



Spatial variability of soil properties, nitrogen balance and nitrate leaching using digital methods on heterogeneous arable fields in southern Germany

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Accepted: 5 October 2022 / Published online: 10 November 2022
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Abstract

In this study, the spatial variability of nitrogen (N) balances and potential nitrate leaching were determined in heterogeneous arable fields in southern Germany using digital methods (tractor-mounted multispectral sensor, satellite data, vegetation indices and models) and measurements of nitrate stocks in deeper zones (1–2.5 m soil depth) with deep drilling. The aim of this study was to achieve precise localisation of N losses at high spatial resolution (sub field level; 10×10 m grid). The spatial variability of plant parameters within uniformly fertilised fields (crop yield, N uptake) was determined for the calculation of the N balances. The spatial variability of soil properties (e.g. soil organic carbon content, soil total nitrogen content) were determined to identify the causes of high or low N surpluses and nitrate leaching in sub-fields. N surplus determined using different digital methods and measured nitrate stocks showed similar spatial patterns. Site-specific N balancing identified zones with high N loss potential (N surplus up to 86 kg ha⁻¹). Deep drilling showed zones with high nitrate loss (nitrate N up to 94 kg ha⁻¹). N surplus and nitrate loss correlated with $r=0.49$. This relationship could be impacted by many other soil and management factors. Soil properties showed considerable spatial variation within the fields. Soil organic carbon (SOC) and soil total nitrogen (TN) content were closely correlated in all fields (up to $r=0.96$) and were most closely positively correlated with crop yield and N uptake (up to $r=0.74$) and negatively correlated with N surplus (up to $r=-0.73$). The sensor data and satellite data (crop yield, N uptake, N surplus) showed similar distribution patterns. Based on these results, digital technologies are suitable for the calculation of site-specific N surplus and estimation of nitrate leaching risk. Satellite or sensor based site-specific and yield-oriented fertilization is one approach to reduce N surplus on sub fields with low yield potential and high nitrate leaching risk.

Keywords Spatial variability · Nitrate leaching · Nitrogen surplus · Satellite data · Multispectral sensor · Deep drilling

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Introduction

Nitrate leaching

Excessive nitrate leaching on cropland endangers ground and drinking water. In Germany, 26.7% of near-surface groundwater bodies exceed the maximum threshold value of 50 mg nitrate per litre (BMEL and BMU 2020). In Germany, the nitrate concentration in groundwater has hardly changed in the last decade (BMEL and BMU 2017, 2020; Sundermann et al., 2020); there are also massive problems with high nitrate losses in other European regions with intensive agriculture (Hansen et al., 2012; Oenema et al., 2004; Wang & Li, 2019). Most of the nitrate input into groundwater is derived from agriculture (Biernat et al., 2020; Sutton et al., 2011).

To solve the nitrate problem, the legal regulations on fertilisation have been tightened several times (Kanter et al., 2020; Kielhorn et al., 2013; Wolters et al., 2021). In particular, in endangered regions in Germany with high levels of nitrate in the groundwater (so-called ‘red areas’), the N fertilisation is limited to 80% of the N fertilisation requirement for the targeted yield (Kirschke et al., 2019).

Further measures have been taken to reduce nitrate leaching. These include crop rotations (soil cover, intercropping), tillage and N fertilisation or measuring soil mineral nitrogen (SMN) stocks in autumn before the beginning of the leaching period (Strebel et al., 1989). Small-scale variability in soil properties, yield potential, and leaching risks have not yet been adequately considered in drinking water protection (Xin et al., 2021).

Research needs

Nitrate losses can be analysed on different spatial scales from the sub-field (10^2 – 10^4 m²) and field (10^4 – 10^6 m²) via the farm (10^5 – 10^7 m²) to drinking water protection areas (10^6 – 10^8 m²) (Schröder et al., 2003). Water protection areas or groundwater bodies are the appropriate level of investigation, if the effects of different land use systems (grassland, cropland, permanent crops, forest), site conditions (Beaudoin et al., 2005), aquifers and denitrification conditions (Cremer et al., 2018) on the nitrate content of a groundwater body are to be analysed (Bechtel, 2008). At the farm level, relationships between farm structures (crop rotation, animal stocking (Hülsbergen et al., 2017), farming systems (Biernat et al., 2020; Drinkwater et al., 1998; Funk et al., 1995) and nitrate losses can be examined. The field level is suited to the investigation of the effects of crop cultivation measures (crop rotation) (Askegaard et al., 2005), catch crops (Tribouillois et al., 2016; Constantin et al., 2010; Tonitto et al., 2006), fertilisation (Perego et al., 2012; Schmidhalter, 2011) and tillage (Hansen et al., 2010; Spiess et al., 2020)) on nitrate leaching.

So far, the sub-field level has received little attention in the analysis of nitrate losses in on-field research, although field variability is known. Kielhorn et al. (2013) modelled the site-specific risk for leaching based on soil data (soil texture, bulk density, humus content and field capacity in the root zone). Hülsbergen et al. (2020) and Mittermayer et al. (2022) analysed nitrogen balances on heterogeneous fields, and found higher nitrogen surpluses in low-yield zones than in high-yield zones. Nitrogen surplus

is used as an indicator of nitrogen losses (Arauzo et al., 2019; Compton et al., 2021; Ju et al., 2006) e.g. nitrate leaching (Zhou & Butterbach-Bahl, 2014; Perego et al., 2012). Thus, increased nitrogen surpluses in low-yield zones could lead to increased nitrate leaching in this areas.

Based on these results, this study focuses on the variability of nitrogen balance and nitrate leaching within uniformly managed fields and their importance in drinking water protection (10×10 m grid).

Modern technologies e.g. the satellite- or sensor-supported reflectance measurement (Finger et al., 2019) enable site specific modelling and calculating of plant parameters. Owing to the advancing digitalisation of crop production, increasing amounts of soil, plant and process data are measured digitally and georeferenced. The question is whether this data can be used to:

- (1) determine the risk of nitrate leaching at the sub-field level and;
- (2) derive measures to reduce nitrate leaching precisely, e.g. site-specific fertilisation.

Study aims

In this study, the relationship between the spatial variability of the N balance as an indicator of nitrogen losses on cropland and nitrate leaching was investigated with a high spatial resolution (10×10 m) in the Burgkirchen water protection area (located 100 km east of Munich). The area is characterised by high N surpluses in agriculture (caused by high animal stocking density in combination with biogas plants), high and rising nitrate levels in the groundwater (>40 mg nitrate litre⁻¹) (Hülsbergen et al., 2022) therefore, in 2020, the region was classified as a 'red area' (LfL and LfU Bayern 2020) associated with restrictions on fertilisation.

The analysis was performed using digital methods for recording plant parameters (tractor-mounted multispectral sensor, vegetation indices, algorithms, satellite data and models) in combination with georeferenced measurement data. The choice of technologies is based on previous studies comparing and validating different digital methods (reflectance measurements from tractor-mounted sensors and satellite data, yield sensing systems for combine harvesters) with ground truth data (yield, N uptake, N surplus) (Mittermayer et al., 2021, 2022).

Based on the current state of knowledge, the following hypotheses were formulated:

- (1) On heterogeneous fields with uniform fertilization, high, environmentally hazardous N surpluses can occur in low-yield zones.
- (2) Site-specific N surplus determined with digital methods is a suitable indicator for nitrate leaching. The N surplus correlates closely with the nitrate stocks in the soil layer 0–2.5 m.
- (3) The spatial distribution of soil organic carbon and soil total nitrogen content are closely related to the spatial distribution of N surpluses and nitrate stocks.

The studies are intended to provide new scientific insights into the variability of nitrogen losses and nitrate leaching within uniformly managed croplands and could provide a basis for new approaches to drinking water protection using digital technologies.

Materials and methods

Site and weather conditions

The investigations were performed on arable fields in a water protection area (48° 16' 56" N 12° 82' 51" E, 450 m a.s.l.) as part of the digisens¹ research project.

