nitrogen (g m^{-2}) for the unfertilized (0 N) and fertilized (90 N) treatments (1984–2019), with median (thick line) and 50 and 95 % uncertainty bands, based on the 30 best/accepted model runs for each treatment.

consistently higher median values. This was especially true for the years following a potato crop (1988, 1993, 2003). In the fertilized treatment, there was no significant trend in the annual total N mineralization. In the unfertilized treatment, there was a decreasing trend in 21 of the accepted model runs, and Sen's slope was -0.02 g N m^{-2} yr^{-1}. The model thus indicates that 0.7 g m^{-2} less N is mineralized per year after 35 years in the unfertilized treatment.

3.4. Simulated mean annual nitrogen balance

Simulated yearly N balances were negative for both treatments (Table 7). The export of N by nitrate leaching was on average 1.4 times larger in the fertilized plots compared with the unfertilized. However, the yield-scaled losses (N leached per unit of N harvested) were larger in the unfertilized treatment than in the fertilized (0.57 compared to 0.29 g N/ g N) due to the smaller yields. The simulated total harvested N (straw and seed) was 2.8 times greater in the fertilized treatment (Table 7). Table 7 also shows that the amount of N lost by deep leaching (nitrate that passes the depth of tile drains) and denitrification was small and similar in both treatments. In the fertilized treatment, more organic N entered both the slow pool (humus formation) and the litter pool, while less N was mineralized from the slow pool compared to the unfertilized treatment. More litter was also produced, both above- and below-ground. However, litter mineralization was also higher in the fertilized treatment (Table 7).

4. Discussion

In this study, we tested and evaluated the performance of a frequently used soil-vegetation model (CoupModel) with respect to two contrasting fertilization treatments in southern Sweden, over a 35-year time period which also covered a significant trend in temperature of 0.06 °C yr^{-1} and one growing season with unusually high temperatures and extremely low rainfall (2018). The model was separately calibrated

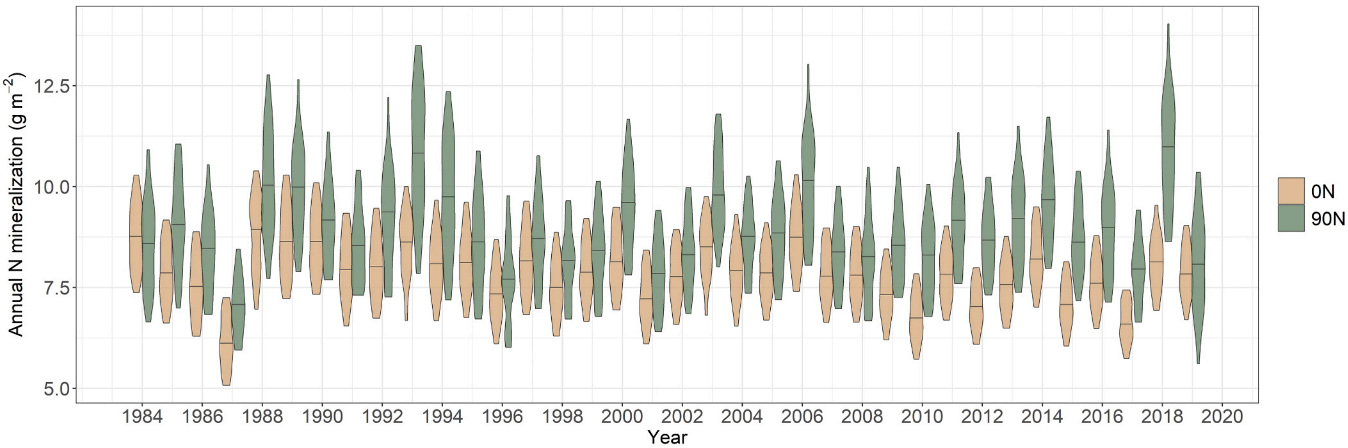

Fig. 5. Simulated annual N mineralization (g m^{-2}) for the fertilized (90 N) and unfertilized (0 N) treatments. Violin plots show the distributions of results from the 30 best/accepted model-runs for each of the treatments. The horizontal line is the median value of the ensemble.

Table 7
Yearly N balance (g N m^{-2}) calculated from the ensemble of the 30 best/accepted model runs for the fertilized and unfertilized treatment (90 N and 0 N), based on 35 years (1984–2019).

