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Spatial-temporal variability in nitrogen use efficiency: Insights from a long-term experiment and crop simulation modeling to support site specific nitrogen management

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ABSTRACT

Within-field soil heterogeneity can lead to large variation in nitrogen use efficiency (NUE). Crop simulation models provide a multi-faceted approach to management considering both soil and plant interactions. However, research using crop models for investigating within field variation in NUE is limited, in part because of challenges quantifying spatially variable soil model parameters. Here soil apparent electrical conductivity (ECa) and measured soil properties were used to map spatial variations in soil characteristics across a Long-Term Experiment in Norfolk, England. The relationship between plot ECa across the 3 ha experiment and agronomic data across three different nitrogen rates (0, 110, and 220 kg N ha^{-1}) over five wheat years (2010–2020) was quantified. The Sirius crop model was parameterized for two soils representing the extremes of ECa. Sirius was validated using recorded plot data. Site-specific optimal nitrogen and associated leaching risks were simulated across 29 years of weather data. Variation in soil properties had significant impact on measured NUE. At 220 kg N ha^{-1} mean observed yields across 5 years ranged from 9.0 to 10.7 t ha^{-1} and grain protein from 11.6% to 11% on the low EC and high EC plots, respectively. On average fertiliser grain N recovery was 19.7 kg N ha^{-1} lower on the low ECa plots. Sirius simulated the variation in yield, grain protein and grain N recovery to a good level of accuracy with RRMSE of 19.5%, 15.4% and 19.5%, respectively. Simulated optimal nitrogen on the low EC soils was on average 12 kg N ha^{-1} lower, with >1 in 4 years with optimal nitrogen <200 kg N ha^{-1}. Our work demonstrated that using a combination of proximal soil EC scans and targeted soil sampling we can optimize the data requirements for model parameterisation to support site-specific N management.

1. Introduction

Nitrogen (N) fertiliser applications exceeding crop requirements lead to reduced N Use Efficiency (NUE) and therefore nutrient surplus, thereby reducing economic margins and increasing the risk of losses to the environment (Van Eerd et al., 2018). N losses can occur through nitrate (NO_3-) leaching to water bodies, damaging aquatic ecosystems and posing a risk to human health (Bijay-Singh and Craswell, 2021; Schullehner et al., 2018). Nitrous oxide (N_2O) emissions from fertiliser applications contribute to greenhouse gas emissions (Rees et al., 2013) while ammonia (NH_3) emissions influence atmospheric particulate matter formation, a major mortality risk factor (Cohen et al., 2017). Improving NUE of cropping systems is therefore a global research priority (Congreves et al., 2021).

The water holding capacity and nutrient content of soils is site-specific and has been shown to vary greatly within fields and farms (Brogi et al., 2020). For wheat (*Triticum aestivum L.*), in the UK, optimal N requirement has been shown to vary by over 150 kg N ha^{-1} and N fertiliser recovery to range between 30% and 100% within a field (Kindred et al., 2017, 2015). Spatially accurate nutrient applications can therefore improve NUE when measured as a whole field/system and forms the foundation of precision agriculture (Nawar et al., 2017). There

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are several methods growers can use to determine an optimal N rate. Variable N applications are currently mainly driven by the balance of cost of inputs and price of grain, with current tools and methods focused on economic return, with little emphasis on any externalities to the environment (Banger et al., 2017). The challenge for farmers, advisors and researchers is balancing these two, often conflicting, demands of applying sufficient N to meet crop demand while minimizing environmental risk (Miao et al., 2018). For example, canopy sensors most commonly apply more N to lower biomass areas to lift yield potential but are unable to take account of the drivers of the initial variation and how prescribed applications might interact with underlying soil properties (Colaço and Bramley, 2018).

It is recognised that crop simulation models (CSM) can help farmers consider both economic and environmental impacts, when used with multi-objective optimisation to identify spatially specific management strategies (Finley et al., 2011; Maestrini and Basso, 2018). Crop simulation models combine soil and plant process models, describing changes in system states in reaction to external drivers, such as weather or management, and how these impact interacting components including crop, soil and system losses (Jones et al., 2017a; Keating and Thorburn, 2018). Despite this potential, there are few reported studies where CSM have been used to explain and manage within field/farm spatial variability (Cammarano et al., 2020; Ma et al., 2016). To our knowledge, to date no studies have been performed to calibrate and/or validate CSM for managing within-field spatial variability in UK wheat crops. A key limitation in the application of CSM for precision agriculture is the data required for model calibration and validation at an appropriate scale, with modelling studies often limited to data from a single season (He et al., 2017). The use of management zones, where yield crop performance is linked to proximally sensed soil data such as soil electrical conductivity (ECa) and targeted samples could help reduce complexity in model parametrisation (Pasquel et al., 2023; Wong and Asseng, 2006). To identify optimal management, models must also accurately simulate the effect of a range of management options (i.e. different N rates) within the range of observed soil heterogeneity and variation in weather (Morarl et al., 2021; Sadler et al., 2000). The accuracy of CSM has been shown to vary across different soils (Thorp et al., 2007) and N rates (Joshi et al., 2019) within the same application context, i.e., field. The accuracy of validation data from other precision agriculture technologies such as combine yield maps also pose problems for spatial validation (Kersebaum et al., 2005). Quantifying the economic and environmental benefits of site-specific management requires an accurate assessment of the spatial variability (Basso et al., 2016).

Long-term experiments (LTE) provide data sets, collected to standardised protocols across a range of treatments (i.e. N rates) and over multiple years, suitable for CSM validation and development (Johnston and Poulton, 2018). They are critical in helping to understand NUE of the cropping systems or experimental treatments (Basso et al., 2009b) for a single soil and climate for which the experiment is situated (e.g. Macholdt et al., 2020). Experiments are however, often situated over underlying spatial variation in soil properties; this is particularly the case for LTE established before field level spatial variation in crop growth could be monitored through combine yield mapping or remote sensing prior to experiment set up (Cassel et al., 2000). Accounting for spatial variability to reduce experimental error through experiment design and/or statistical analysis has been well researched (Stringer et al., 2012) and some of these methods are already employed on the LTE featured in this study. However, this spatial variation, combined with high spatial (plot) and temporal (multiyear) data sets, collected as part of LTE, provide a valuable and currently underutilised resource for understanding the drivers of spatial variation in NUE and developing and validating methods to better manage this on-farm.

In this paper we aimed to quantify the heterogeneity of soil properties within an LTE in the East of England and to link this to the spatial-temporal variation in yield and NUE. The Sirius CSM was calibrated for use at this site and cropping system. We used apparent soil electrical conductivity (ECa) to quantify the spatial heterogeneity of soil properties across the LTE and how crop response correlated to this observed variation using five years of winter wheat data across three contrasting N fertiliser application rates. Measured data sets on soil and crop properties were used to parametrise and validate the CSM across the extremes of this variation. The validated model is used to identify spatially explicit N management strategies and associated environmental risk. We demonstrated how soil proximal sensing, spatial monitoring and targeted soil sampling can be combined with CSM as a tool for on-farm management decisions for UK wheat crops.