The mean annual precipitation (1996–2020) of the site is 870 mm per year and the mean annual temperature is 8.9 °C (online resource 6). Sensor data and ground truth data (soil samples, deep drillings) were measured in 2020, satellite data was recorded in the years 2018 to 2020. The years 2018 and 2019 were characterised by a warm, dry spring. Although cooler temperatures prevailed in May in 2019 and more than 150 mm of precipitation fell, in 2019 it remained warm and dry, above average in the summer months. The research year 2020 was characterised by a dry spring and a wet summer. The temperatures were 0.9 °C above the long-term average. The leachate rates vary from about 280 mm in the dry and warm year 2018 to over 390 mm in the rainy year 2020.

The fields under investigation were located in the Alzplatte, an area in southern Bavaria, which is characterised by thick loess-loam blankets with a low-to-high percentage of mineral fragments over 2 mm in size. The varying proportion of these mineral fragments cause differences in available water capacity (AWC). The soils were cambisols of medium quality (Online resource 1).

Choice of location and crop production

In the study region, two investigation fields were selected according to the criteria for size, crop rotation, fertilisation and soil properties. The fields were over 5 hectares in size, had the same crop rotation (maize (2018)—soybeans (2019)—winter wheat (2020)), were managed uniformly for many years. The study fields were regularly fertilised with high amounts of manure over many years, in accordance with the high animal stocking rates of the study farms [1.5 and 2.25 LU ha⁻¹] (Online resource 1). During the study period, the N supply with organic fertiliser to silage maize was 84 kg ha⁻¹ (Field A) and 126 kg ha⁻¹ (Field B) and to winter wheat 63 kg ha⁻¹ (Field A) and 129 kg ha⁻¹ (Field B) (Online Resource 2). The mineral fertilisation varied depending on the type of crop and the yield target and was applied in accordance with the specifications of the Fertiliser Ordinance. No nitrogen fertiliser was used in the cultivation of soybeans (test year 2019) (Online Resource 2). The heterogeneity of the fields was determined from biomass potential maps (Fig. 1). These maps describe the relative differences in yield potential based on the vegetation index NDVI (normalized difference vegetation index) (Hansen & Schjoerring, 2003), which was measured with satellite data in 2018, 2019 and 2020. The fertilisation of the investigation fields in the years 2018 to 2020 can be found in online resource 2.

Methods of determining plant variables

Satellite data from sentinel 2 and the PROMET model (Mauser & Bach, 2009) provide a methodological basis for analysing the spatial variability of corn, soybean, and wheat

¹ Research project 'Reduction of nitrate leaching through digital nitrogen management and sensor-based fertilization in the model region Burghausen/Burgkirchen', funded by the Bavarian State Ministry for Food and Agriculture (2020–2022).

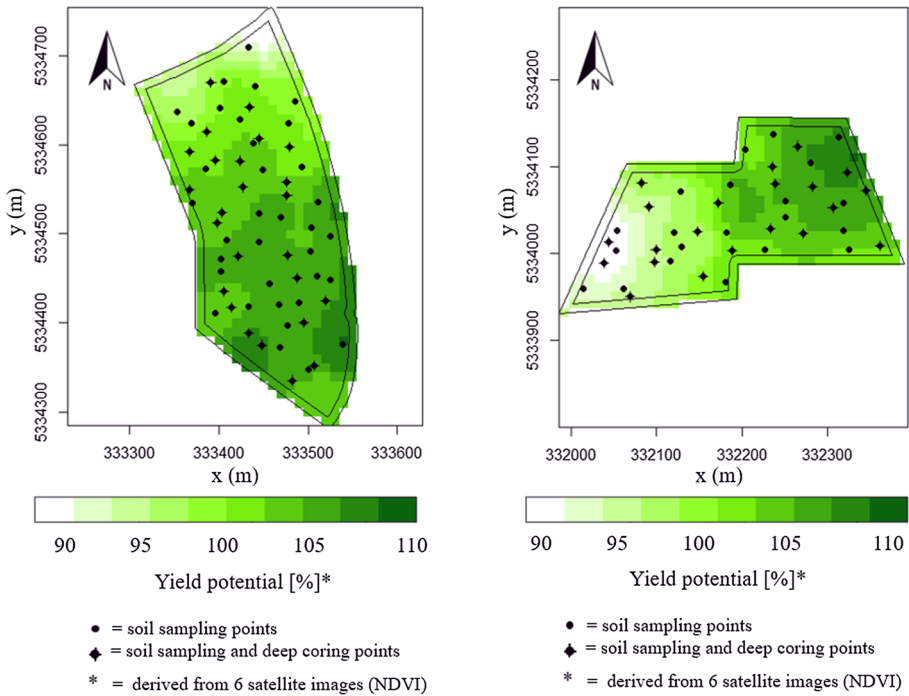


Fig. 1 Maps of the study field A (left) and study field B (right) (Coordinates are expressed using the UTM system). Yield potential derived from satellite images. The outer 10 m of the field were not included in data analysis)

yields (2018 to 2020). Approximately four satellite scenes per growth period were used in the PROMET model as input data for the simulation of grain yield (Hank et al., 2015). PROMET is a coupled hydro-agroecological model, which is capable of tracing the temporal dynamics and spatial heterogeneities of coupled water and carbon fluxes at the arable-field scale (Hank et al., 2015). Using the satellite data, the leaf area index and the crop-specific yield potential are calculated in the model. PROMET is used in the study region to offer various services to farms, e.g. the derivation of satellite-based yield and management maps and recommendations for site-specific nitrogen fertilisation. The yield maps generated with PROMET were taken as the basis for N balancing due to the already wider practical use of these yield maps. This also involves testing the accuracy and error range of the yield maps and the relationships to other soil and plant parameters.

In 2020, a multispectral sensor (TEC 5 2010) and crop-specific algorithms (Maidl et al., 2019) were additionally applied to determine the yield and N uptake of winter wheat on a site-specific basis. This allows a direct comparison of the results of two digital systems—yield determination according to satellite and sensor data. Based on reflectance measurements of winter wheat (at the time of flowering) the rede edge inflection point (REIP) vegetation index was calculated. Numerous scientific studies show that REIP correlates closely with biomass yield, N content and N removal of wheat (Mistele & Schmidhalter, 2008; Prey & Schmidhalter, 2019). The site specific georeferenced

REIP values were processed with a algorithm to calculate site specific N uptakes and yields (see Maidl et al., 2019).

N uptake according to satellite data was calculated by multiplying site-specific yields by mean grain N content; the latter was calculated from sensor data (N uptake/yield). Mean yields on field level were measured on the weighbridge and calculated on the basis of the grain silo volume and specific volume weight of grain.

The methods of determining plant variables used are summarised in online resource 3.

N balancing

N surplus ($\text{kg ha}^{-1} \text{ a}^{-1}$) was determined using N balancing:

$$N \text{ surplus} = N \text{ input} - N \text{ output} \quad (1)$$

$$N \text{ input} = N \text{ deposition} + N \text{ fertilization} + N_2 \text{ fixation} \quad (2)$$

$$N \text{ output} = \text{crop N uptake} \quad (3)$$

N fertilisation of the cultivated crops (Online resource 2) was applied uniformly, in accordance with legal regulations (DüV, 2020). The N input equated the TN supplied with organic and mineral fertilisation, a mean N deposition of 20 kg ha^{-1} (Schaap et al., 2018) and the symbiotically fixed nitrogen. The biological N_2 fixing capacity of the soybeans corresponded to the grain yield multiplied by a factor of 5.3 kg dt^{-1} (Lfl 2018). Total nitrogen from organic fertilisation was taken as N input under the assumption that intensive long-term fertilisation with dairy manure leads to a high mineralisation of nitrogen.

The N output corresponds to the N uptake of the harvested products (e.g., grain or bean). Wheat straw was harvested on both fields. The N uptake of by-products, such as straw, was calculated using the grain-to-straw ratio and the mean N content of the straw (Lfl, 2018).

The N surplus was calculated for each grid element (see “Geostatistical analysis” section).

Methods of determining soil properties

Georeferenced soil samples were taken from the investigated fields after the grain harvest in 2020 (Fig. 1) at a depth of 0–30 cm. The distribution of the soil samples within the field was ‘stratified random’: one single random point was sampled in each grid cell (Thompson, 2002). Eight soil samples were taken within a 50 cm maximum radius around a georeferenced point. All eight samples were combined to form a mixed sample. The location of the sampling points is shown in Fig. 1.

SOC and TN) were analysed by the dumas combustion method (VDLUFA, 2012a) (Online resource 4). The soil texture (soil layer 0–30 cm) was determined using the qualitative feel method (Sponagel, 2005).

