89. Determination of critical nitrogen loss zones in drinking water protection areas with satellite-based algorithms

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Abstract

High nitrate concentrations in groundwater, driven by agricultural nitrogen (N) fertilization, remain a significant concern. This study introduced an N uptake algorithm for winter wheat at harvest, designed to calculate site-specific N surpluses as an indicator of nitrate losses. The algorithm integrated data from plot combine harvesters, Sentinel-2 satellite imagery at various dates, and georeferenced soil properties. A comparison of two statistical models revealed high correlations (R^2=0.77–0.84) and low errors (MAE=8–13 kg/ha) in calculating N uptake. Site-specific N balancing, using the developed algorithm and N fertilization data, enabled the identification of high nitrate leaching risks in low-yield areas within a drinking water protection area (N surplus >90 kg/ha).

Keywords: N uptake, nitrate, satellite data, site-specific N balancing, spatial variability

Introduction

Groundwater contaminated with high nitrate concentrations is mainly due to agricultural nitrogen (N) fertilization (Bijay-Singh and Craswell, 2021). There is evidence linking nitrate contamination in drinking water to health risks, including an increased risk of certain cancers (Picetti *et al.*, 2022). In Germany, efforts such as stricter N fertilizer regulations, the designation of red zones with limitations, and voluntary agreements for drinking water protection (e.g., cover crops in winter, organic farming, conversion of arable land into grassland) have been implemented (Schuster *et al.*, 2022). Despite measures, nitrate concentrations in groundwater have remained largely unchanged in recent decades (Meran *et al.*, 2021; Sundermann *et al.*, 2020). More effective mitigation strategies are needed. The use of digital technologies offers innovative possibilities for more precise and efficient practices to reduce nitrate levels in groundwater. Recent studies have revealed significant variability in nitrate leaching within agricultural fields, with particularly high risks in low-yield areas (Mittermayer *et al.*, 2021; Schuster *et al.*, 2023). In these zones, low yield and N uptake by crops combined with the widespread application of uniform N fertilization often leads to overfertilization and increased nitrate losses. Poor soil quality in such areas further exacerbates the problem by facilitating rapid water movement and nitrate leaching.

Field-level N balancing can mask sub-area variations, because positive and negative balances offset each other. Research on heterogeneous arable fields in southern Germany has shown that even with optimal field-level N balances (≈0 kg/ha per year), sub-areas can exhibit extreme N surpluses (>100 kg/ha per year) or significant negative balances (<-50 kg/ha per year) (Mittermayer *et al.*, 2022). These variations can be effectively captured using digitally calculated site-specific N balances, providing a more accurate representation of nitrate leaching risks. The method of site-specific N balancing is currently available as a scientific method that has been tested on more than 20 arable fields in southern Germany. It has not yet found its way into drinking water protection advice. So far, there are only examples of application in individual arable fields, but not in the entire drinking water protection area. Some prerequisites for practical application in drinking water protection are still lacking, above all proof of applicability under differentiated soil and climatic conditions, as well as an automated and thus cost-effective calculation of the site-specific N balances to determine the nitrate risk areas.

Site-specific N balancing requires at least two essential parameters: the N input (N fertilization) and the N output (N content of the harvested biomass). Various methods for site-specific N balancing were tested, including combine harvesters, tractor-mounted sensors, and satellite-based methods. Mittermayer *et al*. (2022) and Schuster *et al.* (2022) found all three methods suitable, with the highest accuracy from tractor-mounted sensor systems, followed by satellite systems, while combine systems showed greater discrepancies due to calibration issues. The tractor-mounted sensor approach directly measured N uptake at harvest, avoiding reliance on yield estimates. In contrast, combine harvesters and satellite methods estimated N uptake using yield data and average N content (Mittermayer *et al*., 2022), leading to distortions due to spatial variability in protein and N content (Morari *et al*., 2018). However, for large-scale applications, particularly in drinking water protection areas, satellite data remains the most viable option due to its capacity for comprehensive spatial coverage. While there is extensive research on measuring N uptake during vegetation for fertilization purposes, the direct modelling of N uptake at harvest on a large scale is still poorly understood. The aim of this project was to develop and validate satellite-based algorithms for modelling N uptake in winter wheat at the time of harvest for site-specific N balancing. Furthermore, the developed N uptake algorithm will be applied in a drinking water protection area, where site-specific N balances will be calculated, and areas with high nitrate leaching risks will be identified.