2. Materials and methods

2.1. Site description, experimental design and agronomic management

This study used data sets from three long term experiments at The Morley Agricultural Foundation, Morley, Norfolk, U.K (52°33′35″N, 01°01′39″E, 54 m Altitude). The soil is an Endostagnic Luvisol (World Reference Base)/Ashley association with a topsoil sandy loam textural class (Cranfield University, 2023). The NFS Rotations Experiment (NFS-RE) investigates four cover cropping treatments grown prior to spring break crops with three nitrogen rates; 0% (~0 kg N ha^{-1}), 50% (~110 kg N ha^{-1}) and 100% of the recommended N dose (~220 kg N ha^{-1} in winter wheat) (Fig. 1A, Table 1). These will be referred to as 0 N, 110 N and 220 N respectively hereafter. The NFS Cultivations Experiment (NFS-CE) examines four primary cultivation regimes with and without cover cropping before spring break crops under a farm standard N rate (Fig. 1A). N response trials across multiple fields and seasons has shown 220 kg N ha^{-1} to be the economic optimal N rate at Morley, although large temporal (year to year) and spatial (field to field) variation is recorded (Kindred et al., 2018). N rates are split over three timings typically mid-March (~25% of total N), second or third week in April (~60% of total N) and a final dose in early May (~15% of total N). Plots are 12x12m in NFS-RE and 12x36m (split into 12×24 and 12×12 blocks) in NFS-CE to facilitate the use of commercial scale machinery for operations. Each experiment is fully replicated (four repetitions) with a factorial design. All plots received pesticide applications according to local best practice to minimize disease and weed pressures, despite these preventive measures, outbreaks of diseases or weeds still occur, and observations are recorded when such incidents happen. Other nutrients (P, K, Mg) and pH were managed at a field level with all plots receiving the recommended application, with aim to maintain soil indices at levels that are not crop limiting. The Straw Incorporation Experiment (SIE) at Morley was a long term (1984–2018) experiment monitoring changes in soil properties through different quantities of crop residue returns. In the later years, straw return was regulated using different N rates (0–250 kg N ha^{-1} in winter wheat). This experiment was located approximately 150 m south of the NFS-CE (Fig. 1B).

2.2. Data collection and analysis

2.2.1. Soil apparent electrical conductivity (ECa)

Soil apparent electrical conductivity (ECa) was measured across the NFS experiments on 27/01/2020. A Dualem-1S EC scanner (Dualem Inc., Canada) towed behind an all-terrain vehicle equipped with a TOPCON (TOPCON Precision Agriculture, Europe S.L.) GPS device recorded the location of individual ECa measurements at <0.5 m location accuracy. Each experiment was scanned at 6 m intervals perpendicular to the plots (North to South). The timing of the measurements was chosen when soil water content was at or close to field capacity so ECa should reflect soil texture/water holding capacity (McBratney et al., 2005). A cosmic-ray soil moisture sensor situated on-farm at Morley recorded topsoil moisture of 37.3% on the day of scanning and soil temperature was 6.7 °C (Cooper et al., 2021). The maximum recorded topsoil moisture between August 2015 and August 2020 was 40.0%, confirming the scanning took place close to field capacity. ECa was

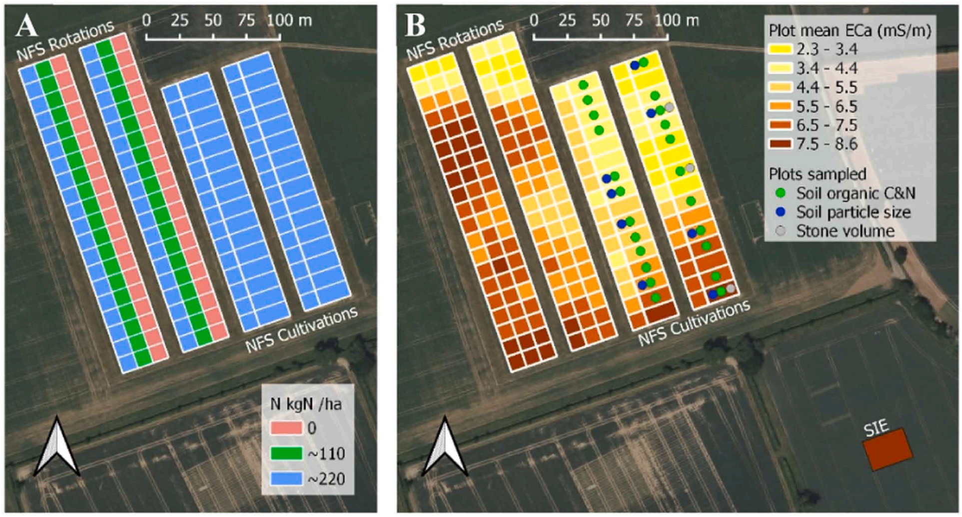

Fig. 1. A. NFS Rotations (NFS-RE) and NFS Cultivations (NFS-CE) experiments with current N rates for winter wheat, B. Plot mean ECa across the NFS-CE and NFS-RE and Straw Incorporation Experiment (SIE). Plots sampled for soil data identified. Areal imagery: © 2024 Microsoft Corporation © 2024 Maxar © CNES (2024) Distribution Airbus DS.

Table 1
NFS-RE wheat crop varieties, drilling date and the N rate at full farm standard N (220 N).

Year	2010	2012	2015	2017	2020
Cultivar	Oakley	JB Diego	Relay	Evolution	KWS Kerrin
Drilling date	14/10/2009	13/09/2011	30/09/2014	23/09/2016	23/10/2019
N rate (kg N ha^{-1})	200	216	210	220	215

averaged for each plot to enable comparison with agronomic and soil measurements collected using a random sampling strategy within each plot. Plot boundaries were extracted from the tractor mounted Trimble RTK guidance system (accuracy <3 cm) used in marking out the experiment and applying experimental treatments (Fig. 1B). A large part of the farm including the NFS Experiments was scanned using a Dualem-1S EC scanner (Dualem Inc., Canada) in February 2023. This showed little variation in soil ECa across the SIE. The mean ECa across the SIE experiment and measured data for soil organic matter was comparable to the higher ECa and organic matter plot values recorded on the NFS experiments (7.5–8.5 mS/m).

2.2.2. *The relationship between soil ECa and soil physical properties and organic C and N*

The site-specific relationships between soil properties and ECa were examined using data from the NFS-CE, which has historically been more intensively sampled than the NFS-RE. Eight plots covering the range in mean plot ECa (Fig. 1A) were sampled for soil particle size at depths of 0–30 cm, 30–60 cm and 60–90 cm. Soil particle size distribution was determined by sedimentation (Rowell, 2014). Soil organic carbon (SOC) and soil organic nitrogen (SON) were measured across the experiment in 2018, at 0–30 cm and 30–60 cm depths (Guo et al., 2018). The linear relationship between soil properties and ECa was tested using Pearson's correlation coefficient (r) and the coefficient of determination (r^2). Soil profile excavations undertaken in previous studies using the NFS-CE (Brown et al., 2021; McKenzie et al., 2017) have noted that stone content varies considerably across the site in line with the observed variation in ECa (personal communications, N. Morris, March 2023). To quantify stone volume for model parameterisation, which is important for accurate water release characteristics, stone volume was measured through profile excavation on high (7.9 mS/m) and low ECa (2.9 mS/m) plots on the NFS-CE. A 2 kg soil sample was taken at depths between 0 and 30 cm, 30–60 cm and 60–90 cm, soil was sieved through a 2 mm sieve and stone volume calculated by water displacement.

2.2.3. *The relationship soil ECa and agronomic data*

The spatial variation in crop performance, unrelated to treatment, across the experiment was quantified by comparing plot ECa and the plot level agronomic dataset for the LTE. The agronomic data from NFS-RE for winter wheat (*Triticum aestivum L.*) in 2010, 2012, 2015, 2017 and 2020 were used. In 2010, 2015, and 2020 the wheat was grown following an oilseed rape crop (*Brassica napus L.*), in 2012 and 2017 the wheat followed a spring bean (*Vicia faba L.*) and spring oat (*Avena sativa L.*) crop, respectively. Ear numbers were assessed annually prior to harvest (not measured in 2017). Plot grain yield was measured using a SAMPO ROSENLEW 2010 (2010–2017) or HALDRUP C-85 (2020) plot combine harvester with a 2 m header. Plot yields are calculated from the mean of two 2 m x 12 m swaths through each plot. Grain protein and specific weight were analyzed from a composite 500 g sample from each plot using FOSS INFRATECH NIR scanner annually calibrated using UK Grain Testing Network (UKGTN) calibrations. The relationship between plot ECa and crop parameters of yield, grain protein, grain specific weight and ear numbers was quantified using linear regression analysis for each year and the 5-year mean. The strength of the linear relationship was tested using Pearson's correlation coefficient (r) and the coefficient of determination (r^2).