The coarse-grained soil proportion (fragments > 2 mm) was estimated. Available water capacity (AWC) was derived from the soil texture and the coarse-grained soil proportion. The leachate rate was calculated as described by Renger et al. (1990) and evapotranspiration was determined as described by Wendling (1993) (Online resource 5).

Nitrate and ammonia stocks in deeper soil layers were determined using a tractor-mounted hydraulic deep drilling advice (Maidl et al., 1991) to generate georeferenced core

soundings on August 13, 2020, for study field Field A and on September 14, 2020, for Field B. 30 (Field A) and 21 (Field B) boreholes were carried out to a depth of 2.5 m; the core samples were divided into 50 cm thick layers. Nitrate and ammonia content was analysed photometrically for each layer (VDLUFA, 2012b).

Descriptive statistics

The mean, median, minimum, maximum and standard deviation were calculated for variables using R (R Core Team, 2020).

Geostatistical analysis

The investigation was carried out on the sub-field level. Therefore, the data were transferred to grids of the same resolution (10×10 m) and with the same raster elements, raster input data by downsampling and point input data by interpolation to the raster elements using block kriging (10×10 m) (Oliver & Webster, 2015). A variogram (variance of the data according to distance classes) of the data was created, which showed the spatial relationship of the variable with increasing separating distance (spatial auto-correlation effect). A model was fitted to the variogram, which is used for weighting data in the kriging neighbourhood to predict values at unsampled places (Oliver & Webster, 2015). The outer 10 m of the field was not included in data analysis to avoid the evaluation of data from areas that did not belong to the field.

A correlation analysis based on the grid elements was performed to check the relationship between the plant and soil variables. The R libraries ‘rgdal’, ‘rgeos’, ‘gstat’ and ‘raster’ were used for spatial analyses and for loading vector or raster files. The correlation coefficients (r) were classified as very strong ($r > 0.9$), strong ($0.9 > r > 0.7$), moderate ($0.7 > r > 0.5$), weak ($0.5 > r > 0.3$) or very weak ($r < 0.3$) according to Mittermayer et al. (2021).

Figure 2 is a flowchart that shows the consecutive work steps for determining plant and N balance variables and soil properties as well as the subsequent geostatistical and correlation analysis.

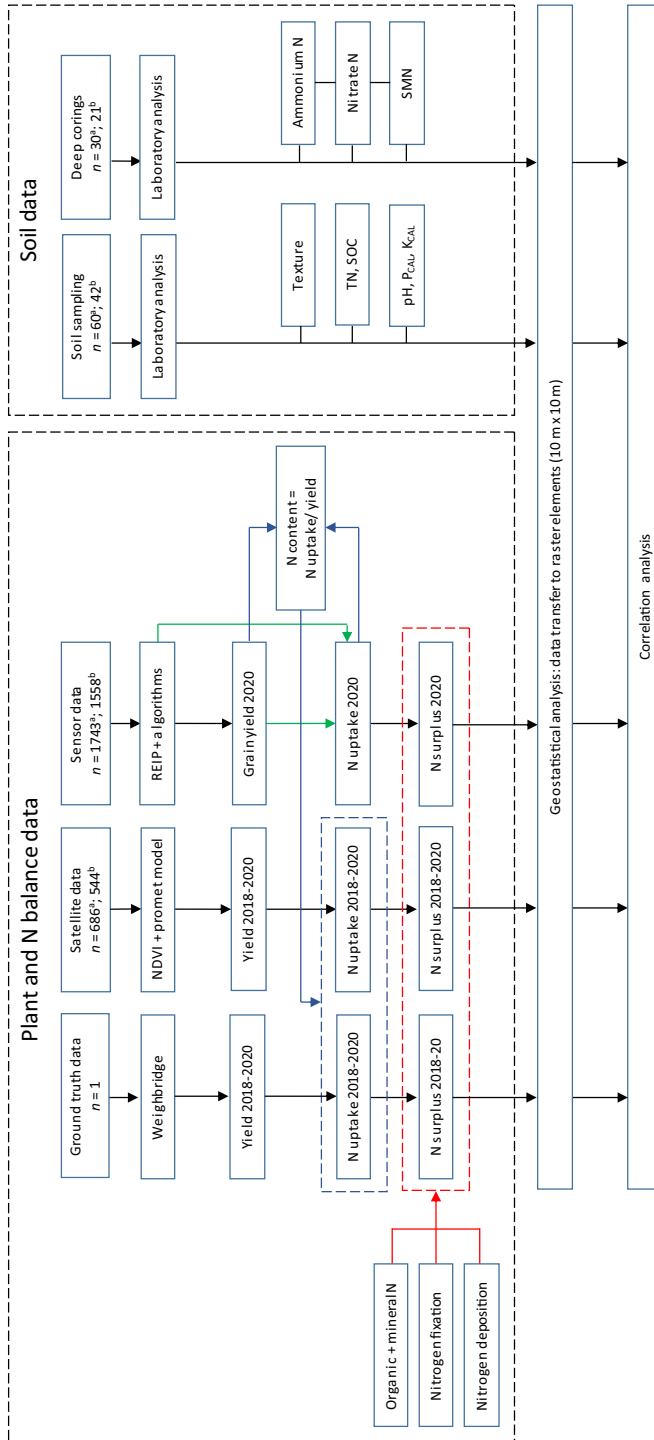
Results

Spatial variation of yield, N uptake and N surplus

2018, maize

The mean maize yields (35% DM content, measured values) were higher (Field A, 48.0 t ha⁻¹, Field B 50.0 t ha⁻¹) than the mean yields calculated from satellite data (43.9 and 44.5 t ha⁻¹, respectively) (Table 1). Within the fields, the yields varied from 21.8 t ha⁻¹ and 27.1 t ha⁻¹, respectively, in low-yield zones to 46.0 t ha⁻¹ and 50.0 t ha⁻¹, respectively, in high-yield zones. Accordingly, the N uptakes ranged from 127.3 to 239.7 kg ha⁻¹ (Field A) (Table 2) and 102.7 to 235.0 kg ha⁻¹ (Field B) (Table 3).

While the mean N surpluses in 2018 were negative in both fields (− 5.1 and − 19.3 kg ha⁻¹, there were strongly negative (− 38.5 and − 45.0 kg ha⁻¹) and strongly positive (73.9 and 87.3 kg ha⁻¹, respectively) N surpluses in sub-fields.



^aField A; ^bField B

Fig. 2 Flow chart of the consecutive work steps in this study

Table 1 Yields on study field A and study field B, 2018–2020

Data	Data source	<i>n</i>	Unit	Mean	Median	Min	Max	Standard Deviation	Skewness
<i>Study year 2018; Silage corn^a</i>									
Field A									
Yield	Weighbridge	1	t ha ⁻¹	48.0					
Yield	Satellite	686	t ha ⁻¹	43.9	44.3	27.1	51.0	4.0	- 1.16
Field B									
Yield	Weighbridge	1	t ha ⁻¹	50.0					
Yield	Satellite	544	t ha ⁻¹	44.5	45.8	21.8	50.0	4.4	- 2.79
<i>Study year 2019; Soybean^b</i>									
Field A									
Yield	Weighbridge	1	t ha ⁻¹	3.7					
Yield	Satellite	686	t ha ⁻¹	3.7	4.0	1.1	4.6	0.6	- 2.24
Field B									
Yield	Weighbridge	1	t ha ⁻¹	4.0					
Yield	Satellite	544	t ha ⁻¹	3.6	3.6	1.5	4.1	0.4	- 1.96
<i>Study year 2020; Winter wheat^c</i>									
Field A									
Yield	Weighbridge	1	t ha ⁻¹	8.5					
Yield	Sensor	1743	t ha ⁻¹	9.1	9.1	8.4	9.8	0.3	- 0.08
Yield	Satellite	686	t ha ⁻¹	10.2	10.4	6.8	12.9	1.0	- 0.89
Field B									
Yield	Weighbridge	1	t ha ⁻¹	10.0					
Yield	Sensor	1558	t ha ⁻¹	9.4	9.4	7.3	12.7	0.7	0.18
Yield	Satellite	544	t ha ⁻¹	8.3	8.2	4.2	11.8	1.1	0.43

