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Evaluation of crop model-based simplified marginal net return maximising nitrogen application rates on site-specific level in maize

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Abstract

Crop growth models such as DSSAT-CERES-Maize have proven to be useful for analysing plant growth and yield within homogenous land units. The paper presents results of newly developed model-based site-specific Soil Profile Optimisation (SPO) tools in combination with an updated version of an already published Nitrogen Prescription Model (NPM). Site-specific soil profiles were generated through an inverse modelling approach based on measured site-specific yield (point-based) and tops weight (above-ground biomass time-series) and evaluated. Site-specific soil profiles generated based only on measured yield variability were able to explain 72% (R^2 0.72) of yield variability (dependent variable) based on selected soil profile input parameters (independent variable). Site-specific soil profiles generated based on measured yield and tops variability simultaneously (multiple target variable) explained 68% of yield variability (R^2 0.68). The NPM uses the SPO generated site-specific soil profiles for economic evaluation of site-specific N application rates. NPM simulated N application rates, aiming at the maximisation of marginal net return (MNR) were 25% lower compared to the uniform N application rates with an assumed grain and N price of 0.17 and 0.3 Euro kg^{-1} respectively, under rainfed conditions over three years based on soil profiles generated via an inverse modelling approach only from measured yield variability (one target variable). N application rates were 28% lower when based on soil profiles generated from simultaneously included grain and tops variability in the inverse modelling approach. The results highlight the importance of site-specific fertilizer management when maximising MNR.

Keywords DSSAT-CERES-Maize · Site-specific N management · Marginal net return

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Introduction

Maize production in Germany plays an important role in society. Aspirations towards plant-based renewable energy supported under the German Renewable Act had an essential impact on maize production while increasing the negative side pressure on the environment (Theuerl et al., 2019). Maize production relies heavily on the use of nitrogen (N) fertilizer for attaining higher yield. Due to problems in the production and supply of N-based fertilizer caused by the coronavirus and the war in Ukraine, prices got unpredictable, with practical implications on maize production for food or energy. Basic premise of Precision Agriculture (PA) and site-specific management of agricultural production inputs (e.g. nitrogen fertiliser) is to maximise marginal net return (MNR) while taking in-field heterogeneity into account. Site-specific units do not necessarily have to be "truly" homogenous in every sense, but homogenous enough to be uniformly treated in practice. Hence, it is important to have means for quantifying the degree of in-field homogeneity/heterogeneity. Historical data of site-specific yield mapping can be a useful indicator of in-field heterogeneity.

Crop growth models are mathematical models that simulate plant growth based on interaction of genetics, environment and management practices on a daily basis in order to simulate in-season biomass accumulation and partitioning among different plant organs (Boote et al., 2010; Hoogenboom et al., 2019). Plant growth is simulated on a daily basis from planting to harvest as a function of specific environmental factors such as solar radiation, temperatures, precipitation, and agricultural production inputs used in crop production. Crop growth models were originally developed for simulating crop growth on a field scale, but are being adapted to work at site-specific level (Batchelor et al., 2002; Gobbo et al., 2022; Paz et al., 1999; Thorp et al., 2008), due to availability of more detailed information measured on site-specific scale (sensor-based) and importance of smaller scales in maximising yield and MNR of already highly productive crop production. Crop growth models offer a unique overview of most factors affecting crop growth and production within the framework of yield defining factors (potential yield) with respect to yield limiting factors (water and nutrients) and reducing factors (pests, leaf diseases etc.). Crop growth models are commonly used for evaluating specific management practice impacts on plant development and yield on a field scale (homogeneous land unit). Thus, in-field site-specific heterogeneity (e.g., heterogenous soil properties) is often averaged to reflect field scale (a form of field-specific soil characterisation). This approach is acceptable for demonstrating the general impact of specific management decisions (e.g. planting date, amount of fertiliser etc.) on a field scale and in cases where the field is relatively homogeneous. More generally, field-scale approaches use *field-specific soil characterisation and initial conditions* for simulating field-specific yields. Here, the entire field is assumed to be a homogeneous land area unit. Site-specific yield variability is relatively easily quantifiable with on-board sensors mounted on combine harvesters with relatively low costs for data acquirement. In cases where in-field soil heterogeneity is present and results in site-specifically variable yield, field specific soil profiles (one soil profile in crop model input) are not able to capture and explain the measured yield variability. In order to capture and explain in-field yield variability either site-specific soil measurements have to be conducted or an *inverse* crop modelling approach can be used for deriving site-specific soil profiles (Braga & Jones, 2004). Within this study, the DSSAT-CERES-Maize crop growth model (Hoogenboom et al., 2021; Jones et al., 2003) was used for evaluating specific aspects of N fertiliser as yield limiting factor under rainfed conditions (observed). Based on the measured site-specific yield and above-ground biomass, in the current study more representative site-specific soil profiles were derived with inverse modelling techniques based on a newly developed Soil Profile Optimisation tool (SPO) (Trenz et al., 2023). An updated version of the published site-specific Nitrogen Prescription Model (NPM) (Memic et al., 2019) that uses SPO generated site-specific soil profiles was used for site-specific MNR maximising N prescription sensitivity analysis based on grain and N fertiliser prices. The NPM tool was used for testing the following hypothesis: *when compared to the common agricultural practice of uniform N application rate, variable N application rates are expected to lead to higher marginal net return while reducing the amount of applied N on site-specific level.*

The hypothesis was tested through crop model-based evaluation of the economic implications of site-specific N management in maize, by comparing two different scenarios: (1) rainfed uniform N application (common agricultural practice), (2) rainfed MNR maximising N application rates based on NPM, with assumed grain and N prices 0.17 and 0.3 Euro kg^{-1}, respectively. The analysis was conducted based on different optimization strategies: site-specific soil characterization based on measured site-specific yield and above-ground biomass. The SPO tool was already made available at GitHub (https://github.com/memicemir). The NPM tool will be made available at the same GitHub account as soon as user guidelines are ready.

The paper is an extended version of the conference contribution presented at 14th European Precision Agriculture Conference in Bologna (Italy) in 2023 (Memic et al., 2023).