2.2.4. *Spatial temporal variation in fertiliser grain N recovery efficiency*

Fertiliser Grain N recovery efficiency RE_{fertN} (Eq. 1) is a metric of NUE, defined as the percentage of N applied as fertiliser within the grain at harvest, accounting for background soil N levels using the unfertilized (0 N) control (Congreves et al., 2021):

$$\boldsymbol{RE}_{\mathbf{fertN}} = \frac{\boldsymbol{u}-\boldsymbol{u}_0}{\boldsymbol{n}} \times \mathbf{100} \quad (1)$$

where u is the total grain N uptake in kg N ha^{-1} (grain yield (kg) × grain N (%)) at a given N treatment, u_0 is the total grain N uptake in kg N ha^{-1} in untreated control and n is total N applied as fertiliser applied to u in kg N ha^{-1}. Grain N is calculated by dividing grain protein by 5.7 (AHDB, 2023). The mean RE_{fertN} across the variability of measured ECa is calculated for the farm standard 220 N plots. Linear regression equations for Plot ECa ~grain yield and ECa~grain protein (see Supplementary Material, S2) were used to generate ECa yield and grain protein

N response functions for ECa ranging from 2.3 to 8.6 mS/m at 0 and 220 kg N/ha for each year. These equations were used to calculate the 5 year mean RE_{fertN} influenced by spatial variation in soil properties quantified by ECa. Not all years demonstrated a significant correlation between yield and grain protein with ECa at 0 N and 220 N. Therefore, mean values at 0 N and 220 N for plots ranging from 2.5 to 3.5 (Low EC), 3.5–4.5, 4.5–5.5, 5.5–6.5, 6.5–7.5 and 7.5–8.5 ECa (High EC) where used to quantify the relationship between plot ECa and RE_{fertN} in each year.

2.3. Crop modeling

2.3.1. Sirius crop simulation model

Sirius is a process-based crop model for wheat (Semenov, 2021). Full details of the model and its processes have previously been described (Brooks et al., 2001; Jamieson et al., 1998). In summary, the model simulates crop biomass production from intercepted photosynthetically active radiation and subsequently radiation use efficiency (RUE). A thermal time sub model determines leaf area index (LAI) and phenological development calculated from leaf appearance rate and final leaf number. Water and nitrogen stress can impact LAI development and subsequent RUE. A proportion of the simulated biomass at anthesis and predominantly new biomass formed at the beginning of grain filling are used to calculate grain yield. Under water stressed conditions, senescence is accelerated restricting grain fill and reducing grain yield. Detailed modeling of soil water and N processes determine root available resources (Brooks et al., 2001; Jamieson et al., 1998). Sirius has previously been validated and applied to evaluate water and weather variations on wheat yields (Clarke et al., 2020) and nitrogen use efficiency (Semenov et al., 2007) in the UK. The Sirius modelling exercises in this study were split into three approaches: i) parameterisation of soil properties from the NFS-CE and validation of cultivar parameters to reproduce yield response to N from two years of wheat data from the SIE, ii) model validation of nitrogen interactions across the measured variation in soil properties in the NFS experiments, and iii) use of the calibrated and validated model with historic weather data to determine economic optimal N management across the spatial variation and associated environmental risk.

2.3.2. Soil parameters

Sirius requires soil parameters including soil horizon depth, water holding characteristics including drained upper limit (DUL), lower limit (LL), saturation water content (KSAT) and percolation coefficient (k_p). Parameters for soil nitrogen processes are also required including organic N content and a mineralization constant. To test the suitability of Sirius for modelling and managing spatial variation in soil N, the modeling exercise was simplified by modeling responses at the extremes of the recorded spatial variation in soil properties quantified using two ranges representing high and low soil ECa. Two representative profiles were created using the measured soil data. A representative high ECa (HEC) was calculated from the mean data from NFS-CE plots with an ECa of 7.5–8.5 mS m^{-1} A representative low ECa (LEC) used the mean data from plots with an ECa of 2.5–3.5 mS m^{-1} (Fig. 2). Its common practice to use measured soil texture and organic carbon to estimate soil water release parameters (Brogi et al., 2020; Joshi et al., 2019). Soil water retention characteristics for each soil layer were calculated using pedotransfer functions of measured soil texture and carbon content (Hollis et al., 2015, 2012). These were corrected for the volume of stones in each soil layer recorded in representative plots (Fig. 3) (Gagkas et al., 2018). Total soil organic N (t ha^{-1}) was calculated using measured organic N content, stone content and estimated soil bulk density. Soil percolation coefficient is dimensionless; therefore, values were used for each soil based on previously calibrated soils with similar available water content in the Sirius soil parameter files (k_p HEC=5, LEC=8). Mineralization constant was set at 7 for both soils, the same as all UK soils in the Sirius soils file. Maximum rooting depth was set at 1.5 m for both profiles, confirmed through root observations from auger samples.

2.3.3. Weather data

Sirius requires daily weather measurements for maximum and minimum temperature, precipitation, solar radiation, wind speed and vapor pressure. A 29-year daily weather data set was compiled for the period between 1990 and 2022 (note no data were available for 2005–2007). Rainfall and temperature data for Morley was extracted for the weather station situated on farm from the MIDAS archive (UK Meteorological Office, 2023). Missing data for daily temperature observations were infilled from a nearby MIDAS station (Norwich airport) and where required from other private stations and a CEH COSMOS station on site (Cooper et al., 2021). Solar radiation, wind speed and vapor pressure have not historically been measured. These parameters were therefore calculated using synthetic measurements extracted from the NASA Prediction of Worldwide Energy Resources (NASA/POWER-NP) series, previously demonstrated as suitable for crop simulation modelling exercises (Monteiro et al., 2018).

2.3.4. Cultivar parameterisation and N response validation on the SIE

It is common practice to use previously calibrated model parameters for cultivars (*cv*) with similar phenological development, yield potential and geographic distribution to the validation data set (Gaso et al., 2021). Sirius has been calibrated and validated for *cv* Claire, which remained on the UK Recommended List (RL) until 2018 (AHDB, 2023b) and has been used extensively in UK wheat breeding programs (Powell et al., 2013). Data from 2017 and 2012 RL trials demonstrated other wheat cultivars (*cv* JB Diego, *cv* Evolution, *cv* KWS Kerrin, *cv* Relay and *cv* Oakley) had similar phonological parameters (e.g. start of stem extension (GS 31: BBCH Scale (Meier, 1997)) and maturity (GS 91) to *cv* Claire. Therefore, the previously calibrated phonological parameters describing crop development for *cv* Claire were used in this study. However, in RL trials, yields of *cv* Claire were on average 2–10% lower compared to the varieties grown on the NFS-RE and SIE (see Supplementary Material, S1). A significant proportion of this gap is likely to be due to reduced yields from poorer disease resistance (Powell et al., 2013) which is not accounted for in Sirius. To reflect the higher yield potential of the modern varieties grown on the NFS-RE the maximum leaf size and maximum grain weight parameters for *cv* Claire were increased from 0.07 to 0.08 and 0.45–0.5, respectively. This is supported by measured data of modern UK elite cultivars in the WIGIN data sets (DEFRA, 2019). All other parameters remain unchanged as previously reported (Clarke et al., 2020; Senapati et al., 2019).

The SIE was cropped with *cv* JB Diego and *cv* Relay in 2014 and 2015 respectively, both varieties were grown on the NFS-RE (Table 1). The incremental N doses and recorded harvest dates provided valuable supplementary validation of Sirius before its application to the NFS-RE experiment. Sirius was validated for maturity date, grain yield, grain protein and grain N offtake, defined by Eq. 2:

$$\boldsymbol{u} = \boldsymbol{y} \quad \times \quad ((\boldsymbol{p}/\mathbf{5.7})/\mathbf{100}) \tag{2}$$

where u is the grain N offtake in kg N ha^{-1}, y is yield in kg ha^{-1}, p is grain protein in % and 5.7 is the conversion factor for converting grain protein to grain N (AHDB, 2023a).

The soil parameters for HEC soil were used for the SIE as the trial mean ECa was comparable to the corresponding plots on the NFS-CE. The agronomy input data (drilling date, nitrogen applications and timings) used in Sirius were as applied in the experiment. Initial soil inorganic mineral N was set at 20 kg N ha^{-1} reflecting the measured soil mineral N (0–90 cm) prior to N fertiliser application in the spring.