Table 1 (Continued)

Data	Data source	<i>n</i>	Unit	Mean	Median	Min	Max	Standard Deviation	Skewness
<i>Study year 2018–2020</i>									
Field A									
Mean relative yield	Satellite	686		1.0	1.0	0.6	1.1	0.1	− 1.81
Field B									
Mean relative yield	Satellite	544		1.0	1.0	0.6	1.2	0.1	− 0.93

Method description in Electronic supplementary material (online resource 3)

^aMoisture content of silage corn, 65%

^bMoisture content of soybean, 8%

^cMoisture content of winter wheat, 14%

Table 2 N balance for the study field A, 2018–2020

Data	Data source	n	Unit	Mean	Median	Min	Max	Standard Deviation	Skewness
<i>Field A, Study year 2018; Silage corn</i>									
N Input									
N fertilization total	Farming system	1	kg ha ⁻¹	181.0					
N deposition	UBA*	1	kg ha ⁻¹	20.0					
N Output									
Silage corn N uptake	Weighbridge	1	kg ha ⁻¹	225.6					
Silage corn N uptake	Satellite, LfL ¹	686	kg ha ⁻¹	206.3	208.4	127.3	239.7	18.9	- 1.16
N surplus	Satellite	686	kg ha ⁻¹	- 5.1	- 7.2	- 38.5	73.9	18.9	1.16
<i>Field A, Study year 2019; Soybean</i>									
N Input									
N ₂ fixation	LfL ²	1	kg ha ⁻¹	198.4	209.7	58.0	241.8	30.8	- 2.24
N deposition	UBA	1	kg ha ⁻¹	20.0					
N Output									
Bean N uptake	Weighbridge	1	kg ha ⁻¹	162.8					
Bean N uptake	Satellite, LfL ³	686	kg ha ⁻¹	164.7	174.7	48.1	200.8	25.6	- 2.24
N surplus	Satellite	686	kg ha ⁻¹	53.7	55.6	29.8	61.1	5.2	- 2.24
<i>Field A, Study year 2020; Winter wheat</i>									
N Input									
N fertilization total	Farming system	1	kg ha ⁻¹	212.0					
N deposition	UBA	1	kg ha ⁻¹	20.0					
N Output									
Grain N uptake	Weighbridge	1	167.4						
Grain N uptake	Sensor	1743	kg ha ⁻¹	179.8	179.9	158.1	200.9	9.2	- 0.01
Straw N uptake	Sensor, LfL ⁴	1743	kg ha ⁻¹	36.5	36.6	33.5	39.3	1.2	- 0.08
Grain N uptake	Satellite	686	kg ha ⁻¹	200.7	205.0	133.0	253.2	19.2	- 0.89
Straw N uptake	Satellite	686	kg ha ⁻¹	40.8	41.7	27.0	51.5	3.9	- 0.89

Table 2 (Continued)

Data	Data source	<i>n</i>	Unit	Mean	Median	Min	Max	Standard Deviation	Skewness
N surplus	Sensor	1743	kg ha ⁻¹	15.7	15.6	- 8.2	40.3	10.5	0.02
N surplus	Satellite	686	kg ha ⁻¹	- 9.5	- 14.7	- 72.7	72.0	23.1	0.89
<i>Mean Study year 2018–2020</i>									
Mean N uptake	Satellite	686	kg ha ⁻¹	190.6	196.0	112.6	214.3	18.5	- 1.78
Mean N surplus	Satellite	686	kg ha ⁻¹	13.0	11.6	- 8.6	60.9	11.1	1.27

^aMethod description in Electronic supplementary material (online resource 3)

¹N content 4.7 kg t⁻¹

²Nitrogen fixation 53.0 kg t⁻¹

³N content 44.0 kg t⁻¹

⁴Grain/straw ratio 0.8, N content straw 5.0 kg t⁻¹

Table 3 N balance for the study field B 2018–2020

Data	Data source	<i>n</i>	Unit	Mean	Median	Min	Max	Standard Derivation	Skewness
<i>Field B, Study year 2018; Crop Silage corn</i>									
N Input									
N fertilization total	Farming system	1	kg ha ⁻¹	170.0					
N deposition	UBA*	1	kg ha ⁻¹	20.0					
N Output									
Silage corn N uptake	Weighbridge	1	kg ha ⁻¹	235.0					
Silage corn N uptake	Satellite, LfL ¹	544	kg ha ⁻¹	209.3	215.2	102.7	235.0	20.5	- 2.79
N surplus	Satellite	544	kg ha ⁻¹	- 19.3	- 25.2	- 45.0	87.3	20.5	2.79
<i>Field B, Study year 2019; Crop Soybean</i>									
N Input									
N ₂ fixation	LfL ²	1	kg ha ⁻¹	188.4	191.6	78.1	219.5	22.1	- 1.96
N deposition	UBA	1	kg ha ⁻¹	20.0					
N Output									
Bean N uptake	Weighbridge	1	kg ha ⁻¹	176.0					
Bean N uptake	Satellite, LfL ³	544	kg ha ⁻¹	156.4	159.0	64.8	182.2	18.3	- 1.96
N surplus	Satellite	544	kg ha ⁻¹	52.0	52.5	33.3	57.3	3.8	- 1.96
<i>Field B, Study year 2020; Crop Winter wheat</i>									
N Input									
N fertilization total	Farming system	1	kg ha ⁻¹	251.2					
N deposition	UBA	1	kg ha ⁻¹	20.0					
N Output									
Grain N uptake	Weighbridge	1	kg ha ⁻¹	200.0					
Grain N uptake	Sensor	1558	kg ha ⁻¹	187.9	188.0	146.7	229.2	18.0	- 0.02
Straw N uptake	Sensor, LfL ⁴	1558	kg ha ⁻¹	37.8	37.8	29.2	50.7	2.7	0.17
Grain N uptake	Satellite	544	kg ha ⁻¹	165.6	163.4	83.5	236.3	22.6	0.43

Table 3 (Continued)

Data	Data source	n	Unit	Mean	Median	Min	Max	Standard Derivation	Skewness
Straw N uptake	Satellite	544	kg ha ⁻¹	33.1	32.7	16.7	47.2	4.5	0.43
N surplus	Sensor	1558	kg ha ⁻¹	45.5	45.6	-1.7	91.0	18.8	-0.05
N surplus	Satellite	544	kg ha ⁻¹	72.5	75.1	-12.3	171.0	27.1	-0.43
<i>Mean Study year 2018–2020</i>									
Mean N uptake	Satellite	544	kg ha ⁻¹	177.1	179.4	111.5	211.0	15.9	-1.07
Mean N surplus	Satellite	544	kg ha ⁻¹	35.1	36.1	3.8	85.9	12.7	0.86

^aMethod description in Electronic supplementary material (online resource 3)

¹N content 4.7 kg t⁻¹

²Nitrogen fixation 53.0 kg t⁻¹

³N content 44.0 kg t⁻¹

⁴Grain/straw ratio 0.8, N content straw 5.0 kg t⁻¹

2019, soybean

In the case of soy yields, the mean measured soybean yields (3.7–4.0 t ha⁻¹) agreed well with the yields modelled from satellite data (3.6–3.7 t ha⁻¹). Within the fields yield zones with lower yields (1.1–1.5 t ha⁻¹) and higher yields (4.1–4.6 t ha⁻¹) were detectable.

The N surpluses were positive owing to symbiotic N₂ fixation. They varied from 29.8 to 61.1 kg ha⁻¹ (Field A) and from 33.3 to 57.3 kg ha⁻¹ (Field B).

2020, Winter wheat

On the weighbridge, mean wheat yields from Field A and Field B were 8.5 t ha⁻¹ and 10.0 t ha⁻¹, respectively (Table 1). The mean yields from satellite data (10.2 and 8.3 t ha⁻¹) differed more from the measured values from weighbridge than the yields based on sensor measurements (9.1 and 9.4 t ha⁻¹).

The high and low yield zones were identifiable within the fields. The yields from sensor varied only slightly, between 8.4 and 9.8 t ha⁻¹ (SD: 0.3) in Field A, whereas the differences were more pronounced in Field B (7.3 to 12.7 t ha⁻¹, SD: 1.0). The differences in yield were even higher for the satellite data (Table 1).