Materials and methods

Case study description—Riech field

Maize was planted in 2006, 2007 and 2008 at University of Hohenheim agricultural research station Ihinger Hof (Germany). The field was divided into 80 site-specific units (0.125 ha) to investigate the potential of variable N management. Variable N management was compared to a control treatment representing the common farmers' N management practice of 160 kg N ha^{-1} (uniform N application of 30 kg N shortly before planting and 130 kg N ha^{-1} approximately two weeks after planting) (Link et al., 2013). Size and positioning of designated site-specific units were kept constant over three years. Yield was measured site-specifically with yield mapping technology on a combine harvester over three years. In addition, above-ground biomass sample cuts were made three times in 20 site-specific units during the vegetation period, at 4th leaf stage (BBCH 14), flowering (BBCH 65) and at maturity (BBCH 90), for additional crop model evaluation (Link et al., 2013) over three years. The focus of this study was kept on these 20 site-specific units due to availability of the destructively collected biomass-related samples. The soil at the experimental site, as determined based on soil texture analysis, was characterised as heavy calcareous brown earth. This soil contains high clay and silt amounts (Link et al., 2013). 20 site-specific units investigated within the current study were classified as silty clay and silty clay loam with 7.2 pH and average soil organic matter being 2.6%. Weather data was collected at a weather station located at Ihinger Hof. Soil preparation, planting, harvest, fertiliser and plant protection management was conducted according to common agricultural practice at the time (for more information refer to Link et al., 2013). The precipitation patterns of the three seasons are shown in a form of cumulative amount in mm as days after planting Fig. 1.

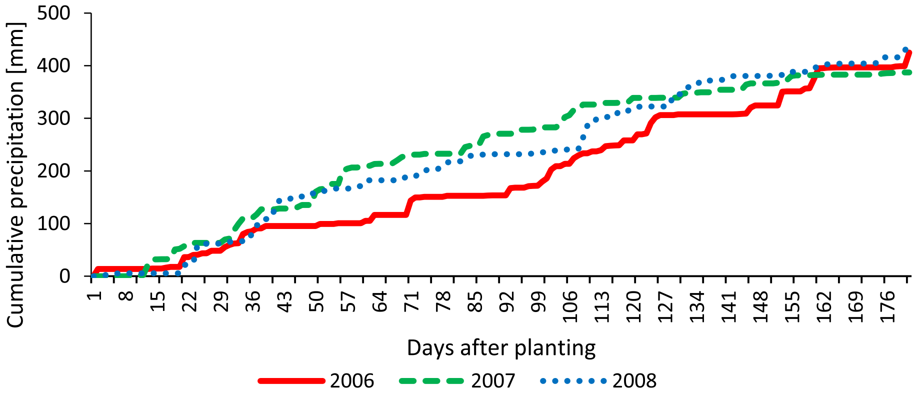


Fig. 1 Cumulative precipitation [mm] observed at the local weather station (2006–2008)

Site-specific soil characterisation—invers modelling

The SPO allows users to optimise soil profile parameters in the standard DSSAT soil profile. The software offers the capability to optimise parameters, both those defined for the entire soil profile (e.g. runoff curve) and layer-based parameters (e.g. soil water lower limit, upper limit, root growth factor, etc.) (Trenz et al., 2023). Soil profile characterisation used in DSSAT models is commonly conducted based on measurements of soil texture, bulk density etc., which are then used for estimating soil layer-based water lower limit, upper limit, etc. based on pedo-transfer functions (Saxton et al., 1986).The pedo-transfer function approach is commonly used due to costly and labours nature of acquiring soil related data required for crop modelling. Because of this minimum input data approach (only soil texture), potential uncertainty may occur in pedo-transfer function-based soil input parameters that might be improved indirectly based on indicators easier to measure. *The SPO approach enables the user to adjust soil layer-based parameters affecting soil water holding capacity estimated based on pedo-transfer functions, to a certain degree.* For this study, soil water lower limit (SLLL), root growth factor (SRGF) and runoff curve (SLRO) were targeted for optimisation in 20 site-specific units over three years, due to available site-specific yield and tops (above-ground biomass) measurements.

In order to set an inverse *modelling* technique into place, it was assumed that measured crop data could indirectly provide insight into soil water holding capacity and thus contribute to the explanation of measured yield variability by minimising the difference between simulated and measured yield and tops weight at site-specific level (Trenz et al., 2023). The inverse modelling approach implemented in the SPO tool enables users to use all available measured in-season above-ground biomass data (e.g. leaf area index, canopy weight, leaf weight, etc.). Normalised root mean square error minimisation technique implemented in Time-Series cultivar coefficient Estimation tool for DSSAT (Memic et al., 2021) was implemented in SPO as it enables the use of measured plant biomass (destructive sampling) or sensor data with different unit scales as target variable for estimating indirectly specific crop model input parameters from observations (multiple target variables).

The user can use a field-specific soil profile and modify it with SPO to provide a better statistical fit based on measured site-specific yield or other crop variables on a site-specific level. The main premise of site-specific zone delineation is the creation of sub-field units that are "homogenous" enough and can be treated in management practices homogenously. In cases when in-field soil heterogeneity is present and results in site-specifically variable yield, field specific soil profile (one soil profile in crop model input) is not able to capture and explain the yield variability measured (Fig. 2 a and b). In order to capture and explain in-field yield variability either site-specific soil measurements have to be conducted or an *inverse crop modelling approach* can be used for generating site-specific soil profiles based on measured yield variability. Based on the measurable end-of-season yield on site-specific level more representative site-specific crop model soil profiles can be generated with inverse modelling techniques (Fig. 2c).

Inverse modelling techniques can be depicted as optimisation of objective functions by means of input parameter sensitivity analysis based on measured variables (targets), which are easier attainable. The SPO is used for modifying specific soil profile parameters in the process of repetitive execution of the crop growth model and subsequent comparison and error minimization between simulations and measurements of target variables. A more detailed description of the SPO inverse modelling can be found in Trenz et al. (2023). For this study, in addition to the published grain target variable (end-of-season) approach in Trenz et al. (2023) tops weight target variable (time-series) and a combination of the grain and tops weight target variables approach were investigated:

1. Target variable GRAIN **(G)**—*end-of-season (point-based)*
2. Target variable TOPS **(T)—multiple in-season (time-series-based)**
3. Target variables GRAIN and TOPS **(G–T)—combination**

Input parameters sensitivity analysis—exhaustive gridding

Technically speaking crop growth models are a set of equations describing the behaviour of specific natural phenomena (in this case plant) under specific conditions over time. Equations in crop growth models are commonly the result of direct measurements or regression-based correlations used for mimicking biomass accumulation and plant development in digital form. All equations used in crop models rely on input parameter values that can meaningfully reflect physical and physiological processes with respect to soil and atmosphere conditions. Due to the nature of correlation regressions and mathematical frameworks underlying the crop growth model, input parameters have limited range (minima and maxima range), if physics and physiology engraved in the crop modelling algorithm are to be sustained. As a result, this means that pure mathematical fit cannot overrule basic agronomic restraints reflecting real natural phenomena (e.g., plant