2.3.5. Validating Sirius cross the spatial variation on the NFS-RE

Sirius was validated with measured data of mean yield, grain protein and total grain N offtake for plots with HEC and LEC on the NFS-RE the using the model parametrised for measured soils data.

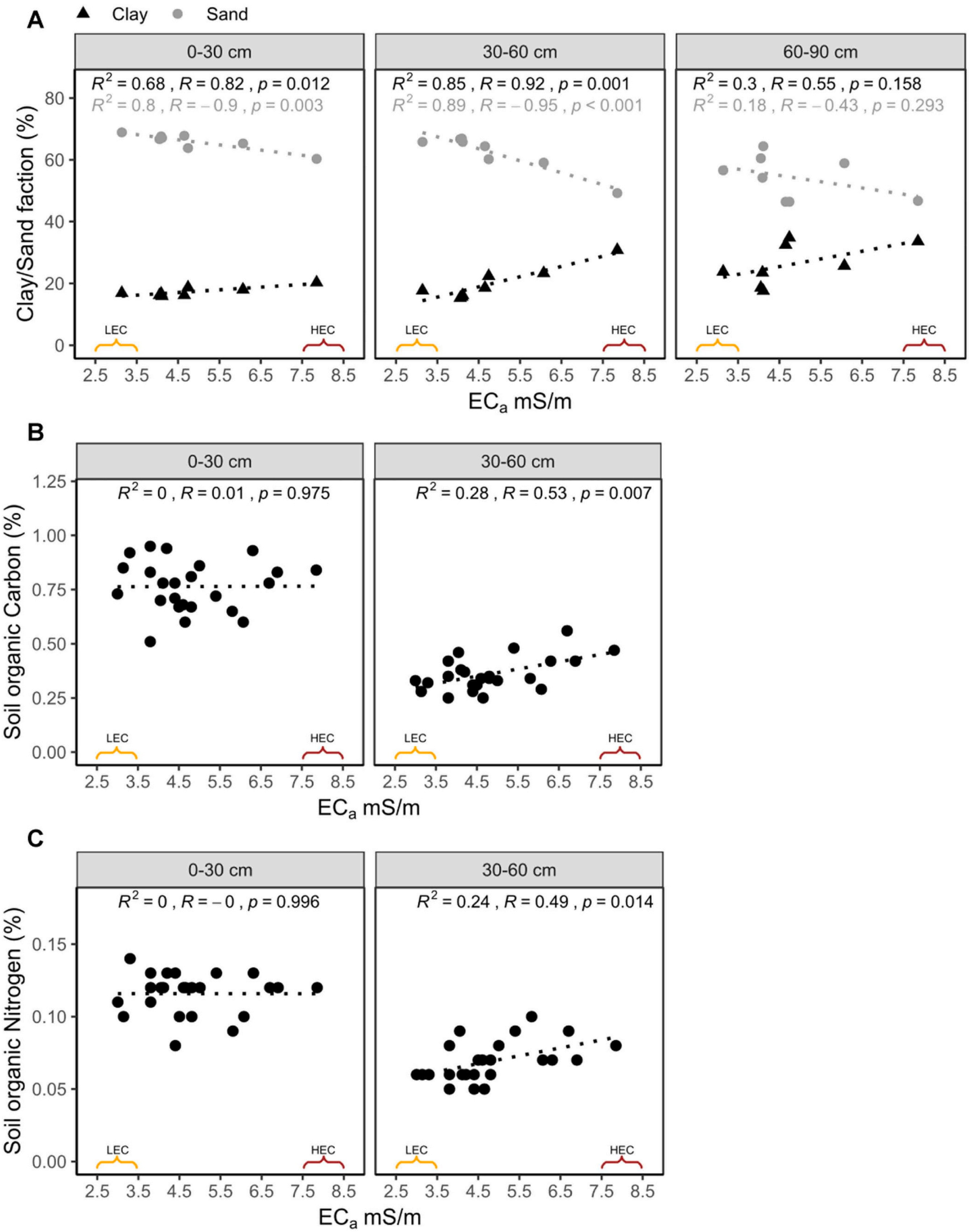

Fig. 2. linear relationship between Soil ECa and A. clay and sand factions, B. soil organic Carbon, C. soil organic Nitrogen at 30 cm depth intervals to 90 cm on the NFS-CE. Braces represent the range of data points used to generate Soil parameters for Sirius representative of the Low ECa (LEC) and High ECa (HEC) plots across the NFS experiments.

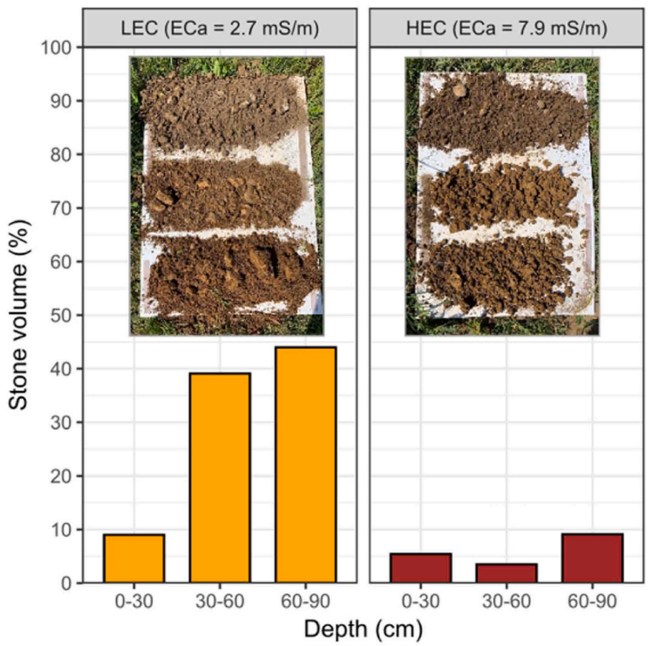

Fig. 3. Stone volume by 30 cm soil depth (0–90 cm) and images of reconstructed profile excavation for HEC (7.5–8.5 mS/m) and LEC (2.5–3.5 mS/m).

Drilling dates, nitrogen applications and timings were taken from agronomic farm data and expected ear numbers were adjusted based on recorded ear counts. Measured soil mineral N was set at 20 kg N ha^{-1}. Model accuracy was assessed using the Root Mean Square Error (RMSE), as defined by Eq. 3:

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}(y_i - \widehat{y}_i)^2} \tag{3}$$

where y_i is the observed data, $\widehat{y}_i$ is the simulated data and n is the number of comparisons. The RMSE was normalised (RRMSE) by dividing by the mean of observed data for easier cross study comparisons and can be assessed against quantitative performance criteria. Model performance is considered “excellent” if RRMSE <10%, “good” between 10% and 20%, “fair” if between 20% and 30%, and “poor” if >30% (Jamieson, 1991).

2.3.6. Soil specific modelled response to N

To determine the economic optimal N for both soil types, an industry standard N response experiment was simulated for the 29-year weather record. Treatments and timings were as set out according to Kindred et al., (2018) and comprised of six N treatments ranging from 0 to 360 kg N ha^{-1}, including an estimated optimum N of 220 kg N ha^{-1}. The linear plus exponential function (George, 1984) was used to estimate yield response to N, as defined in Eq. 4:

$$y = a + b.rN + c.N \tag{4}$$

where y is yield in t ha^{-1} at 85% dry matter, N is fertiliser rate in kg N ha^{-1} and a, b, c and r are parameters determined by statistical fitting. Optimum N rates were derived through Eq. 5:

$$NOpt = [\ln(k - c) - \ln(b(\ln(r)))]/\ln(r) \tag{5}$$

where k is the breakeven ratio between fertiliser N (£/kg) and grain(£/t), here a breakeven ratio of 0.006 (tonnes grain per additional kg N) was based on 2023 grain and fertiliser prices (AHDB), n, b, c and r are defined in Eq. 4.

Sirius was run for the 29-year weather data set at the mean soil specific NOpt, simulating wheat grain yield, in-season N leaching and soil mineral N at harvest.