N uptake on Field A amounted to 201 kg ha⁻¹ (133–253 kg ha⁻¹) and was higher than N uptake from sensor, which amounted to an average of 180 kg ha⁻¹ (158–201 kg ha⁻¹). In Field B, N uptake determined from satellite data, with an average of 166 kg ha⁻¹ (84–236 kg ha⁻¹) below the N uptake from sensor measurement, which was 188 kg ha⁻¹ (147–229 kg ha⁻¹). Based on the mean yields (weighbridge), the following N uptake was calculated: Field A: 167 kg ha⁻¹, Field B: 200 kg ha⁻¹. Thus, N uptake determined with the sensor and the weighbridge agreed well.

The N surpluses balanced for each grid element with different methods and input data were slightly negative on average (satellite, -10 kg ha⁻¹) or positive (sensor, 16 kg ha⁻¹) for Field A and strongly positive for Field B (satellite and sensor) (73 and 46 kg ha⁻¹, respectively). Analogous to N uptake, the N surplus varied on a small scale, whereby zones with high and low N surpluses could be identified within the fields. In the high-yield zone of Field A, the lowest N surplus was as low as -8 kg ha⁻¹ (sensor) and -73 kg ha⁻¹ (satellite). In the low-yield zone, the N surplus ranged up to 40 kg ha⁻¹ (sensor) or 70 kg ha⁻¹ (satellite). The standard deviation of the N surplus was higher for the satellite data than for the sensor data. In Field B, the N surpluses were higher than in the Field A and showed minimum values of -2 kg ha⁻¹ (sensor) and -12 kg ha⁻¹ (satellite). In the low-yield zone, N surplus up to 91 kg ha⁻¹ (sensor) and 171 kg ha⁻¹ (satellite) were observed. The standard deviation was also higher for the satellite data than for the sensor data. The minima and maxima (Tables 2 and 3) represented extreme values that occurred only in a few grid elements (Figs. 3 and 4).

2018–2020: crop rotation

In the mean of the 3-year crop rotation, the relative yields varied between 60% and 110% at Field A, respectively and between 60% and 120% at Field B (Table 1). The mean N surpluses were moderate (Field A: 13 kg ha⁻¹; Field B: 35 kg ha⁻¹) and varied from -9 to 61 kg ha⁻¹ (Field A) and 4 to 86 kg ha⁻¹ (Field B).

Table 4 Descriptive statistics of the soil data acquired on Field A and Field B

Soil properties	<i>n</i>	Unit	Mean	Median	Minimum	Maximum	Standard Deviation	Skewness
<i>Field A</i>								
Soil organic carbon content (0–30 cm)	60	% DM	1.53	1.54	1.26	2.01	0.15	0.45
Soil total nitrogen content (0–30 cm)	60	% DM	0.15	0.16	0.12	0.21	0.02	0.62
Nitrate content 0–2.5 m	30	kg ha ⁻¹	76.6	72.2	33.7	159.1	30.6	1.16
Nitrate content 1–2.5 m	30	kg ha ⁻¹	36.5	32.7	11.4	85.3	16.7	1.01
Ammonium content 0–2.5 m	30	kg ha ⁻¹	76.0	70.1	12.6	219.1	58.7	1.20
Ammonium content 1–2.5 m	30	kg ha ⁻¹	26.8	20.0	7.5	134.3	24.2	3.23
P (0–30 cm)	60	mg (100 g) ⁻¹	4.09	4.05	2.22	7.55	1.03	0.79
K (0–30 cm)	60	mg (100 g) ⁻¹	7.58	7.43	2.90	15.00	2.41	0.68
pH (0–30 cm)	60		6.50	6.51	5.94	6.99	0.20	-0.29
<i>Field B</i>								
Soil organic carbon content (0–30 cm)	42	% DM	1.71	1.71	1.37	2.03	0.14	-0.32
Soil total nitrogen content (0–30 cm)	42	% DM	0.17	0.17	0.13	0.20	0.01	-0.16
Nitrate content 0–2.5 m	21	kg ha ⁻¹	121.0	109.2	35.7	281.2	60.7	0.92
Nitrate content 1–2.5 m	21	kg ha ⁻¹	42.5	37.0	6.3	94.1	22.0	0.72
Ammonium content 0–2.5 m	21	kg ha ⁻¹	18.0	17.5	10.1	40.4	6.9	1.86
Ammonium content 1–2.5 m	21	kg ha ⁻¹	6.5	5.3	3.9	18.0	3.0	2.91
P (0–30 cm)	42	mg (100 g) ⁻¹	5.15	5.12	2.96	10.45	1.25	1.87
K (0–30 cm)	42	mg (100 g) ⁻¹	8.93	9.08	4.16	16.46	2.88	0.61
pH (0–30 cm)	42		6.40	6.42	5.72	6.73	0.19	-1.19

Method description in electronic supplementary material (online resource 4)

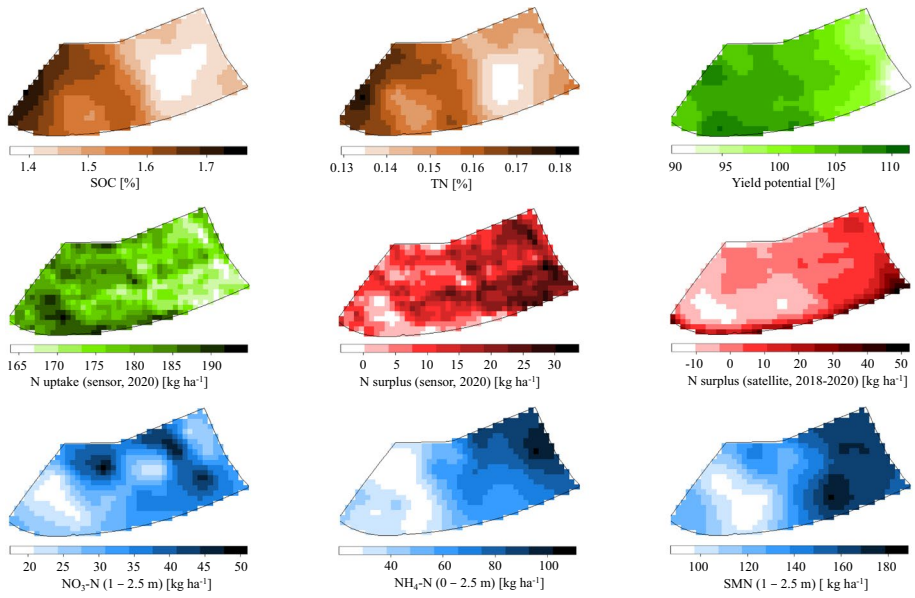


Fig. 3 Kriged maps of spatial distribution of yield potential, soil organic carbon content (SOC), soil total nitrogen content (TN), N uptake (sensor, 2020), N surplus (sensor, 2020), N surplus (satellite 2018–2020), nitrate, ammonium and SMN content on field A

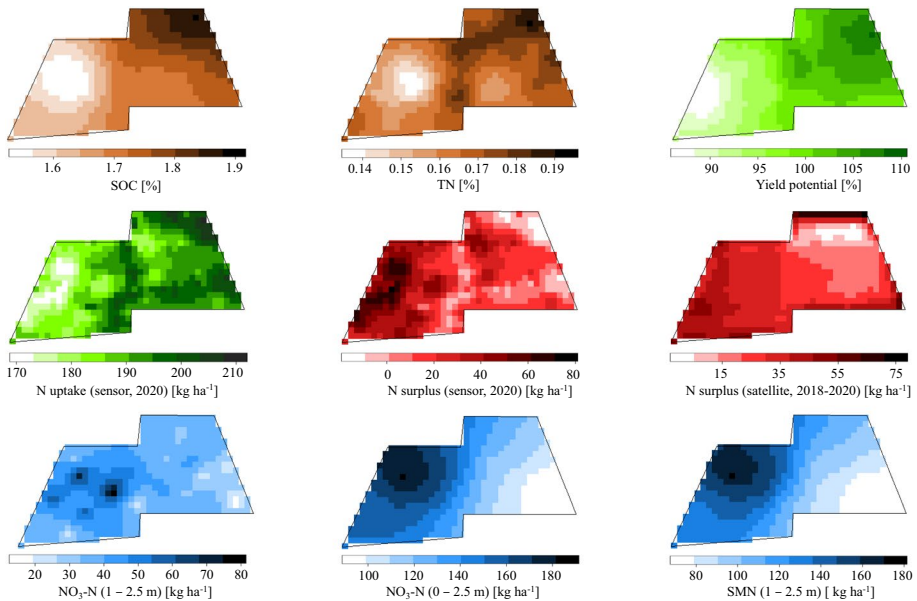


Fig. 4 Kriged maps of spatial distribution of yield potential, soil organic carbon content (SOC), soil total nitrogen content (TN), N uptake (sensor 2020) N surplus (sensor 2020), N surplus (satellite 2018–2020), nitrate, ammonium and SMN content on field B