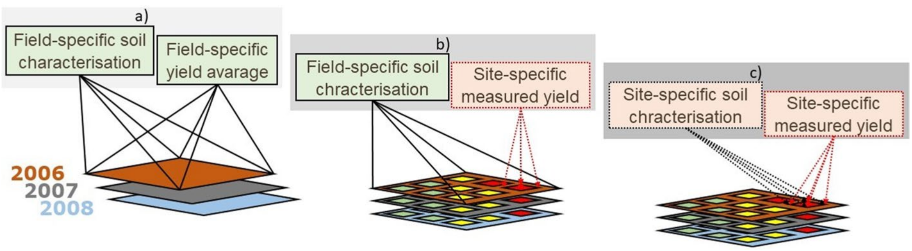


Fig. 2 Conceptual framework of transition from field-scale soil characterisation to site-specific soil characterisation based on measured site-specific biomass variability

growth and biomass accumulation). This means in concrete example of crop modelling that every input parameter has minimum and maximum input parameter values that have to be respected (e.g. input parameters defining size of a leaf have to obey observation-based minimum and maximum size). Due to crop model complexity, huge number of parameters with sometimes large gaps between minimum and maximum values of input parameters can result in extremely challenging sensitivity analysis and potential multiple optima solutions. The SPO algorithm was designed in a way that enables users to conduct semi-automatically sensitivity analysis of specific input parameters in a user-friendly manner. Among various methods used for defining potential scenarios based on minima and maxima range, random probabilistic methods or exhaustive gridding methods can be used to explore how the algorithm reacts to changes in input values. Even though exhaustive gridding method is a primitive and deterministic approach (Duan et al., 1992) in search of optima it was selected for SPO algorithm because it enables the users to conduct more systemic sensitivity analysis of input parameters and their influence on output variables. If not used carefully exhaustive gridding method may lead to long time-consuming analysis due to amount of discretization steps for every parameter range (number of scenarios) and over-fitting of the data. However, if used strategically it can be fast (e.g. range reduction methods) and provide systemic insight into parameter sensitivity in more systemic way when compared to any other randomised or probabilistic methods. Two applications of exhaustive gridding method are shown in Table 1: high density (HD) (Trenz et al., 2023) and sufficient density (SD) of number of discretization steps for demonstrating the meaning of the exhaustive gridding method with respect to number of scenarios resulting from minima and maxima range with respect to intermediate steps. The HD sensitivity analysis was published and described in detail by Trenz et al. (2023). As it can be seen in Table 1, primitive deterministic application of exhaustive gridding method with *high density (HD)* of discretization steps in specific range when considered in the context of three years (each year 20 site-specific units) will require crop model to be executed *196 800* times *(60* $\times$ *3280)*. Further *sufficient density (SD)* of discretization steps range will require the model to be executed *11 340* times *(60* $\times$ *189)*. The number of executed scenarios have practical implications in the context of computational power and required time. For example, the values for SLLL in Table 1 and SPO interface are used as a form of multipliers which modify the available parameter values in crop model input files (Trenz et al., 2023). This means that if field scale SLLL (original SLLL) in the existing DSSAT soil profile is multiplied with 0.8,

Table 1 Exhaustive gridding methods HD (Trenz et al., 2023) and SD with corresponding minima, maxima ranges based on discretization steps

Exhaustive gridding	Param	Minima	Maxima	Step	# scenarios
High density (HD)	SLRO	60	100	10	5
	SLLL	0.8	1.2	0.01	41
	SRGF	0.7	1.3	0.05	16
Total number					3280
Sufficient density (SD)	SLRO	60	100	20	3
	SLLL	0.8	1.2	0.05	9
	SRGF	0.7	1.3	0.10	7
Total number					189

Table 2 Example of SPO sensitivity analysis based on minima/maxima and discretization step: 0.8 (minima), 1.2 (maxima) and 0.05 (step) Table 1 SD section

Number of scenarios	1	2	3	4	5	6	7	8	9
SPO coeff. setup (interface—multipliers)	0.80	0.85	0.90	0.95	1.00	1.05	1.10	1.15	1.20
Percentage equivalent	− 20	− 15	− 10	− 5	Original SLLL	+5	+10	+15	+20

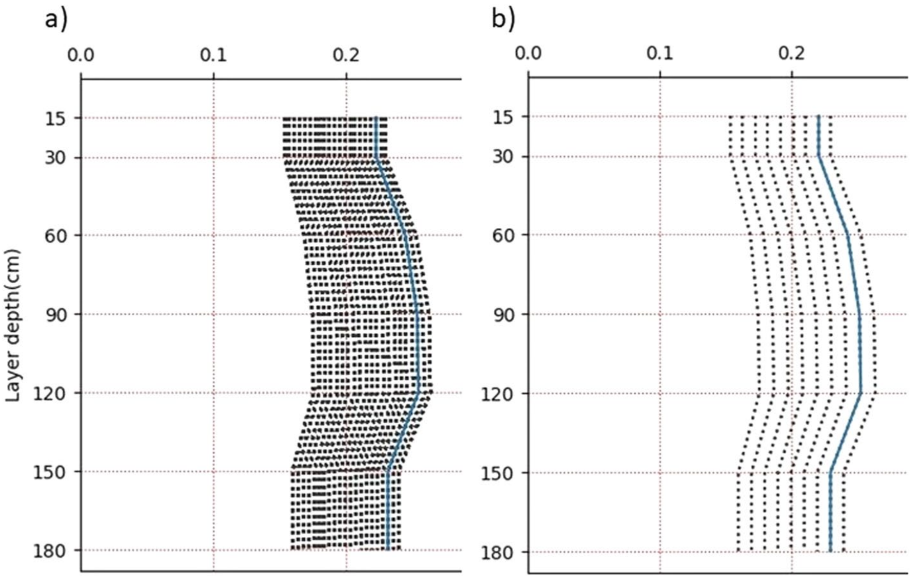


Fig. 3 High density (HD) (**a**) and Sufficient Density SD (**b**) exhaustive gridding example for SLLL based on discretization steps with respect to minima and maxima range

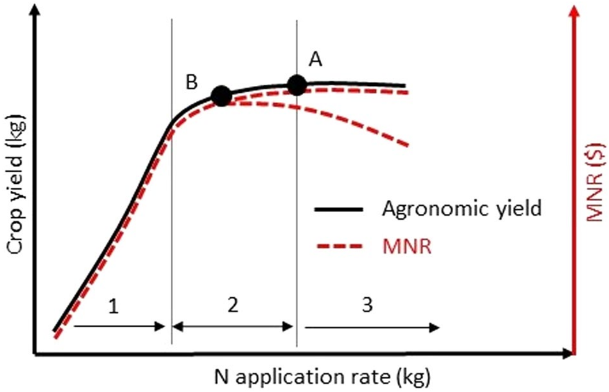
0.85 etc., it is effectively reduced by 20%, 15% etc. Table 2 shows the process of input parameter sensitivity analysis in search of optima, as it was described in detail in Trenz et al., (2023).