Material and methods

The data used in this study were gathered at various sites in southern Germany, including two research stations of the Technical University of Munich – Thalhausen (A) and Roggenstein (B) – which were used to develop an N uptake algorithm for winter wheat. These sites, located about 30 km north and west of Munich, have distinct soils and climates. Site C, located in Burghausen, about 100 km east of Munich in a drinking water protection area, was used to calculate site-specific N surpluses. Data were collected in 2018, 2019, 2021, 2022, 2023 and 2024. Crop yields were measured using a plot combine harvester as ground truth data for algorithm development. To complement these measurements, additional samples were collected from the harvested material in the cabin after each plot. These samples were allocated for laboratory analysis to primarily determine N content for calculating N uptake.

Figure 1. Collection of ground truth data at Field A5 (2023).

The study utilized Sentinel-2 satellite data, the German soil estimation survey (Blume *et al.*, 2016), georeferenced soil samples, elevation and climatic data to analyze N uptake at harvest. Sentinel-2 data from key growth stages (BBCH 31, 55, 65) (Meier 2018) were used, with the red edge inflection point (REIP) vegetation index as a primary indicator:

$$REIP = 700 + 40 * (((B4 + B7)/2) - B5)/(B6 - B5) \quad (1)$$

The REIP formula utilizes specific spectral bands from the Sentinel-2 satellite. These include the red band (B4) with a wavelength of 665 nm, as well as three red-edge bands: the first red-edge band (B5) at 705 nm, the second red-edge band (B6) at 740 nm, and the third red-edge band (B7) at 783 nm.

The German soil survey provides soil quality ratings (0–100) based on type, structure, and water availability (Blume *et al.*, 2016). Temperature and precipitation data from January to July were incorporated, along with field elevation data. Georeferenced soil samples were collected (depth: 0.3 m, 8 per hectare) from fields A2 and A3 to measure soil organic carbon (SOC), total Nitrogen (TN), phosphorus (P), potassium (K), and pH. Sample points were arranged in a systematic-random pattern and interpolated using kriging (to a 20 m×20 m resolution) matching Sentinel-2 grids. A variogram quantified spatial autocorrelation effects (Oliver and Webster 2015).

A linear model was derived using statistical regression considering all available predictors. To optimize the model, stepwise backward selection based on the Akaike Information Criterion (AIC) was applied, eliminating irrelevant or less informative variables. The dataset was split into 80% training data and 20% test data to validate the model's performance. Two models were developed to predict grain N uptake at harvest. Model 1 utilized open-access data, including Sentinel-2 imagery from BBCH 31, 55 and 65, elevation, temperature and precipitation data from January to July, and the German soil survey. Model 2 extended Model 1 by incorporating georeferenced soil properties (SOC, TN, P, K pH). The statistical models were evaluated using R-squared, mean absolute error (MAE), p-values, AIC to assess their fit and predictive performance.

For N balancing, the results of the newly developed N uptake algorithm were employed as N output. The N surplus (kg/ha per a) was determined by N balancing:

$$N\ surplus = N\text{-}Input - N\text{-}Output \quad (2)$$

The N input was the amount of N fertilizer uniformly applied to winter wheat test fields 2022 (at Site C in a drinking water protection area), with data provided directly by farmers. The N uptake and N

Table 1. Study fields for plot combine harvesting and ground truth data generation for algorithm development.

Year	Name	Size (ha)	Coordinates
2018	A1[1]	12.7	48°28′00.5″N 11°48′25.7″E
2019	A2[1]	6.1	48°25′46.3″N 11°40′40.7″E
2021	A3[1]	9.4	48°18′237.0″N 11°339442″E
2022	B1[2]	31.0	48°18′0534″N 11°339439″E
2023	A4[1]	5.3	48°429203″N 11°678326″E
2023	A5[1]	6.1	48°430931″N 11°681762″E
2024	A6[1]	4.4	48°431522″N 11°666526″E

[1] 30 km north of Munich, [2] 30 km west of Munich. A, research station Thalhausen; B, research station Roggenstein.

surplus calculations (Figures 2 and 3) at the drinking water protection area (Site C) are presented for the year 2022. N surplus was calculated at a high resolution for each 20×20-m grid cell, aligned with the Sentinel-2 raster data.