Unlike the modeling in 2.3.5 and 2.3.4, in which some plots have historically received below optimal N, this modeling exercise assumed previous crops had crop specific optimal N. Therefore, soil mineral N at sowing was assumed to be 30 kg N ha^{-1} in line with the long term average autumn soil N recorded on farm (TMAF, 2023). Cumulative probability functions were used to interpret the variation in NOpt between the two soil types as well as modeling results. All data handling and statistical analysis was performed in R programing language (R Core Team, 2023). Crop modeling was performed through the native windows application for Sirius (Sirius, 2023).

3. Results

3.1. Spatial variation across a LTE

3.1.1. Spatial variation in soil properties

Plot mean soil ECa ranged from 2.3 mS/m to 8.6 mS/m across the NFS experiments (Fig. 1B). Soil ECa was significantly correlated to both clay and sand content at 0–30 cm and 30–60 cm depths (Fig. 2 A) accounting for 68%-89% of the variation in sand and clay content at these depth intervals. ECa was not significantly correlated to sand and clay content at 60–90 cm depth. Clay and sand content ranged from 15.9% to 20.3% and 60.3–68.9% respectively at 0–30 cm depth, and from 15.3% to 30.8% and 49.2–66.9% respectively at 30–60 cm depth. There was no significant relationship between ECa and soil organic C or N at 0–30 cm, however both were significantly correlated to ECa at 30–60 cm, with ECa explaining 36% of the recorded plot variation in C and 27% of the recorded plot variation in N at 30–60 cm depth (Fig. 2B&C). Stone content was higher on the lower ECa plots (Fig. 3), especially at depth (39% and 44% at 30–60 cm and 60–90 cm depth, respectively). The measured soil data was used to parametrise Sirius for two soil profiles representing the variation in ECa across the NFS-RE (see Supplementary Material, S3). The calculated available water capacity (150 cm) was 105 mm for LEC and 148 mm for HEC profiles. The significantly lower soil organic N at 30–60 cm combined with the higher stone volume (lower fine earth material) resulted in slightly smaller pools of soil organic N in the LEC (6 t ha^{-1}) compared to HEC (7 t ha^{-1}).

3.1.2. Spatial temporal variation in crop performance

The variation in soil properties across the NFS-RE quantified through ECa showed significant relationships to key crop measures and their interactions with N rate (Fig. 4). Except for 2012 at 220 N, a significant correlation between ECa and grain yield was observed at all N rates in all years (Fig. 4A). Across the 5 years, plot ECa explained 71%, 87% and 79% of the variation in plot yield at 0 N, 110 N and 220 N, respectively. The range of 5-year mean yield between the LEC and HEC plots was 9.0–10.7 t ha^{-1} at 220 N, 7.5–9.5 t ha^{-1} for 110 N and 4.2 and 5.5 t ha^{-1} at 0 N, respectively. In 2012, 110 N and 220 N yields were similar and 0 N yields were similar to other years at 110 N. In 2017 and 2020 the yield response at 220 N compared to 110 N appeared to be smaller on plots with lower ECa than those with relatively higher ECa.

The relationship between grain protein and plot ECa was generally the inverse for that of yield (Fig. 4B). In 2010, 2017 and 2020 a significant negative correlation between ECa and grain protein was recorded at 220 N. No significant correlation was recorded in 2012 and 2015. At 110 N a significant negative correlation was recorded in 2010 and 2020, a significant positive correlation in 2012 and no correlation in 2015. At 0 N a significant negative correlation was recorded in 2010, 2015, 2017, and 2020. Across the 5-year mean there was a significant negative correlation between grain protein and plot ECa at 220 N and 0 N explaining 36 and 43% of the plot variation in grain protein, respectively. The mean grain protein for the measured range in plot ECa ranged from 11.6% to 11% at 220 N and 7.8% and 7.2% at 0 N ha. The plots defined as LEC on average exceed the 11% optimal grain protein for yield for feed wheats (AHDB, 2023a).

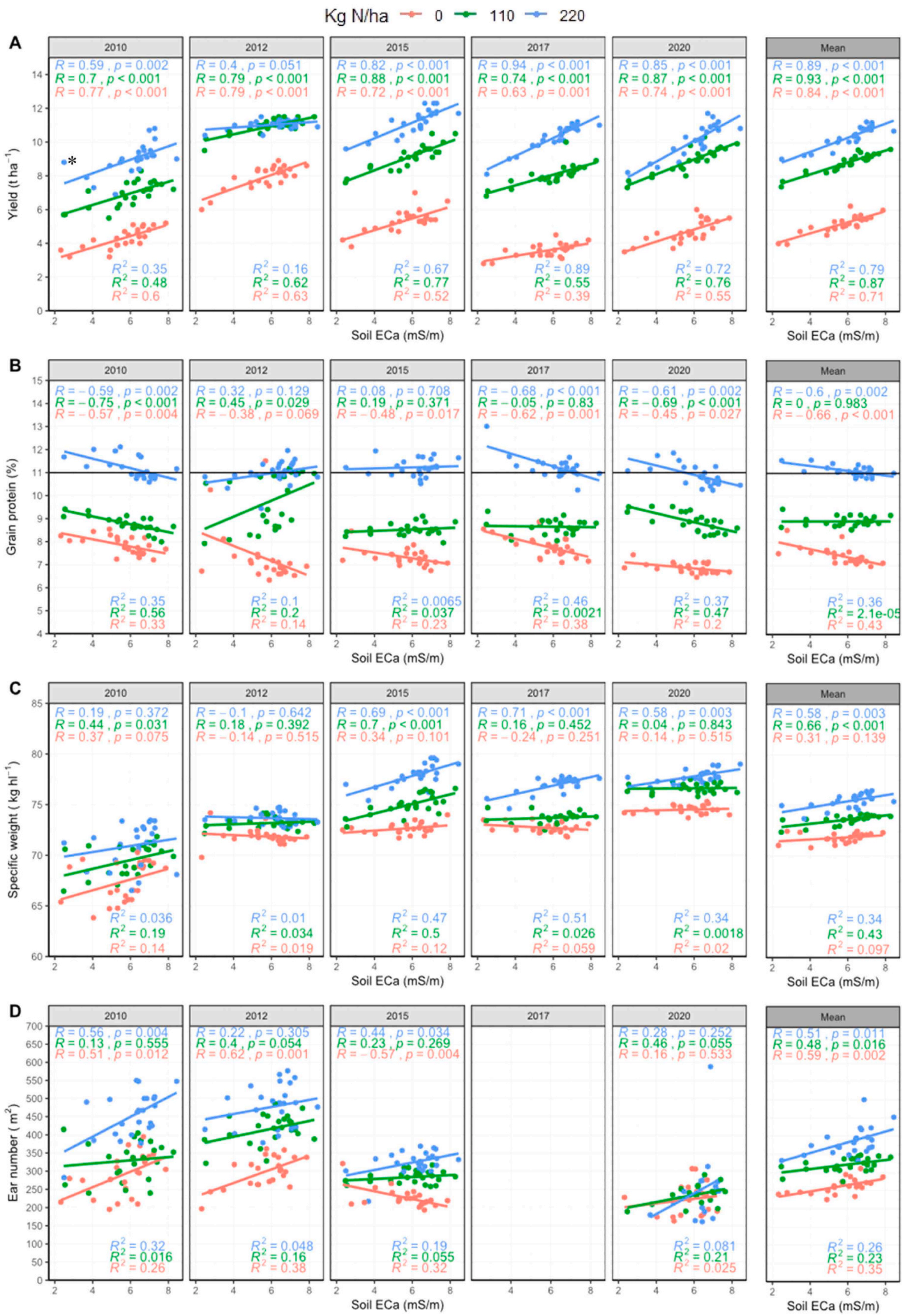

Fig. 4. Linear relationship between plot ECa and wheat performance metrics (2010–2020) and their 5-year means, (A) grain yield, (B) grain protein, where the black line at 11% represents the optimal grain protein for yield, (C) grain specific weight and (D) ear numbers (no ear numbers were recorded 2017). The asterisk (*) in 2010 yield plot represents influential outlier when calculating grain N fertiliser recovery.