In Fig. 3, specifically for SLLL parameter, this principle is shown graphically with respect to HD and SD number of sensitivity analysis scenarios described in Table 1.

Site-specific Nitrogen Prescription Model (NPM)

Based on the assumption of water stress-free conditions, yield response to applied N can be depicted in three phases: (i) at lower N application rates yield response to applied N is exponential-like (high N utilisation efficiency, Fig. 4, segment 1), (ii) after a certain amount of applied N, yield response is still positive but decreasing (lower N utilisation efficiency) (Fig. 4, segment 2); (iii) at specific N application rate, yield response reaches a plateau where additional N application does not lead to further yield increases (N utilisation efficiency equals zero, Fig. 4, segment 3).

Fig. 4 Yield response to N application with corresponding MNR



The basic NPM theoretical assumption is: *Crop yield in a fully parameterised crop model is the result of applied N.* The updated NPM is based on the same principle as the former version. Sensitivity analysis is conducted by investigating yield response to different N kg ha^{-1} amounts (e.g. 0, 10, 20, …). The NPM algorithm was designed as a form of marginal return analysis tool. Marginal return analysis looks into the marginal increase of specific outputs resulting from additional one-unit increase (this case additional 10 kg N ha^{-1} at each run) of variable input, without other crop model input parameters being modified (ceteris paribus). In the process of analysing marginal return of additional N unit, crop model is repeatedly executed and yield response for every marginal N input unit is calculated. The crop model is executed for each application rate and simulated yield is extracted for calculating simplified MNR (Eq. 1). For the study, original parametrisation of crop model was based on common N practice (160 kg N ha^{-1}), measured weather data, cultivar genetics and in- and end-of-season destructive above-ground biomass cuts collected over three years. Fully parametrised crop model in-season above-ground biomass and end-of-season yield was expected to correctly respond to different N amounts and enable analysis of simplified MNR maximising N application rates. In this simplified MNR analysis, N application rate with highest MNR, based on prices, was selected as optimal N prescription rate for each site-specific unit (Basso et al., 2012; Paz et al., 1999).

$$\text{MNR} = \text{Grain (kg)} * \text{Grain Price (€/kg)} - \text{N (kg)} * \text{N Price (€/kg)} \tag{1}$$

If N price was zero, agronomic yield maximising N application rate would also maximise MNR (Fig. 4, point A). Since N price was not zero, MNR maximising N application rate was always lower than the one maximising agronomic yield. After a certain N application rate, even though there was the potential of increasing agronomic yield, additional kg of N did not produce enough yield to cover the costs of applied N (Fig. 4, point B).

Results

Site-specific yield based on field-scale soil characterisation

Figure 5a shows simulated and measured yield results on a field-scale over three years. Field-scale measurement was a result of an average of 20 site-specific measured yields for each year. Field-specific soil profile was a result of averaging 20 soil profiles that were

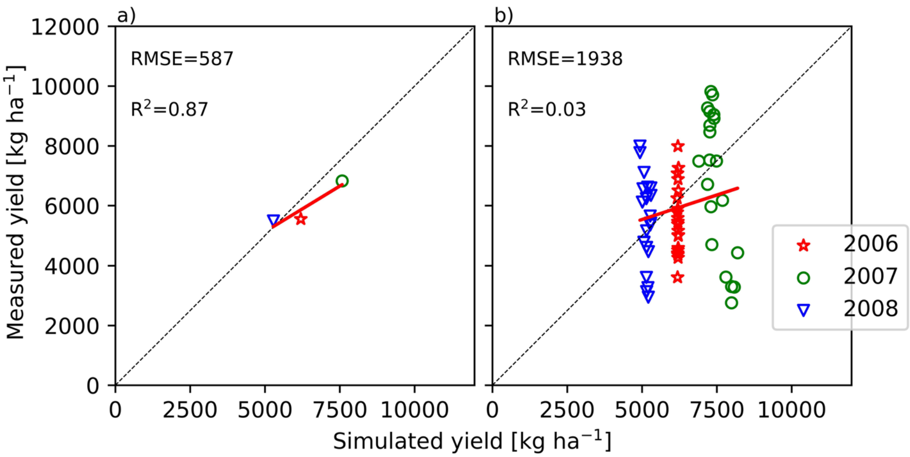


Fig. 5 Simulated and measured yield shown in 1:1 graphs for: field-specific soil characterisation and field-specific measured yield (**a**), field-specific soil characterisation with site-specific measured yield (**b**)

used. Field-specific regression fit indicated a relatively good agreement of simulated and measured yield with R^2 of 0.87 and RMSE of 587 kg ha^{-1} (n = 3) (Fig. 5a). Based on the field-scale analysis (Fig. 5a), it can be concluded that the model performed well and the results seem to be consistent. Since field-specific yield was a result of 20 site-specific units average, therefore, further analysis was conducted to understand how homogenous the field "truly" was. In Fig. 5b, the DSSAT crop model was used with field-specific soil profile for simulating yield for 20 site-specific units over three years. Model results were compared to the site-specific measured yield of 20 site-specific units over three years. Figure 5b indicated that field-specific soil profile was not able to explain site-specific yield variability with R^2 0.03 and RMSE 1938 kg ha^{-1} (n = 60) over three years.