Table 5 Satellite- and sensor-data in relation to soil an N balance parameters*, Correlation matrix (r) based on 10 m × 10 m raster

Field A	N surplus 18–20 (satellite)	N surplus plus 20 (satellite)	TN	pH	P	K	NH ₄ N 0–2.5 m	NH ₄ N 1–2.5 m	NO ₃ -N 0–2.5 m	NO ₃ -N 1–2.5 m	SMN 0–2.5 m	SMN 1–2.5 m
<i>Field A (n=671)</i>												
Biomass potential map	-0.70	-0.68	0.51	0.17	0.16	-0.05	-0.58	-0.22	-0.30	-0.23		
Yield 18–20 (satellite)	-0.90	-0.80	0.41	0.17	0.16	-0.05	-0.58	-0.22	-0.09	-0.24	-0.59	-0.20
Yield 20 (satellite)	-0.92	-0.54	0.54	-0.10	0.26	0.06	-0.47	-0.21	-0.11	-0.33	-0.57	-0.33
N uptake 20 (sensor)	-0.46	-0.55	0.63	0.10	0.24	-0.18	-0.63	-0.38	-0.11	-0.20	-0.55	-0.24
N surplus 18–20 (satellite)	0.92	0.46	-0.51	-0.17	-0.27	-0.04	0.49	0.15	0.10	0.30	0.56	0.25
N surplus 20 (sensor)	0.55	-0.63	-0.63	-0.10	-0.24	0.18	0.55	0.33	0.11	0.20	0.55	0.24
SOC	-0.51	0.96	0.96	0.04	0.09	-0.23	-0.83	-0.45	-0.10	-0.28	-0.80	-0.36
<i>Field B (n=523)</i>												
Biomass potential map	-0.77	-0.67	0.68	-0.18	0.14	0.49	0.07	0.09	-0.71	-0.50		
Yield 18–20 (satellite)	-0.80	-0.72	0.47	-0.18	0.14	0.49	0.07	0.09	-0.45	-0.28	-0.16	-0.20
Yield 20 (satellite)	-0.94	-0.39	0.74	-0.60	0.04	0.65	-0.10	-0.16	-0.36	-0.36	-0.21	-0.27
N uptake 20 (sensor)	-0.48	-0.39	0.72	-0.09	0.43	0.60	0.12	0.14	-0.65	-0.49	-0.65	-0.42
N surplus 18–20 (satellite)	0.94	0.48	-0.73	0.43	-0.12	-0.65	0.05	-0.03	0.50	0.39	0.24	0.28
N surplus 20 (sensor)	0.39	-0.70	-0.70	0.09	-0.43	-0.60	-0.12	-0.14	0.65	0.49	0.65	0.42
SOC	-0.74	0.94	0.94	-0.37	0.41	0.91	-0.10	-0.05	-0.71	-0.60	-0.56	-0.50

*SOC: soil organic carbon content, TN soil total nitrogen content, SMN soil mineral nitrogen, ammonium-N + nitrate-N

Spatial variation of soil properties

The soil texture varied only slightly within the fields. It was mainly silty loam and partly sandy loamy silt. However, the coarse-grained soil proportions in the soil profile fluctuated up to a soil depth of 2.5 m within the fields, as shown by the deep drilling. The modelled leachate rate ranged from 251 mm year⁻¹ (1% coarse soil) and 269 mm yr⁻¹ (25% coarse soil) in 2019 to 372 mm year⁻¹ (1% coarse soil) and 390 mm year⁻¹ (25% coarse soil) in 2020. This leads to ranging exchange factors of soil water from 0.7 to 2019 to 1.1 in 2020 as a function of the coarse-grained soil proportion (Online resource 5). Thus, the soil depth of 2.5 m roughly corresponds to the modelled displacement distance of leachate water in the three years of investigation (2018–2020). The modelled displacement distance is higher in sub-fields with higher coarse-grained soil proportion than in sub-fields with lower coarse-grained soil proportion.

The soil carbon and nitrogen properties showed high spatial variability (Figs. 3 and 4). The variation range of the SOC contents within the investigation fields was considerable from 1.26 to 2.01%, in Field A and from 1.37 to 2.03% in Field B (the TN contents varied accordingly). The other soil parameters investigated (P, K, pH) also showed high levels of spatial variability (Table 4).

The nitrate and ammonium stocks are shown in Table 4 as the sum of the total sampled soil profile depth (0–2.5 m) and for the 1 to 2.5 m soil layer. The nitrate and ammonium stocks showed extreme variation and showed site-specific differences. There was a very different displacement of nitrate, but also of ammonium through the soil profile. For example, in Field A, nitrate N stocks of 34 to 159 kg ha⁻¹ (soil layer 0–2.5 m) and 11 to 85 kg ha⁻¹ (soil layer 1–2.5 m) were measured, and in Field B, nitrate N stocks of 36–281 kg ha⁻¹ (soil layer 0–2.5 m) and 6 to 94 kg ha⁻¹ (soil layer 1–2.5 m) were measured. In addition, very high ammonium N stocks of 13 to 219 kg ha⁻¹ (soil layer 0–2.5 m) and 7 to 134 kg ha⁻¹ (soil layer 1–2.5 m) occurred. A comparison of the maps (Figs. 3 and 4) showed that the highest mineral nitrogen stocks occurred in the field areas that had high N surpluses, low yields and low N uptakes, as well as low SOC and low TN contents. These were the low-yield zones (Fig. 1).

Correlations

Very strong correlations were found between the soil properties SOC and TN ($r=0.94\text{--}0.96$) (Table 5) in the investigated fields. No correlations were calculated for the soil texture and the clay, silt and sand proportions, since hardly any differences were found within the fields.

The multi-year NDVI satellite data (biomass potential maps) showed the best correlations of all methods used (Field A: SOC $r=0.64$; TN $r=0.51$; N surplus satellite 18–20 $r=-0.70$; N surplus sensor $r=-0.70$ and Field B: SOC $r=0.86$; TN $r=0.68$; N surplus satellite 18–20 $r=-0.77$; N surplus sensor $r=-0.78$).

The crop yields from satellite data showed similar distribution patterns in the years of investigation (Field A: silage maize/soybean $r=0.73$; silage maize/winter wheat $r=0.55$; soybean/winter wheat $r=0.60$; Field B: silage maize/soybean $r=0.44$; silage maize/winter wheat $r=0.38$; soybean/winter wheat $r=0.39$). Weak to moderate correlations were also found between satellite and sensor data in 2020 (Field A, $r=0.54$; Field B, $r=0.39$).

Yields and N uptake correlated positively with SOC contents. The crop rotation yield (2018–2020) according to satellite data showed moderate correlations with the SOC content ($r=0.53$ and 0.62). Winter wheat yield (2020) according to satellite data correlated more closely with SOC content ($r=0.57$ and 0.74) and TN content (0.54 and 0.63).

In 2020, the N uptake sensor showed moderate-to-strong correlations with the SOC content ($r=0.63$ and 0.72) and TN content ($r=0.61$ and 0.62). Other soil properties (pH, P) showed only weak or very weak correlations with the yield. There was a moderate correlation with the grain yield only for the P content on Field B (Table 5).

In 2020, the SOC contents correlated negatively with the N surpluses according to sensor data ($r = -0.63$ and -0.70) and according to satellite data (2018–2020) ($r = -0.51$ and -0.73), the correlations between the TN content and the N surpluses according to the sensor or satellite were weaker ($r = -0.43$ to -0.62 , Table 5).