		Fertilized (90 N)	**Unfertilized (0 N)**
Input	Fertilization	10.32	0
	Deposition	1.53 ± 0.004	1.52 ± 0.004
	Seeds	0.53	0.53
Σ		**12.35 ± 0.03**	**2.06 ± 0.004**
Export	Nitrogen Harvest	−9.64 ± 0.33	−3.46 ± 0.2
	Min N Leaching	−2.75 ± 0.32	−2.03 ± 0.13
	Deep N leaching	−0.16 ± 0.03	−0.16 ± 0.03
	Denitrification	−0.2 ± 0.01	−0.18 ± 0.01
Σ		**−12.74 ± 0.41**	**−5.83 ± 0.32**
Storage			
	Soil organic N	−0.28 ± 0.42	−3.48 ± 0.32
	Mineral N	−0.23 ± 0.02	−0.30 ± 0.02
Σ		**−0.51 ± 0.42**	**−3.78 ± 0.32**
Organic transformation			
	Humus formation	3.54 ± 0.99	2.23 ± 0.6
	Humus mineralisation	−3.76 ± 1.09	−5.59 ± 0.77
	Aboveground input to litter	2.24 ± 0.38	1.62 ± 0.19
	Belowground input to litter	6.70 ± 0.64	2.96 ± 0.31
	Litter mineralisation	−5.13 ± 0.92	−2.20 ± 0.57

on data from each of the treatments (spring cereals on sandy soil, with and without N fertilizer). The obtained differences between the treatments in key parameter values and simulated outputs are discussed below with a focus on long-term crop yields, nitrate leaching, and soil nitrogen dynamics.

4.1. Grain yield and N grain

No significant trends were identified in observed grain yield or N in harvested grain in the unfertilized treatment. Generally, it seems that after an initial drop in yield of about 250 g m^{-2}, the unfertilized system was able to sustain this lower yield level for a considerable time (>30 years) as a consequence of the mineralization of organic N. In contrast, the model simulations did suggest a small decreasing trend for both grain yield and N in grain in the unfertilized treatment due to the decreasing trend in net N mineralization. That this trend was not significant in the observations may be due to additional factors affecting yields in individual years that are not accounted for by the model (e.g. pathogens, pests, and diseases (Bregaglio et al., 2021)).

The model reproduced a reduction in yield observed in both treatments in 2018 due to extremely low rainfall amounts and high temperatures during the growing season, although the extent of the reduction was not as great as in the measurements (65–223 g m^{-2} in the simulations compared to 150–379 g m^{-2} in the measurements). There may be several reasons for this, but a plausible explanation is that the model underestimated the effects of combined water and heat stress or that it does not consider certain plant responses to water or heat stress, such as an earlier onset of heading and flowering. Improving predictions of phenology as a function of climate is therefore an important task for future research (Wallach et al., 2023).

4.2. Results of the calibration

The calibration resulted in significant differences between the two treatments in the posterior values and ranges of some critical parameters. The smaller value of *LeafMassPerArea* indicates thinner leaves following N fertilization, which is supported by previous studies (e.g. Knops and Reinhart, 2000). To reproduce the observed yields, *CleaftoGrain and CStemtoGrain* were required to be higher in the fertilized treatment, while *CritThresholdDry and NUptFlexibilityDeg* were lower. The model thus suggests, as expected, that the crop in the fertilized treatment shows less sensitivity to N stress. At the same time, the fertilized treatment showed a higher sensitivity to water stress (lower *CritThresholdDry)* which might be consistent with a higher transpiration rate from a larger leaf area and above ground biomass.

CoupModel does not come with any ready-to-use crop-specific parameterizations that are included in other models such as APSIM and STICS (Brisson et al., 2009; Keating et al., 2003). Such templates are typically developed from detailed field experiments with measurements of several phenological variables. However, such field experiments are scarce at higher latitudes, where both growing conditions and cultivars differ (Kumar et al., 2021). In this regard, allowing key allocation parameters to vary during calibration was seen as a viable alternative. Indeed, crop yields during the 35 years were reproduced with satisfactory accuracy by the mean of the 30 best simulations in both fertilized and unfertilized treatments, even though we did not distinguish between crops, other than the fact that potato haulm was left on the field. This simplification most likely contributed to some of the deviations between the simulated and measured yields in single years (Fig. 3). Furthermore, the allocation coefficients and critical N concentrations were kept constant during the growing season which caused the stem to have a lower C/N ratio at the time of harvest than is normal for spring cereals (30 and 50 for the fertilized and unfertilized, respectively). This was likely the reason behind the trade-offs between N total harvest, N grain, and nitrate leaching seen in the calibration (Table 6). The allocation of C and N to roots may also have been an important source of error in the simulations. Hansson et al. (1987) found root biomass at harvest for a barley crop to be 16 % and 23 % of total biomass and N in roots to be 21 % and 28 % of total N content for a fertilized (120 kg N/ha) and unfertilized treatment, respectively. The simulated values for root biomass obtained in this study (27 $\pm$ 2 % and 29 $\pm$ 1 % of total biomass) and N in roots (30 $\pm$ 3 % and 33 $\pm$ 3 % of total N content for the fertilized and unfertilized, respectively) thus seem to be at the higher end for both root biomass and N. Future model applications would benefit from the development of crop-specific allocation patterns based on datasets that contain more data on root biomass and phenology.