In 2006, yield average over 20 site-specific units was 5548 kg ha^{-1} with standard deviation of 1156 kg ha^{-1} (Fig. 6). In 2007, yield average was 6824 kg ha^{-1}, and 5485 kg ha^{-1} in 2008 with a standard deviation of 2391 kg ha^{-1} and 1493 kg ha^{-1}, respectively (Fig. 6). These values are an important indicator of the given field heterogeneity, while they are indirectly estimated based on measured site-specific yield. In 2006, 2007, and 2008, yield medians were 5417, 7488, and 5532 kg ha^{-1}, respectively (Fig. 6). Large differences

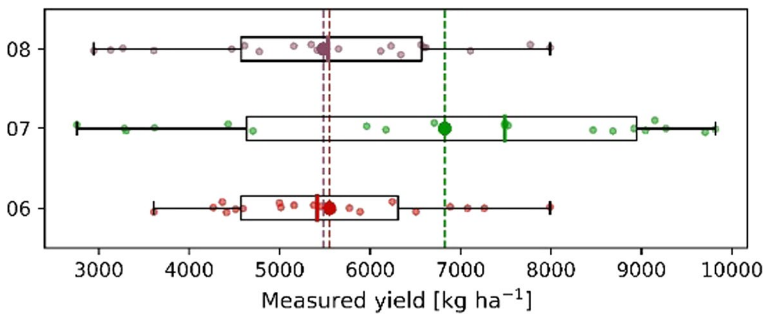


Fig. 6 Boxplot for three seasons 2006 (06), 2007 (07) and 2008 (08) with corresponding yield measurements, average and median values

between the median and average yield in 2007 with a standard deviation of 2391 kg ha^{-1} raised additional concerns on the representativeness of the determined field average.

Target variable GRAIN (G)—SD gridding based site-specific soil characterisation

In Fig. 7a, results of the implemented SPO inverse modelling approach are shown where site-specific yield variability (n = 60, yield as explanatory target variable) measured over three years was used for deriving site-specific soil profiles (n = 20) with R^2 0.72 and RMSE 937 kg ha^{-1}. The main assumption of the approach was that site-specific soil profiles used over three years can reflect and capture yield variability (dependent variable) caused by varying factors from season to season with respect to spatial and temporal variability. Within this study, spatial variability refers to the site-specific yield variability within a field during one season and temporal variability to the impact of seasons from year-to-year yield variability. Temporal variability at small scale within one season (year) may have huge impact on yield variability as well but was not investigated in detail. The interpretation of the results when considered within the used crop model R^2 0.72 and RMSE 973 kg ha^{-1} indicated that the model was able to explain 72% of site-specific yield variability (dependent variable yield) by soil profile parameterization (independent variable) conducted with SD gridding. Overall analysis of the data for 20 site-specific units over 3 years (60 measurements in total) is a good indicator of crop model "prediction" ability with respect to spatial variability. To understand the ability of site-specific soil profiles to reflect seasonality (temporal variability) each year was investigated independently (20 yield measurements). As it can be seen in Fig. 7b the ability of site-specific soil profiles was evaluated at seasonal level. Based on the results, it looks like site-specific soil profiles were able to explain around 95% of site-specific yield variability in 2007 and 2008, with only 2% of site-specific yield variability in 2006.

Due to a high temporal variability in 2006, the explanatory power of the model in this specific year was quite low wherefore the overall, good accuracy or ability of site-specific soil profiles to explain site-specific yield variability over three years might not have practical implications.

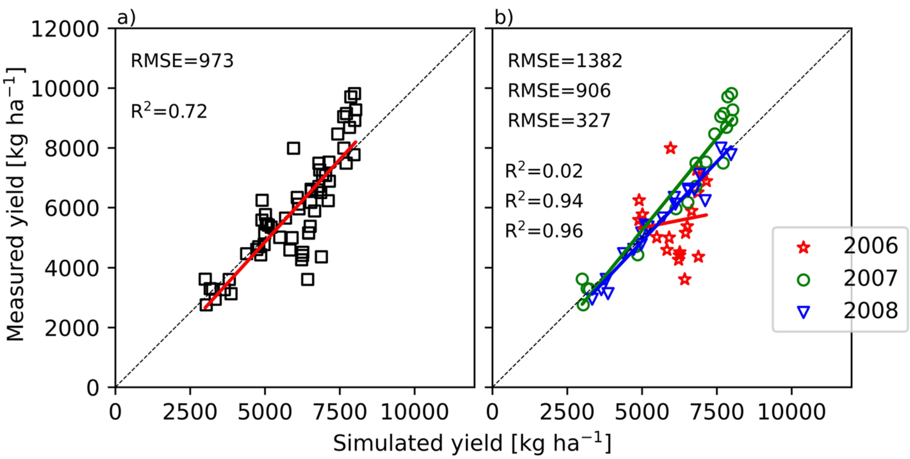


Fig. 7 Simulated and measured yield for site-specific soil profiles with all three seasons (n = 60) (**a**) and season based for three seasons, (**b**) based on site-specific grain variability as target variable

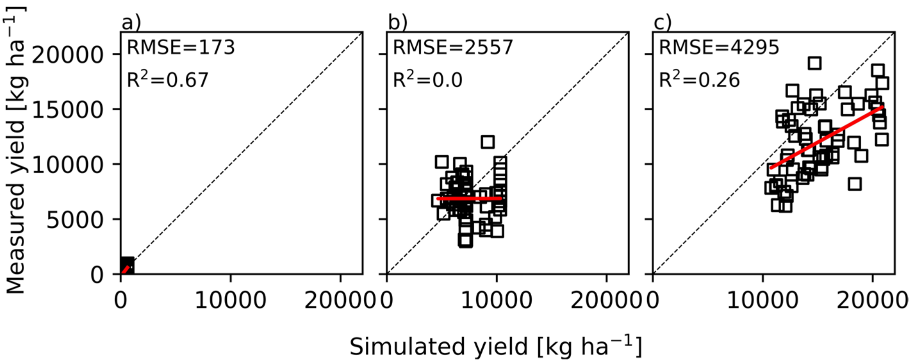


Fig. 8 Simulated and measured tops weight (above-ground biomass) for three sample cuts: BBCH14 (**a**), 65 (**b**), and 90 (**c**), with a total 180 measurements over three years (each sample cut 60 measurements)

To understand crop model parametrization success rate, additional time-series data of above-ground biomass was used with three in-season sample cuts for each site-specific unit over three years of evaluation. In Fig. 8 three sample cuts at BBCH-14 (a), BBCH-65 (b) and BBCH-90 (c) are shown. Ideally if crop growth model parametrization is correct it would mean that all ratios in the model are accurate and adjustment of any of those factors would result in correct biomass accumulation response. As we can see in Fig. 8 above-ground biomass was not simulated satisfactory overall. To delve deeper into the underlying issues, the subsequent section of this paper will focus on concurrently targeting grain and tops weight during the derivation of site-specific soil profiles.