Results

Model 2 outperforms Model 1 with a higher R^2 (0.84 vs. 0.77) and a lower MAE (8 kg/ha vs. 13 kg/ha) (Table 2). Including georeferenced soil properties (e.g., SOC) in Model 2 improves prediction accuracy compared to the freely available data used in Model 1. Model 2 achieves better model fit, as indicated by a lower AIC, demonstrating the added value of detailed soil data.

Table 2. Comparison of models for derivation of N uptake algorithm.

Model	Initial variables included	Final predictors used	R^2	MAE (kg/ha)
1	Sentinel-2 BBCH 31, 55, 65; German soil appraisal; Weather data (temperature and precipitation January–July); Height	Sentinel-2, BBCH 31 BBCH 55, BBCH 65; German soil appraisal; Height; Temperature (January–May)	0.77	13
2	Sentinel-2 BBCH 31, 55, 65; German soil appraisal; Weather data; (SOC, TN, P, K pH).	Sentinel-2 BBCH 31, BBCH 55, BBCH 65; SOC; Temperature (Feb–May)	0.84	7

For site-specific N uptake calculation, Model 1 was chosen because there are no georeferenced soil samples in site C (drinking water protection area in Burghausen), which is also a common limitation in practical applications.

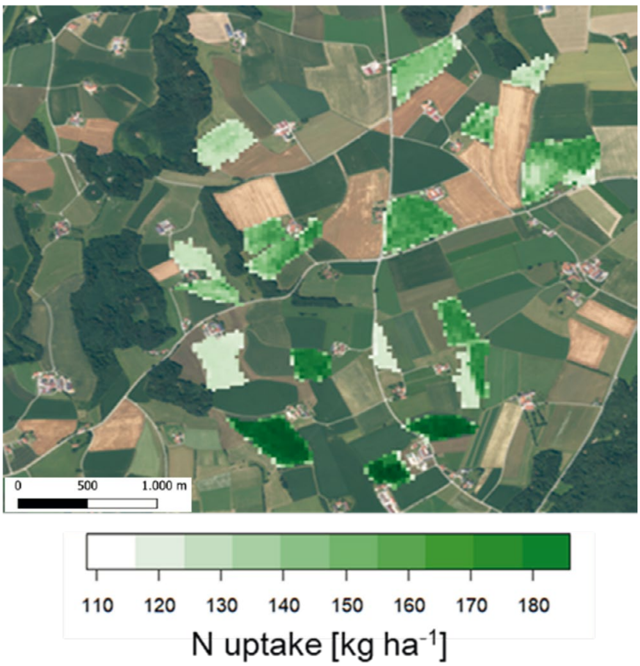

Figure 2. N uptake from Model 1 in winter wheat fields (2022) at Site C within drinking water protection area.

The N uptake in winter wheat fields at Site C during 2022 shows significant spatial variability (Figure 2). The colour scale ranges from white/light green (low N uptake: <110 kg/ha) to dark green (high N uptake: >180 kg/ha). The mean N uptake across all fields is 160 kg/ha.
By N balancing (N-Input–N-Output), significant differences in the N surplus are evident. The color scale ranges from white/light pink (low N surplus: <20 kg/ha) to dark red/black (high surplus: >90 kg/ha). N Surplus patterns are also observed across continuous zones that extend beyond individual field boundaries. The mean N surplus across all fields is 65 kg/ha.

Discussion

In recent years, many approaches to reducing nitrate pollution in drinking water protection areas have shown limited effectiveness, often due to the implementation of uniform measures that fail to account for spatial variability within fields. This is despite the well-established knowledge that many croplands exhibit spatial differences in yields (Blackmore *et al.*, 2003). This study demonstrates how satellite-based algorithms and site-specific N balancing can address these shortcomings. By identifying critical nitrate leaching zones, these tools offer targeted solutions for effective groundwater protection.
In this study, georeferenced SOC data outperforms the German soil survey (Model 2 vs. Model 1). However, the reliance on labour-intensive soil sampling limits its widespread application. To address this limitation, the development and adoption of devices capable of automatically measuring SOC (Tavakoli *et al.*, 2024), would provide substantial benefits.
Site-specific N balancing has shown strong potential for addressing nitrate leaching risks, with studies by Mittermayer *et al.* (2021) and Schuster *et al.* (2022) shown correlations of up to r=0.82 between N surpluses and measured nitrate concentrations, particularly in low-yield areas.