The nitrate N and ammonium N stocks in different soil layers correlated weakly to strongly with the examined plant and N balance parameters and soil properties. In Field A, there was no or a weak relationship between the N surplus (2018–2020) (satellite) and the nitrate N stocks at soil layer 0–2.5 m ($r=0.10$) or soil layer 1–2.5 m depth ($r=0.30$). In Field B, this relationship was moderate ($r=0.50$, soil layer 0–2.5 m) or weak ($r=0.39$, soil layer 1–2.5 m). (Table 5). The soil mineral N stocks (ammonium + nitrate) in 0–2.5 m correlated with the N surpluses ($r=0.55$ (Field A) to 0.65 (Field B)).

There were very weak to strong correlations between SOC, TN and the nitrate and ammonium stocks. The correlation of the SOC content with nitrate in the soil layer 0–2.5 and 1–2.5 m depth in Field A was very weak ($r = -0.10$ and $r = -0.28$, respectively) and with ammonium strong to moderate ($r = -0.83$ and $r = -0.45$). In Field B, there were moderate-to-strong correlations between SOC and nitrate N stocks (soil layer 0–2.5 m: $r = -0.71$; soil layer 1–2.5 m: $r = -0.60$). Ammonium stocks were low overall. Correlations could not be determined.

The correlations between the biomass potential maps and nitrate stocks showed different results in both fields. In Field A there were weak negative correlations between the biomass potential map and nitrate stocks. In Field B the negative correlation was moderate to strong (Table 5).

Discussion

Site selection

Site-specific differences in yield and N efficiency within arable fields are caused and influenced by physical, chemical and biological soil properties, soil genesis and cultivation (crop rotation, tillage and fertilisation) (Mzuku et al., 2005; Casanova et al., 1999). Accordingly, the choice of investigation fields (size, soil heterogeneity) significantly influences the results of studies on the spatial variability of plant and N balance parameters.

To test whether the study plots were sufficiently heterogeneous and therefore suitable for analyses of spatial variability of nitrogen balances, biomass potential maps based on satellite data (Georgi et al., 2018) were used to approximate the variability of biomass formation in previous years.

Nevertheless, the variability was slightly below that of previous studies in southern Germany (Mittermayer et al., 2021; Schmidhalter et al., 2002). This was due to the lower

variability of yield-relevant soil properties (AWC, SOC, TN, texture) of the investigated fields. There are only site specific differences in the coarse-grained soil proportion (fragments > 2 mm), which are higher in the low-yield areas. The nearly flat surfaces of the fields do not indicate surface runoff or lateral water flows in the subsoil that would complicate interpretation of deep drilling data.

The rainy weather in the study years 2019 and 2020 (without pronounced dry periods in the growing season) is a further reason for the lower yield variability than observed in previous studies, for example in 2018, which had extremely hot and dry periods in the growing season (Hülsbergen et al., 2020; Mittermayer et al., 2022).

Another factor that determined the choice of the investigated fields was their long-term management. The arable fields are cultivated from farms with high animal stocks and intensive manure fertilisation, which is expected to result in high nitrogen mineralisation potential and a risk of nitrogen loss (Salo & Turtola, 2006; Hülsbergen et al., 2017).

Origin of data and technologies used

The digital methods used (tractor-mounted multispectral sensor, satellite data, vegetation indices and models) are suitable for modelling yields and N uptakes and the subsequent calculation of N surplus as other studies also show (Mittermayer et al., 2021, 2022). The comparison of the mean yields calculated with sensor and satellite data with ground truth data shows good agreement. In this study the digital methods were compared to mean yields of the fields. The correlation analysis with measured soil data in a high spatial resolution is an indirect validation of the digital methods.

The comparison of satellite and sensor data (mean values, minima, maxima, standard deviation; Table 1) and distribution patterns (Figs. 3 and 4; Online resource 7) revealed some considerable deviations. Especially the absolute level of yields determined by satellite data and weak to moderate correlations of $r=0.39$ to $r=0.55$ shows the need for further development and optimisation of these systems. In line with previous studies (Mittermayer et al., 2022), it can be confirmed that the accuracy of digital systems should be further improved, for which there are many methodological approaches, including higher spatial resolution, better vegetation indices, algorithms and models (Mulla, 2013; Diacono et al., 2013). One approach could be to create biomass potential maps by using multi-year NDVI satellite data. By combining the spatial distribution of the multi-year satellite data with one average yield value (e.g. determined by weighbridge) it is possible to identify zones with increasing risk of nitrogen losses in the past. For this creation it is not necessary to estimate yields with algorithms or models. The validation of this methodological adaptation and development of algorithms to transfer the relative distribution of BMP into plant parameters e.g. yields is in progress.

One advantage of using satellite data (compared with sensor data) is that yields can be modelled retrospectively. To represent the 2.5 m depth of the drillings it was necessary to balance three years of the crop rotation by satellite data.

The satellite data were used to model the yields with the PROMET model. To calculate N uptake, grain N content is needed in addition to yield, which in this study corresponded to the mean grain N content calculated from the sensor data. It should be noted that the grain N content can also vary greatly in small areas, e.g. owing to dilution effects in the high-yield areas (Morari et al., 2018). In contrast, for the sensor data, both the yield and the N uptake were calculated using specific algorithms, so that varying N contents were also recorded on a site specific basis. The sensor-based method is therefore more suitable for

site specific N balancing; it also shows closer correlations to measured data (Mittermayer et al., 2021). Further N inputs and N outputs were calculated in the N balance. Nitrogen fixation of legumes, N deposition and other N balance variables can also vary site specific depending on soil properties e.g. soil nitrogen content (Larue & Patterson, 1981; Heuwinkele et al., 2005). In general, N balances are subject to numerous errors and inaccuracies (Oenema et al., 2003). In addition, some N fluxes that could not yet be digitally determined were missing in the this N balancing; in particular, the change in the soil nitrogen stocks owing to mineralisation or immobilisation, which were recorded as relevant variables for other N balances (Küstermann et al., 2008; Lin & Hülsbergen, 2017) A consideration of these variables could improve the correlations of N surplus and nitrate stocks. In this study N surplus is regarded as indicator of N loss potential. The relation to the measured nitrate stocks was investigated. Other potential N losses on the sub-field level such as denitrification were not taken into account. Thus, the accounting approach presented in this study still offers numerous opportunities for improvement of precision.

While satellite and sensor data were measured in high spatial resolution on the fields, the time required for soil sampling limited the number of measuring points for the soil properties (e.g. SOC content and nitrate stocks). Therefore, the soil maps created by kriging are not as differentiated as the satellite data (Figs. 3 and 4).

Spatial variation of N surplus in relation to soil parameters

Spatial variability in yields, N uptakes and N surpluses was determined in the arable fields using the sensor and satellite supported methods. The 3-year N surpluses were at moderate to medium level ($> 50 \text{ kg N ha}^{-1}$). Extremely high N surpluses (as in some other studies (Hülsbergen et al., 2017) were not found. In the field areas with low N uptakes and high N surpluses, correspondingly high nitrate stocks in the soil were to be expected. In these areas, more nitrate nitrogen was also measured using the deep drilling. Of all the soil properties surveyed, the strongest positive correlation exists between the SOC and TN contents and the yields and N uptakes, and, accordingly, the closest negative correlation to the N surpluses. SOC and TN are indicators of humus content. In numerous studies, close correlations have been found between SOC and TN contents (or humus contents), important soil properties and soil processes (Körschens et al., 1998; Hülsbergen, 2003) and the crop yield (Leithold et al., 2015; Usowicz & Lipiec, 2017). However, most of these studies took place in field experiments, especially long-term field experiments. However, there are also scientific studies that have demonstrated these relationships in arable fields, e.g. in georeferenced test plots (Hülsbergen, 2003).

As the SOC contents and their spatial distribution are relatively stable and changeable only over the long term (Wiesmeier et al., 2019), they may be suitable indicators for yield and N uptake potentials on the sub-field level. However, there are many factors influencing the yield that can overlay the effects of SOC and TN. The spatial variability of AWC, which is also of great importance for soil processes and yield formation (Godwin & Miller, 2003; Harrach, 2016) was not determined on the sub-field level for the whole soil profile. The modelled leachate rates and exchange factors based on estimated coarse-grained soil proportion (fragments $> 2 \text{ mm}$) indicate that the displacement of soil water, and thus nitrate, is greater in sub-fields with higher coarse-grained soil proportion in low-yield zones. The comparison of nitrate stocks from deep drillings of the same depth represents different periods. In low-yield zones the nitrate stocks from deep drilling are from shorter periods because the displacement of leachate water and thus nitrate is greater.