Target variable TOPS (T)—SD gridding based site-specific soil characterization

Site-specific soil profiles for 20 site-specific units have been derived based on time-series site-specific tops weight measurements (180 in total over three years). In Fig. 9, three sample cuts at BBCH-14 (a), BBCH-65 (b) and BBCH-90 (c) are shown after SPO calibration. Time-series data of three sample cuts and simulations are shown separately in 1:1 graphs

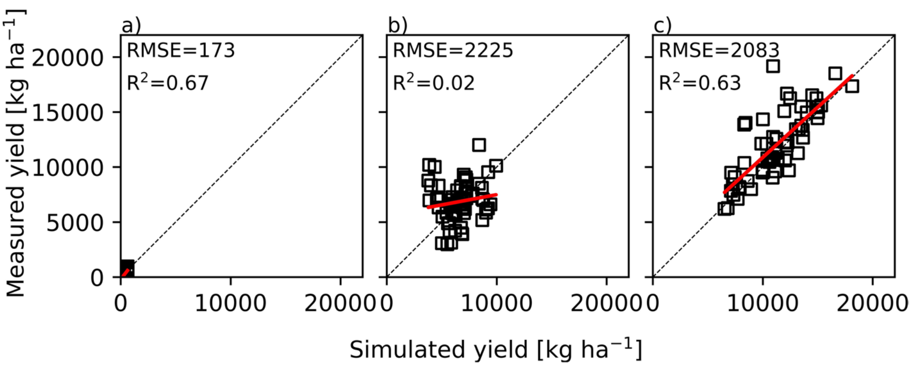


Fig. 9 Simulated and measured tops weight (above-ground biomass) for three sample cuts: BBCH14 (**a**), 65 (**b**) and 90 (**c**), with in total 180 measurements over three years

to show efficiency of the optimisation for each of them separately. As it can be seen in the Fig. 9 simulations of: BBCH-14 cut (a) and end-of-season cut (c) (BBCH-90) with R^2 0.67 and 0.63, respectively are satisfactory. The BBCH-65 sample cut in Fig. 9b has very low R^2 0.02. This is an optimisation challenge commonly faced when evaluating and optimising crop models with time-series data.

During site-specific soil profile optimization based on one target variable "tops" the other output variable grain weight got less accurate with R^2 0.34 (Fig. 10).

Target GRAIN and TOPS simultaneously (G-T)—SD gridding based site-specific soil characterization

The SPO software was used for deriving site-specific soil profiles based on end-of-season grain yield and in-season observations of tops weight (three sample cuts) simultaneously. Multi target variable based soil profile optimization was conducted in principle as described in Memic et al. (2021). As it can be seen in Fig. 11 overall explanatory power of site-specific soil profiles when it comes to grain was reduced, with R^2 0.68, when compared to 0.72 (Fig. 7a). Season-based explanatory power of newly derived site-specific soil profiles based on grain and tops weight had minor changes when compared to the scenario where only grain was the target variable of optimization. It is expected that multi-target variable based site-specific soil profiles have better practical application potential when used for site-specific N optimization, due to expected better underlying crop model parametrization.

When it comes to tops weight as shown in Fig. 12, three different sample cuts were shown separately. In the process of multiple target variable based site-specific soil profile optimization usually mathematical compromises based on error minimization methods are achieved, and it seems that soil profile parameters were more effective in explaining grain yield variability than above-ground biomass. Above-ground biomass parameters include different plant organs: leaf, stem, pod, etc. Further analysis into leaf the stem to pod ratio is required to understand the reason for lower explanatory power of above-ground biomass measurements when it comes to site-specific soil profiling.

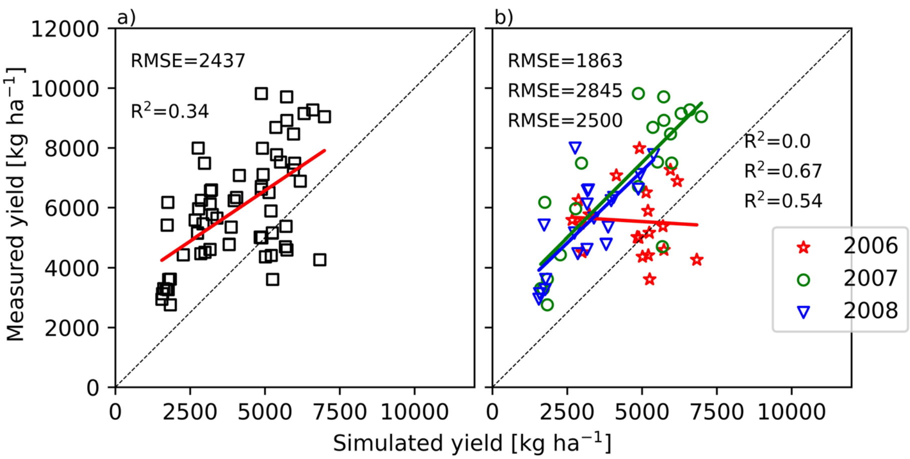


Fig. 10 Simulated and measured yield for site-specific soil profiles with all three seasons (n = 60) (**a**) and season-based for three seasons (**b**)

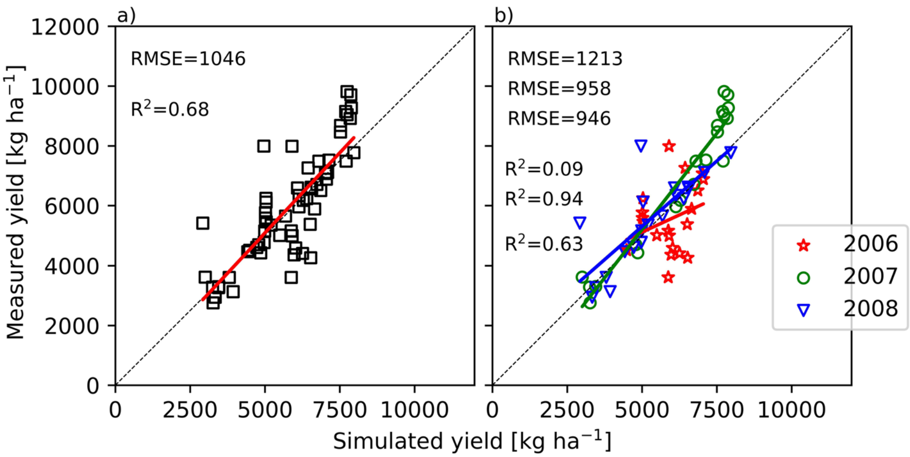


Fig. 11 Simulated and measured yield for site-specific soil profiles with all three seasons (n = 60) (**a**) and season-based for three seasons (**b**)