Plot mean ECa was significantly correlated to grain specific weight in 2015, 2017 and 2020 at 220 N, in 2010 and 2015 at 110 N and in no years at 0 N (Fig. 4C). Across the five years on average there was a significant correlation with ECa and specific weight at 220 N and 110 N explaining 34% and 43% of the variation, respectively. ECa was significantly correlated to ear numbers in 2010 and 2015, but not in 2020 at 220 N (Fig. 4D). No significant correlation was recorded in any years at 110 N but was significantly positively correlated in 2010 and 2012 at 0 N and negatively correlated in 2015. On average across the 5 years ECa was positively correlated to ear numbers at all N rates.

3.1.3. Spatial temporal variation in grain fertiliser N recovery

The 5-year mean grain fertiliser N recovery (calculated using regression equations for the linear relationship between ECa, grain yield and grain protein at 0 N and 220 N) ranged from 46.7% to 56.0% from low to high ECa (Fig. 5). This equates to an average 19.7 kg N ha^{-1} variation in RE_{fertN}. LEC plots had 8% lower RE_{fertN} in 2015, 2017 and 13% in 2020 compared to the HEC plots. Smaller (0–5%) differences were recorded in 2010 and 2012. In 2010 the LEC plots were strongly influenced by an outlier in the yield data (Fig. 4A), resulting in higher RE_{fertN}, this observation contradicts the overall trend of lower yields on the low ECa plots in that year.

3.2. Crop simulation modeling

3.2.1. Sirius validation SIE

The updated parameters for *cv* Claire simulated maturity date within one day of recorded harvest date in 2014 and 3 days in 2015 for *cv* JB Diego (2014) and *cv* Relay (2015). Correctly simulating the longer growing season in 2015 (Fig. 6A). The calibrated parameters explained 82% of the variation in yield across the two years (Fig. 6B). Sirius showed good model performance in describing variation in yield (RRMSE of 10.8%), grain protein (RRMSE of 18.1%) and grain N offtake (RRMSE of 18.9%) under different N rates across the two years with the updated cultivar parameters (Fig. 6A, B and C).

3.2.2. Sirius validation across spatial variation on the NFS -RE

Sirius was validated for its ability to simulate the observed spatial variation in crop growth in response to the extremes in variation in soil

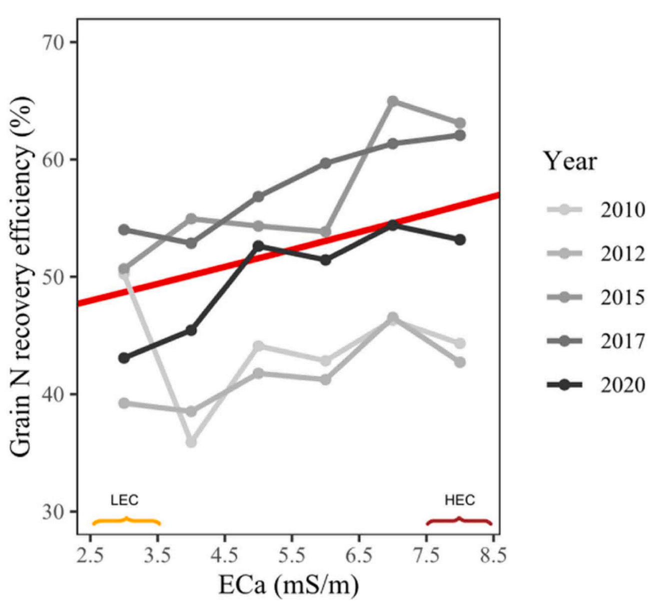

Fig. 5. Grain N recovery efficiency (2010–2020) by plot ECa ranges 2.5–3.5 (LEC), 3.5–4.5, 4.5–5.5, 5.5–6.5, 6.5–7.5 and 7.5–8.5 (HEC). Red line = Grain N recovery efficiency across range of ECa from regression equations for the five year mean grain yield and protein.

available water capacity and organic N across the NFS-RE using two soil profiles representative of the extremes of the spatial variation in soil properties (LEC and HEC). Sirius showed good model performance at simulating yield (RRMSE: 19.5%), grain protein (RRMSE: 15.4%), and total grain N offtake (RRMSE: 19.5%) across both soils profiles, N rates and years (Table 2).

At 110 N and 220 N Sirius overestimated yields on both soils, primarily because of higher simulated yields in 2012 and 2017 (Fig. 7A). Whilst simulated yields were slightly worse on LEC soils, the influence of the different soil properties on yield, grain protein and grain N offtake was captured in model performance (Fig. 7A). At 220 N across all years Sirius simulated 1.2 t ha^{-1} lower yields, 0.6% higher grain protein and 18 kgN ha- lower grain N offtake on the LEC soils compared to HEC soils. These values were similar to LEC soil observed data that showed 1.5 t ha^{-1} lower yields, 0.6% higher protein and 23 kg N ha $^{-1}$ grain N offtake compared to HEC soil. On the HEC plots observed yields were higher at 110 N than 220 N on the LEC plots (7.9 t ha^{-1} compared with 7.7 t ha^{-1}). The mean simulated yields align with this pattern, with simulated yields of 8.3 t ha^{-1} at 110 N on the HEC, surpassing the 8.1 t ha^{-1} simulated yields on LEC plots at 220 N (Table 2).

Sirius overestimated grain protein at all N rates and on average by 0.7% at 220 N for both soils. Sirius was unable to simulate proteins lower than 8.55% (1.5% grain N) despite recorded grain proteins being recorded as low as 6.3% (1.1% grain N) at 0 N in the observed data set (Fig. 7B). The errors in grain yield and grain protein did not seem to propagate to total grain N offtake which showed comparable RRMSE (Fig. 7C).

3.2.3. Modelling soil specific economic optima N rates and environmental

The mean NOpt across 29 years of simulated N response trials was 12 kg N ha^{-1} lower on the lower available water capacity LEC soil (234 kg N ha^{-1} and 222 kg N ha^{-1} for the HEC and LEC soils, respectively) (Fig. 8A). Large seasonal variation was observed on both soil types. The cumulative frequency distributions for NOpt were similar above c. 235 kg N ha^{-1} on both soil types, although there was a smaller cumulative probability at NOpt on the LEC soil (HEC=0.46, LEC=0.35). For the LEC soil there was a greater distribution of seasons with NOpt below 200 kg N ha $^{-1}$ (cumulative probability: 0.31/greater than 1 in 4 seasons) compared to the HEC (cumulative probability 0.1/1 in 10 seasons). The mean simulated yield was 10.8 t ha^{-1} and 12.3 t ha^{-1} for the LEC and HEC respectively (Fig. 8B). Simulated growing season N leaching (sowing-harvest) was higher on the LEC soil with a mean leaching loss of 20.7 kg N ha^{-1} compared to 12.8 kg N ha^{-1} on the HEC soil (Fig. 8C). Small difference in surplus soil N at harvest were simulated with higher (78.5 kg N ha^{-1}) values on the LEC soil compared to the HEC soil (66.9 kg N ha^{-1}) (Fig. 8D).