4.3. Drainage and nitrate leaching

The calibrated model simulated drainage and nitrate leaching satisfactorily for both treatments in most years (Fig. 2). In the first 11 years, the observed nitrate leaching in the unfertilized treatment was systematically higher compared with the subsequent years. This may be due to the history of the field site where farmyard manure had been applied for a long time. Additionally, until 1998, grab sampling was used instead of flow proportional sampling. Grab sampling has been found to give higher N concentrations (Stone et al., 2000). This change in measurement method may have caused a trade-off between the two periods in the parameterization of the model.

4.4. Soil organic nitrogen dynamics

The model indicates a faster degradation of organic matter (a higher value for the parameter *RateCoefHumus*) in the unfertilized treatment compared to the treatment supplied with mineral fertilizer (Fig. 1 & Figs. 4–5). This may indicate a difference in the composition and type or function of microbial communities between the two treatments. Spohn et al. (2016) found that N fertilization reduced microbial respiration in a temperate grassland in Austria. Similarly, Janssens et al. (2010) found a decrease in forest soil respiration following N deposition. N fertilization may increase the relative contribution of root-derived C to microbial biomass and reduce soil organic matter losses (Zang et al., 2017) as well as promote conversion of mineral N to organic N (Liang et al., 2022). The *RateCoefHumus* parameter was relatively well-constrained in both treatments (Fig. 1). However, in the fertilized treatment there was a larger spread in simulated mineralization and the development of SON was less certain, and positive instead of negative for seven of the accepted model runs (Figs. 4–5). This was likely because the variables used for the calibration were not as sensitive in the fertilized treatment as in the unfertilized. Adding mineral fertilizer to the system thus allowed for a broader range of parameter value combinations, and will therefore require additional types of observations to constrain the model efficiently. Calibration against reliable estimates of SOC or SON, which are often missing in many field studies, would be necessary to further constrain the mineralization. Large uncertainties in the simulation of N mineralization were also found in a model comparison study in northern France (Yin et al., 2020b). Thus, both model uncertainty and parameter uncertainty might contribute to the overall uncertainty in modeled mineralization of nitrogen in arable soils, which makes predictions of N mineralization in response to changed management or climate highly uncertain, despite calibration against long-term data sets including key variables such as yield and nitrate leaching.

The high C/N ratio (varying from 19 to 25) at the field site posed a challenge for the initialization of the organic pools. We opted for the recommendation given by Springob and Kirchmann (2010) and considered the slow pool to have a C/N of 10 and the inert pool a C/N ratio of 35. The parameter *CN microbe*, representing the C/N ratio of microbial biomass and "humified" products was set to its default value of 10. With this setup, the C/N ratio of the slow pool did not change over time. Assuming an additional pool to be inert as was done here, seems to be a good solution for this type of old heathland soil. However, other solutions might be required for soils with high C/N originating from other land use histories, and thereby other types of particulate organic matter.

5. Conclusions

Long-term field measurements of yield and nitrate leaching in fertilized and unfertilized cropping systems provided robust support for the calibration of a process-oriented agroecosystem model with respect to a period covering a systematic trend in the climate (air temperature) as well as an extreme year (2018) with severe drought. It allowed us to establish and compare the budgets of internal and external fluxes of nitrogen in the two systems over more than three decades and also to identify where the model structure and parameterization could be improved.

Yields, drainage, and nitrate leaching were generally well captured by the model during the 35 years. The model simulated substantial yield reductions in the severe drought year of 2018 in both treatments, although not to the extent indicated by the measurements. This highlights the importance of model testing and model improvements to accurately account for the combined impact of both water and heat stress on crop yields in exceptionally hot and dry years. Moreover, our study suggests that the representation of year-to-year variations could be improved by developing crop-specific parameterizations in CoupModel, in particular with respect to phenology and the allocation of assimilate to above- and below-ground biomass.

Separate long-term calibrations of the fertilized and unfertilized cropping systems resulted in substantially different posterior parameter means and ranges for some key parameters, for example, the decomposition rate constant for the slow organic pool, the leaf mass per area, and nitrogen uptake flexibility. We conclude that changes in soil and crop management can trigger changes in key functions of the system, especially in the long-term, which are currently not considered by the model, for example, the composition and function of microbial populations in the soil. This means that we cannot assume that model parameter values will remain unchanged when the management of an agricultural system changes. It remains a challenge to include these kinds of feedback responses in soil-crop models in a sufficiently parsimonious way.

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CRediT authorship contribution statement

Nimblad Svensson David: Writing – original draft, Visualization, Software, Methodology, Formal analysis, Data curation. **Aronsson Helena:** Writing – review & editing, Supervision, Investigation, Funding acquisition, Data curation. **Jansson Per-Erik:** Writing – review & editing, Software, Methodology. **Lewan Elisabet:** Writing – review & editing, Supervision, Project administration, Methodology, Funding acquisition, Conceptualization.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.fcr.2025.109856.

Data availability

Data will be made available on request.

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