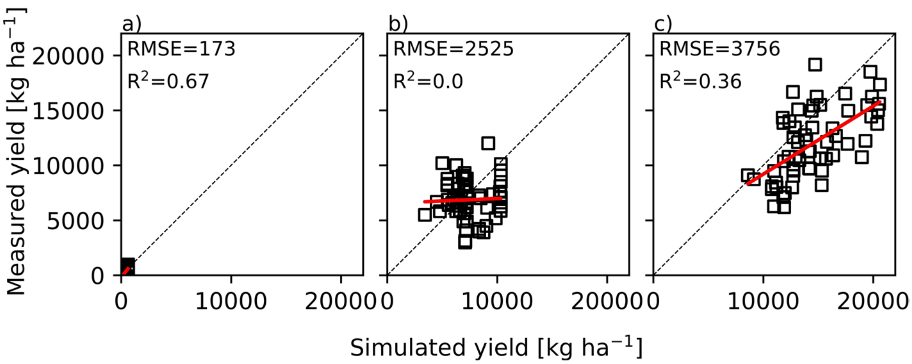


Fig. 12 Simulated and measured tops weight (above-ground biomass) for three sample cuts: BBCH14 (**a**), 65 (**b**), and 90 (**c**), with in total 180 measurements over three years

NPM results

Site-specific N prescription is expected to deliver meaningful results only if crop growth model parametrization is conducted properly. Specific soil input parameters were estimated indirectly based on the observed site-specific yield and above-ground biomass variability. The statistics summary of three soil profile calibration scenarios: target variable GRAIN (G), target variable TOPS (T) (above-ground biomass) and simultaneously targeting GRAIN and TOPS (G-T) are shown in Table 2. Based on the R^2 and RMSE statistics shown in Table 3 we can see different levels of seasonal accuracy. The statistics indicate the ability of derived soil profiles to explain site-specific grain variability over three years based on this crop model analysis. All three years were used for deriving site-specific soil profiles in order to understand to what degree site-specific soil profiles can explain observed variability with respect to seasonality factor (weather-related seasonality). Based on the seasonal performance (2006, 2007 and 2008) of the site-specific soil profiles we

Table 3 Optimization strategies based on target variables used in the inverse modelling approach

Optimization targets	2006	2007	2008
R^2			
GRAIN (G)	0.02	0.94	0.96
TOPS (T)	0.0	0.67	0.54
GRAIN and TOPS (G&T)	0.09	0.94	0.63
RMSE (kg ha^{-1})			
GRAIN (G)	1382	906	327
TOPS (T)	1863	2845	2500
GRAIN and TOPS (G&T)	1213	958	946

can see that site-specific soil profiles perform differently. Based on the seasonal accuracy of explaining site-specific yield, two scenarios were selected for estimating site-specific N prescriptions: target variable GRAIN and target variable GRAIN and TOPS. Even though all optimization scenarios underperformed for 2006 season it was still included in the N prescription evaluation. The issue with 2006 season is addressed in discussion.

Site-specific MNR maximising N application rates were estimated for 20 site-specific units over three years. Yearly averages of 20 site-specific units are shown in Table 4 for two different scenarios: (1) rainfed uniform N application (common agricultural practice) and (2) rainfed MNR maximising N application rates based on NPM, with assumed grain and N prices 0.17 and 0.3 Euro kg^{-1}, respectively based on optimization strategies: G and G-T shown in Table 3. N was applied on two different dates: N1—shortly before planting, and N2—approximately two weeks after planting. The first scenario shows yield, revenue, costs and MNR for uniform N application rate (160 kg N ha^{-1} (30 + 130)). The second scenario shows the results of site-specific NPM optimisation under rainfed conditions where the amounts of applied N were varied for N-1 and N-2 from 0 to 200 kg N ha^{-1} with increments of 10 kg ha^{-1} in the form of marginal return analysis where marginal input unit was 10 kg N ha^{-1}.The N application rates, based on the assumed prices, providing the highest MNR were selected as “optimum” and used for calculating 20 site-specific unit yearly averages.

Based on the post-processing analysis of the rainfed data for 20 site-specific units over three years with simplified MNR analysis it can be concluded that variable N application over three years would lead to 10% higher MNR with a 25% lower N application rate for G optimization strategy. For G-T optimization strategy site-specific N prescriptions resulted in 11% higher MNR with 28% lower N application rates, when compared to the uniform (common agricultural practice) N application strategy.

Discussion

Braga and Jones (2004) used an inverse modelling approach for deriving soil water holding capacity-related parameters (all three together: lower limit, upper limit and saturated rate) based on two different target variables: measured site-specific end-of-season yield and time-series of soil water content. It was concluded that soil parameters estimated from end-of-season yield led to acceptable estimates of end-of-season yield. However, soil water content was not accurate when compared to measured values due to errors in estimated

Table 4 Simulation outputs of MNR maximising N application rate yearly averages for two different scenarios with grain and N prices 0.17 and 0.3 € kg^{-1}, respectively

Scenario	Year	N-1 (kg ha^{-1})	N-2	N-sum	Yield	Revenue (€ kg^{-1})	Cost	MNR
G	2006[a]	30	130	160	6128	1042	48	994
	2006	81	29	110	6410	1090	33	1057
	2007[a]	30	130	160	6285	1068	48	1020
	2007	100	13	113	6913	1175	34	1141
	2008[a]	30	130	160	5571	947	48	899
	2008	96	40	135	6084	1034	41	994
	Avg.[a]	30	130	160	5995	1019	48	971
	Avg	92	27	119	6469	1100	36	1064
				− 25%				+ 10%
G&T	2006[a]	30	130	160	5948	1011	48	963
	2006	75	29	103	6269	1066	31	1035
	2007[a]	30	130	160	6262	1064	48	1016
	2007	100	15	115	6959	1183	34	1149
	2008[a]	30	130	160	5211	886	48	836
	2008	85	43	128	5810	988	38	949
	Avg.[a]	30	130	160	5807	987	48	938
	Avg	87	29	115	6346	1079	34	1044
				− 28%				+ 11%

Crop model-based grain yield predictions do not contain protein content. The model-based N application favoured N-1 higher values for total biomass accumulation and grain yield without insight into protein content. It is possible that, during grain filling period, there was not enough N to enable higher concentration of protein in grain

[a]Common agricultural practice (uniform N rate)

soil water holding limits. To avoid problems encountered in the study of Braga and Jones (2004), the current study focussed only on the optimisation of the lower limit in combination with root growth factor and runoff, based on end-of-season yield. Upper limit and saturation rates were kept fixed, as determined based on the field-specific reference (field specific texture). This approach still has to be tested with more detailed ground-truth data as soil water measurements were not available. As designed in the current version, the SPO algorithm can be used for optimising specific parameters based on time-series data (including soil water content) (Trenz et al., 2023), and as soon as data is available, it will be tested. However, on a field-scale, it is not realistic to expect the availability of time-series data collected with soil moisture sensors on a site-specific level, wherefore the potential of inverse modelling has to be further investigated with end-of-season yield in combination with field-scale measured texture in the process of site-specific soil profile derivation.