4. Discussion

4.1. Spatial variation in soil properties and influence on grain yield and NUE

Variations in ECa measured across the NFS-RE exhibited a strong correlation with sand and clay factions at 0–30 cm and 30–60 cm depths. This aligns with previous research demonstrating a positive linear relationship between soil ECa and clay content (Domsch and Giebel, 2004; McBratney et al., 2005). However, these relationships are likely to be site-specific, as ECa is also influenced by soil mineralogy, depth (Mcbratney et al., 2005) and, as observed in this study stone content. The stone content was considerably higher in the LEC soil and increased with depth and was likely to have a large influence on soil hydraulic properties and other soil physical processes (Naseri et al., 2019). Stones (>2 mm) are not easily sampled during most regular restricted diameter soil core sampling and often, as performed here, more intrusive pits are required (Rytter, 2012). It would have been desirable to quantify stone content at depth across the entire range of

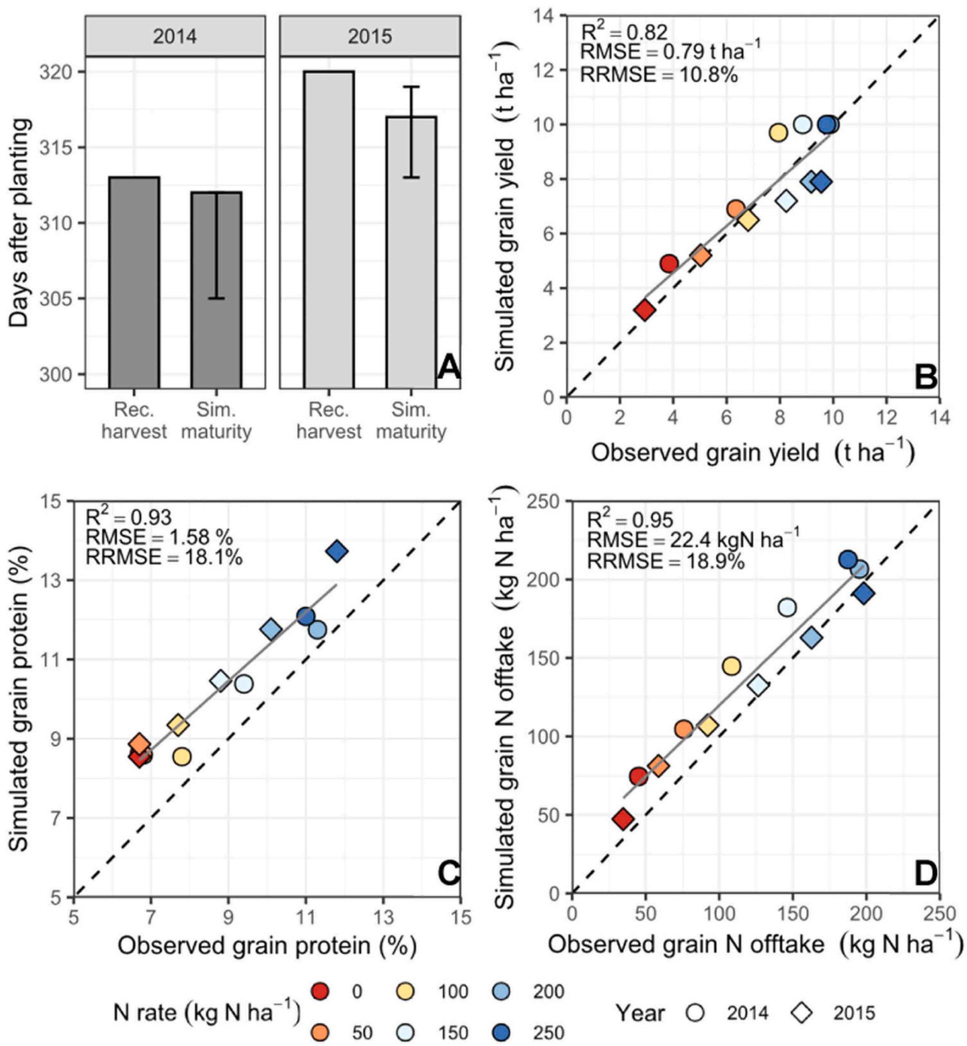

Fig. 6. Comparison of observed and simulated data for wheat performance. (A) Recorded date of harvest compared to simulated maturity date at 200 kg N ha-1, with error bars representing the maximum and minimum across N rates. (B) Observed yield compared to simulated yield. (C) Simulated grain protein compared to observed grain protein. (D) Observed grain N offtake compared to simulated grain N offtake (Eq. 2).

Table 2
Model validation across 5 wheat years on the NFS-RE for the two representative soil profiles, High ECa (HEC= plots 7.5–8.5 mS/m) and Low ECa (LEC=plots 2.5–3.5 mS/m).

	N (kgN ha^{-1})	0		110		220		
	Soil	HEC	LEC	HEC	LEC	HEC	LEC	Mean
Yield	Observed	5.0	3.7	7.9	6.5	9.2	7.7	6.7
(t ha)	Simulated	4.3	3.5	8.3	7.4	9.3	8.1	6.8
	RMSE	1.2	0.8	1.3	0.1	1.5	1.7	1.1
	RRMSE	24.6	22.0	16.2	17.5	16.7	21.8	19.5
Grain protein	Observed	7.1	8.1	9.1	9.4	11.0	11.6	9.4
(%)	Simulated	8.6	8.6	9.2	9.5	11.7	12.3	10.0
	RMSE	1.5	0.8	1.6	1.2	1.6	1.9	1.4
	RRMSE	20.6	10.8	17.3	13.1	14.3	16.1	15.4
Grain N offtake	Observed	62	54	128	109	178	155	114.2
(kgN ha)	Simulated	65	53	132	122	188	170	121.9
	RMSE	15	12	19	19	33	30	21.3
	RRMSE	24.0	22.9	15.1	17.5	18.5	19.1	19.5

ECa, however at a field or farm scale this is labor intensive, at an experimental level it also is destructive of natural soil formation, with likely long-term impacts on the sampled area. Where multiple factors such as variation in texture and stone content or soil depth influence ECa, relying on pre-described models derived from soil databases or non-local data sets might lead to inaccuracies in soil parameter estimation. It is more reliable to develop farm or even field specific relationships/regressions for field zones derived from proximal data (e.g. ECa) and specific soil properties that consider all local influences on water retention characteristics of a soil (Brogi et al., 2020; Wong and Asseng, 2006). Here, we used sampled data from the extremes of the ECa range across the NFS experiments to reflect how targeted samples across