In addition, the question arose whether the higher yields in these field zones with increased humus content were due to the higher humus content or whether the higher humus content was a result of the higher yields in these zones for many years. The SOC content depends on climatic conditions as well as numerous soil properties (Jobbágy & Jackson, 2000), including the soil texture (Hassink, 1997; Hülsbergen, 2003; Mittermayer et al., 2022) found a positive relationship between the clay content and SOC content and a negative relationship between the sand content and SOC content in heterogeneous fields.

From the results of this study it can be concluded that SOC is not only a suitable indicator for yield potential on heterogeneous soils, but also correlates positively with N efficiency and negatively with nitrate leaching potential. With uniform N fertilisation, more nitrogen is taken up from the soil and/or the applied N fertiliser in the zones with high yields and N withdrawals. This results in lower N losses in these zones.

However, these correlations need to be further investigated, also under other soil, climate and management conditions.

The influence of the study site can be overlaid by the land use (crop rotation, tillage and fertilisation (Guo & Gifford, 2002; Poeplau et al., 2011). For example, higher SOC contents can be found under permanent grassland than under arable land with otherwise identical site conditions (Martin et al., 2011; Jacobs et al., 2018), which can be determined long time after a change in land use. Organic fertilisation over many years can also have a positive effect on SOC content (Körschens, 1997). Differentiated SOC content within the investigated fields can be caused by historical permanent grassland or increased organic fertilisation of sub-fields near farms. The differences found (0.2–0.3% SOC) were of an order of magnitude that can be explained by management (Martin et al., 2011). The interdependence of SOC contents and yields could not be clarified with the methods in this study. However, the repeatedly determine close correlation between SOC content and yield (Mittermayer et al., 2022; Hausherr Lüder et al., 2018; Usowicz & Lipiec, 2017) confirms the suitability of SOC as an indicator for the identification of yield zones.

Spatial variation of nitrate contents in relation to soil properties and plant variables

In this study, nitrate stocks in deeper soil layers were first measured in high spatial resolution on arable fields to analyse the relationships between N surpluses and nitrate stocks under practical conditions. By examining the spatial variability of N surpluses, sub-fields with high risk for nitrogen losses can be localised and site specific measures can be derived to reduce nitrate leaching in the ground- and drinking water.

The soil layer (0–1 m) of the drilling profile was defined simplifying as the evapotranspiration zone (Funk et al., 1995). Accordingly, the layers below were assigned to the leachate zone. Thus, the nitrate stocks measured in the leachate zone were defined as being at risk of loss.

In the low yield areas, the nitrate and ammonium stocks were higher than in the high-yield areas of the fields (Fig. 3 und 4). In Field A, a weak correlation was found ($r=0.30$) between N surplus and nitrate stocks (Fig. 3). In addition, high ammonium stocks were found in the deeper soil layers. Closer correlations of N surplus and nitrate stocks can be seen in the Field B. While SOC content can explain the plant and N balance parameters well ($r=0.74$) and the nitrate stocks moderately ($r=-0.60$), the correlation between N surplus and nitrate stocks was weaker ($r=0.39$). Similar to Field A, the stable soil properties (SOC, TN) can explain nitrate losses better than the N balance parameters. The weak-to-moderate (Field A) or moderate-to-strong correlations (Field B) were due to the complexity

of the nitrate leaching, as there are many influencing factors, such as denitrification (Cremer et al., 2018), hydrodynamic dispersion and molecular diffusion (Geries, 1989).

Further effects could cause differentiated nitrate leaching within heterogeneous fields. In addition to the yields of the main crops, the growth of catch crops in the high-yield zones can also benefit and thus more nitrate can be bound and saved from leaching (Ritter et al., 1998). Increased denitrification in these zones is also possible. However, the opposite effects could also occur. Increased TN content increase the N mineralisation potential. Incorrect post-harvest management (Askegaard et al., 2011), bare fallows (Tonitto et al., 2006), or poorly timed tillage (Hansen & Djurhuus, 1997) can result increased nitrate leaching in the high-yield zones.

Conclusion, outlook and further research

The examination of the hypothesis yielded the following results:

Hypothesis 1 On heterogeneous fields with uniform fertilization, high, environmentally hazardous N surpluses can occur in low-yield zones.

Higher N surpluses occurred on both study plots due to uniform N fertilization but lower yields and N uptakes in the low-yield zones.

Hypothesis 2 Site-specific N surplus determined with digital methods is a suitable indicator for nitrate leaching. The N surplus correlates closely with the nitrate stocks in the soil layer 0–2.5 m.

Weak positive correlations were found ($r=0.30$; $r=0.39$). There is a relation of the parameters but the correlations were not strong enough.

Hypothesis 3 The spatial distribution of soil organic carbon and soil total nitrogen content are closely related to the spatial distribution of N surpluses and nitrate stocks.

The SOC content correlated moderate with the yield and N uptake ($r=0.53$; $r=0.62$), similar as N surplus ($r=-0.51$; $r=-0.73$). The nitrate stocks in Field A could be explained by the SOC content equally, in Field B better than by N balancing (SOC: Field A: $r=-0.28$; Field B: $r=-0.60$; N surpluses: Field A: $r=0.30$; Field B: $r=0.39$). The spatial distribution of soil organic carbon and soil total nitrogen correlates negatively with nitrate stocks from deep drilling. In zones with higher soil organic carbon contents higher yields and N uptakes and thus lower N surpluses and less nitrate occurs.

Thus, hypotheses 1 and 3 were confirmed, hypothesis 2 was rejected.

The results of this work show that site-specific N balancing based on sensor and satellite data can be used to identify areas with a higher risk of nitrate leaching within arable fields.

Further approaches could be used to assess spatial nitrate leaching risk. A first validation of biomass potential maps (BPM) by multiyear sensor data showed stronger correlations to ground truth data than satellite data and the PROMET model. For spatial N balancing an algorithm is needed to transfer the relative distribution of NDVI to spatial N uptake.

The variation of N surpluses and nitrate stocks in uniformly managed fields with higher surpluses and nitrate stocks in low-yield zones arose the question if uniform fertilisation

of fields overestimates the yield potentials of low yield zones. Variable rate technologies could solve this issue if applying less nitrogen fertiliser in low yield zones. For example, in large, heterogeneous fields and in ecologically sensitive regions (water protection areas or soils with a high risk of nitrate leaching), this can help to determine the actual risk of nitrate losses more precisely and to reduce them through suitable measures. Sub-fields with high nitrate-leaching risk could be farmed more extensively or less fertilised.

However, further studies are necessary to enable the targeted use of digital methods to reduce nitrogen surplus. When used in water protection areas, the leachate rate should be modelled in a site-specific way to allow the analysis of nitrate profiles. The evaluation of hydrodynamic dispersion and molecular diffusion (Gerjes, 1989) and matrix flow is a major challenge. Therefore, a study was conducted using chloride as a tracer to investigate the leaching in different zones within the studied fields A and B.

Furthermore, the methodology must be comprehensively tested under various site and management conditions and, if necessary, adapted. Corresponding studies are currently being performed under the conditions of organic farming in the model region of Burghausen. Particular methodological challenges arise here from the modelling of the nitrogen fixation of legumes, the N transfer in the crop rotation and the lower crop yields, which require appropriate adjustment and calibration of the models. Perhaps more complex N balances are necessary to improve the relation between N surpluses and ground truth nitrate leaching measurements.

In the future, soil properties (SOC, TN) can also be recorded on a site-specific basis using digital methods. Heil & Schmidhalter (2021) provided that sufficient measurement accuracy is achieved. This would further expand the application possibilities of the methodological approach presented here.

Supplementary Information The online version contains supplementary material available at <https://doi.org/10.1007/s11119-022-09967-3>.

Funding Open Access funding enabled and organized by Projekt DEAL. This study was funded by the Bavarian State Ministry of Food, Agriculture and Forestry (Bayerisches Staatsministerium für Ernährung, Landwirtschaft und Forsten).

Declarations

Conflict of interest The authors declare that they have no conflict of interest.

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