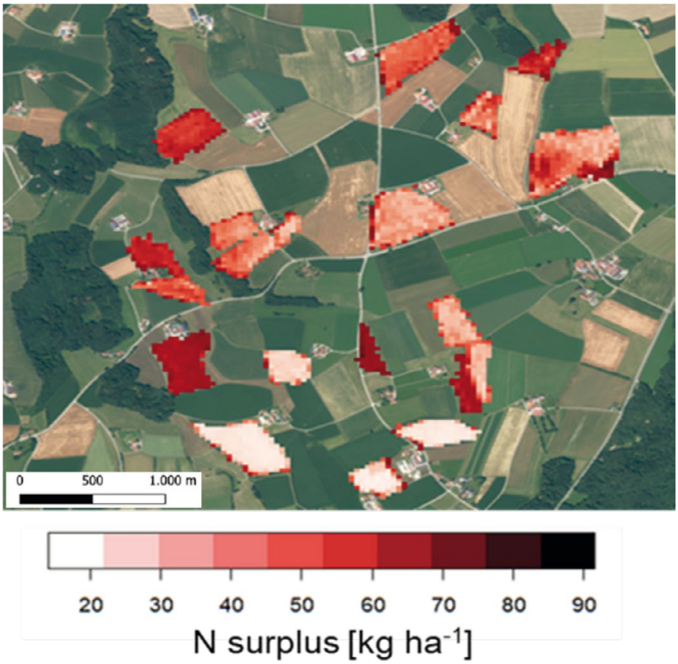

Figure 3. N surplus in winter wheat fields (2022) at Site C within drinking water protection areas, calculated by N balancing (N input–N uptake).

The site-specific N surplus calculated in this study often exceeds the recommended threshold of 50 kg/ha, particularly in low-yield areas. At Site C, nitrate levels in the groundwater are critically high, reaching 50 mg/l. Removing sub-areas with high N surpluses and implementing targeted measures – such as extensification, agroforestry, and reducing mineral N fertilization in low-yield areas – can significantly enhance the effectiveness of these measures. Calculating and modelling such scenarios is essential to understand their influence on nitrate leaching comprehensively. For instance, reducing the N surplus from 65 kg/ha to 30 kg/ha on average could lead to significant reductions in nitrate leaching and improve groundwater quality. Integrating these data into models assessing nitrate leaching risks is essential for accurately identifying high-risk areas and developing more effective management strategies. Such modelling provides valuable
insights into the environmental benefits of optimized N management practices and supports informed decision-making for sustainable agriculture (Donauer *et al.*, 2023). These advancements can improve both the precision and scalability of N balancing in agricultural systems.

Conclusions

The developed N uptake algorithm, based on satellite data, delivers reliable results and establishes a strong foundation for effective site-specific N balancing. By integrating data from plot combine harvesters, Sentinel-2 imagery, and georeferenced soil properties, the algorithm demonstrates the potential of satellite-based approaches to identify critical N loss zones in drinking water protection areas. The N uptake algorithm demonstrates high accuracy, validated with ground-truth data, with Model 2 achieving an R^2 of 0.84 and an MAE of 8 kg/ha. While Model 2 outperformed Model 1 by incorporating georeferenced soil properties, Model 1 proved more practical for large-scale applications where detailed soil data is unavailable.
The site-specific N balancing approach revealed substantial heterogeneity in N surpluses within fields, particularly in low-yield zones, where higher N surpluses were observed. By utilizing satellite-based data, this approach provides a scalable and cost-effective solution to identify high-risk areas and improve N use efficiency in drinking water protection areas. It accounts for spatial variability and enables the implementation of more targeted measures, avoiding the inefficiencies of a uniform application strategy.

Acknowledgment

This study was funded by the Bavarian State Ministry of Food, Agriculture, and Forestry.

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