In the process of deriving site-specific soil profiles in Trenz et al. (2023) aiming at investigating the concept of overall yield explanatory power of specific soil parameters and the ability of SPO algorithm to assist in that task, HD optimization strategy was pursued. The HD strategy resulted in optimization runs that lasted hours with high computational demand. For this study various SD scenarios were tested and the one used and demonstrated in this study (Table 1) show good balance in trade-off with required time and results accuracy. The SD strategy used in this study required 94% less executed scenarios when compared to HD with minor impact on resulting statistics. If this SPO algorithm is to be used in the future in combination with season-based measurements in some kind of "real time" approach of optimizing soil profiles, there must be a compromise between speed and accuracy. The HD scenario tend to over-fit the data. However, this aspect of HD and SD optimization strategies was not investigated in detail in this study.

As already mentioned, crop model parametrization is extremely important if crop growth model is going to be used as decision support tool for future management of crops. If crop growth model is "correctly" parametrized it is expected to be able to accurately simulate yield response to system inputs such as N-based fertilizer. The problem is that crop growth models can rarely be accurately parametrized and because of that model evaluation cannot be conducted only with end-of-season yield, due to complexity of in-season physical and physiological process involved in plant growth. To investigate the implications of different plant aspects additional parameters such as tops weight (total above-ground biomass) was included in the process of deriving site-specific soil profiles as it provides additional insight into the in-season plant biomass dynamics. Ideally, if crop growth model was accurately parametrized additional in-season information about above-ground biomass should contribute to better representation of in-season dynamics enabling more accurate recommendation of in-season plant N demand.

Based on the results of the different optimization strategies used in this study, the season 2006 was underperforming. There are two potential reasons for low predictability power of site-specific soil profiles for season 2006: (1) SPO designated minima and maxima-based discretization scenarios were not effective and (2) seasonality factor (temporal variability—weather related) was not explainable by soil profile input parameters selected within this study. To understand point one (effectiveness of SPO) 20 site-specific soil profiles (n = 20) were estimated based only on the site-specific yield variability from season 2006 (n = 20) for grain (G) (Fig. 13). Based on the perfect fit of 2006 yield variability-based optimization with R^2 of 0.99 and RMSE 151 kg ha^{-1} it can

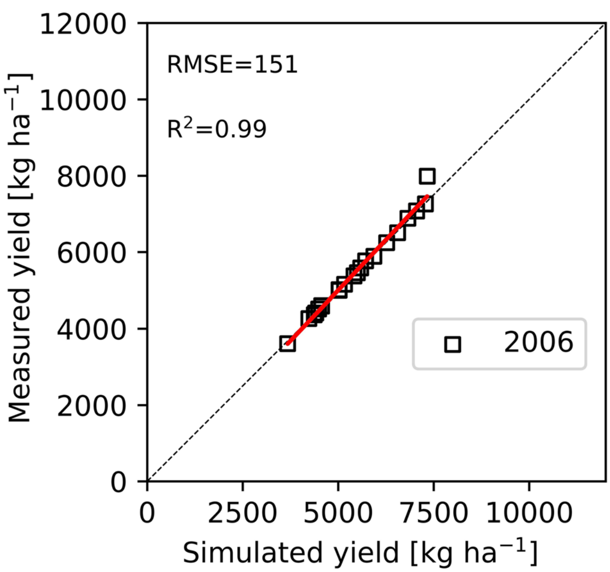


Fig. 13 Simulated and measured yield based on site-specific soil profiles derived from one season of yield (n = 20)

be concluded that SPO was very effective technically. Unfortunately, technical effectiveness of a specific algorithm if not supported by agronomic conditions is meaningless.

As it can be seen in Fig. 1 in 2006 there was less rain from end of juvenile phase to anthesis. This might have had an impact on plant growth that was not captured well by the crop growth model (e.g. lower pollen fertility due to water stress), and subsequently was not explainable via SPO based soil profiles. More detailed analysis has to be conducted into temporal variability within one season, in order to understand implications of specific weather patterns throughout various plant growth stages (impact of temporal variability with respect to plant phenological development).

Common optimisation of N fertiliser under rainfed conditions causes difficulties due to the interplay of yield limiting factors such as N and water. Wang et al. (2020) conducted a study in maize with two different soil types and investigated the effect on economic optimal N rate with respect to weather and planting density. It was found that N rates optimised for soil, year and planting density would reduce applied N and improve N use efficiency without significant impact on yield (Wang et al., 2020). Different studies indicated the importance of soil type on optimal economic N management, but without additional analysis of available water in different plant growth stages, they might be misleading. Post processing analysis indicating the importance of plant, soil, weather and management for deriving MNR maximising N rates do not seem to be a straightforward solution for site-specific management of N in future, as major factors like precipitation are difficult to predict in rainfed crop production. One of the greatest problems of ceteris paribus analysis in which only one parameter is analysed, such as yield response to N, is that it does not properly reflect the interaction of yield limiting factors such as soil water and N.

Conclusion

The study evaluated a combination of the recently developed software solutions SPO and NPM aiming at creating a base for user-friendly crop model-based site-specific field delineation (site-specific soil profiles) and N optimization. Within this post-processing analysis, the results indicated that variable N management would have led to higher MNR for the field investigated in this study when compared to uniform N application, due to existing in-field site-specific soil heterogeneity.

The potential of site-specific N management can only be fully realised if in-field heterogeneity exists, and further if it can be accurately quantified, and causes correctly identified. The crop model-based inverse modelling approach (SPO) was used for identifying potential "causes" of spatial yield variability based on three years of data to estimate plant requirement-based fertilizer recommendations. The use of an inverse modelling approach for estimating site-specific soil parameters based on end-of-season yield and tops weight (in-season measurements) clearly showed potential for deriving site-specific soil profiles that can be used for the optimization of N fertilizer rates on site-specific levels.

More "accurate" in-season crop model parameterization can be achieved by including additional canopy-related in-season measurements and might lead to more consistent N recommendations. Future work will focus on understanding the impact of in-season precipitation patterns on in-season plant growth and NPM N prescriptions based on SPO soil profiles.

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Declarations

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

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