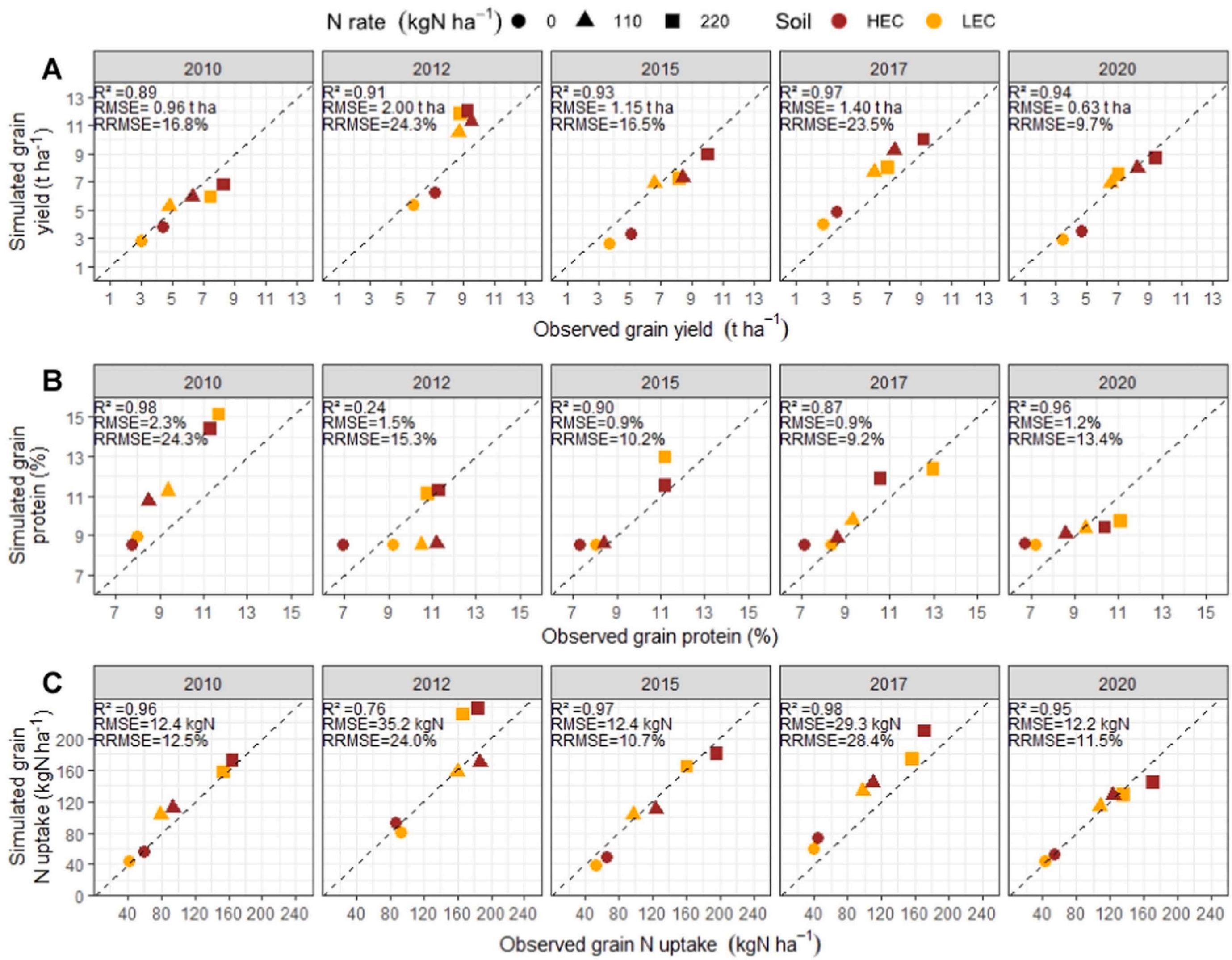

Fig. 7. Sirius validation for the NFS-RE at 0 N, 110 N and 220 N on the Low ECa (LEC=plots 2.5–3.5 mS/m) and High ECa (HEC=plots 7.5–8.5 mS/m) plots for A; grain yield, B; grain protein, C: grain N uptake.

observed variation could be used to parametrize CSM spatially. The variation in ECa was explained by observed variation in texture, stone content and organic C resulting in soil with contrasting available water capacities (LEC=105, HEC=148 mm) and inorganic N. This is particularly important when these variations in soil properties, mapped through proximal sensors such as ECa, have a strong and temporally stable influence on crop performance, as seen in this study.

The NFS experiments were situated in the relatively dry, east of England with an average annual rainfall of 676 mm at Morley. It is estimated that 30% of UK wheat is grown on drought prone soils, causing average yield losses of 10% (Ober et al., 2013). In four of the five years, a lower ECa, here demonstrated to represent a lower plant available water capacity, resulted in a significant reduction in yield at all N rates. In 2012 no significant correlation between ECa and yield was recorded at 220 kgN ha^{-1} and only a small significant yield response was recorded at 150 kg N ha^{-1}. April to July 2012 was the wettest summer on record in England, therefore it is likely that, even on the lowest ECa soils, soil water was not a limiting factor where N was applied. However, a significant correlation and large yield response between soil ECa and yield was still recorded at 0 N. The relationship between NUE and water uptake efficiency (WUE) is understood to be co-limiting (Quemada and Gabriel, 2016; Sadras, 2004) with N fertilization shown to improve WUE in cereals (Cossani et al., 2012). This co-limitation likely explains why we still see higher grain yield on high ECa soils compared to low ECa soils at 110 N and 0 N. Using the linear regression equations for the five-year mean regressions between soil ECa and yield and grain protein, RE_{fertN} was estimated to be 9.3% lower on the plots with the lowest ECa compared to the highest. This correlation raises environmental concerns, as it implies that under standard nitrogen application rates, areas with the lowest NUE also align with elevated leaching risk, primarily due to their increased sand and stone content. These correlations and inferences, drawn from an LTE dataset, can be applied on the farm. By integrating ECa measurements with targeted soil sampling (e.g. Brogi et al., 2020), combine yield mapping (Adhikari et al., 2023), and technologies such as on-the-go near-infrared spectroscopy for grain protein/N mapping (Long and McCallum, 2015), farms can initiate the spatial mapping of NUE. This process would allow the identification of areas with elevated environmental risks and potential economic inefficiencies. Although such analysis can help farms identify areas where a change in management might be required, determining economic and environmental optimal management strategies is still difficult.

One method is to use grain protein concentrations as a retrospective diagnostic tool. Current UK feed wheat recommendations specify that optimal grain protein content for yield is 11% (equivalent to 1.9% N), and N rates could be adjusted by 25 kg N ha^{-1} for every 0.5% above or below this benchmark (AHDB, 2023a). Using the 5 year mean linear

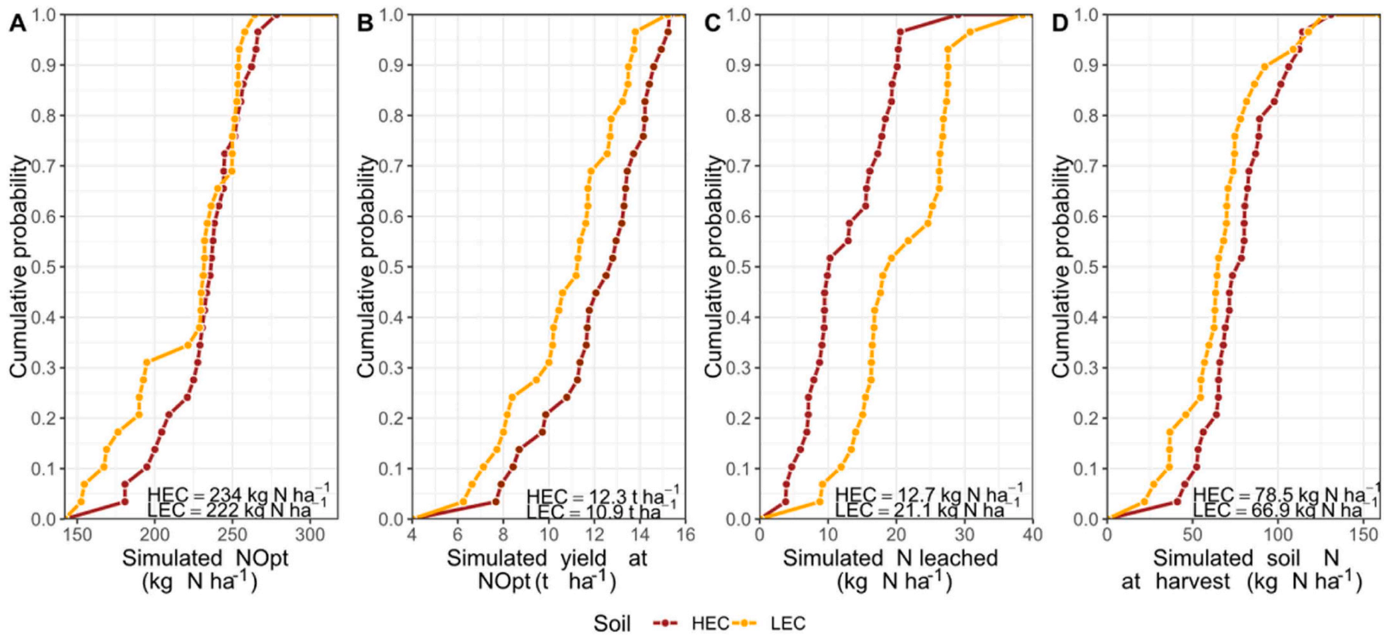

Fig. 8. Sirius simulation results for HEC (brown) and LEC (yellow) soils displayed as cumulative probability using 29 years of weather data. (A) simulated NOpt, (B) simulated yield at NOpt, (C) simulated within growing season N leached, (D) simulated surplus N.

relationship, grain proteins ranged from 11.5% in the lowest EC plots to 10.8% in the plots with the highest ECa under current farm standard N rates. Therefore, based on current recommendations, N rate could potentially be lowered by 25 kg N ha^{-1} on areas with the lowest ECa. This conclusion is potentially supported by the relationship between yield and ECa in 2020 and 2017. In 2020, only a small increase in yield is recorded from 220 N compared with 110 N in plots with the lowest ECa. A similar, but less pronounced trend is seen in 2017. In these years the smaller response to 220 N on the low ECa soils suggests NOpt rates might be below the farm standard 220 N as suggested by the grain protein data. However, the effectiveness of grain protein as a N management tool is still debated. Sylvester-Bradley and Clarke (2009) showed that grain protein explained NOpt in 70–80% of small plot N response experiments and was useful in indicating NOpt. However, within a precision agriculture context (Kindred and Sylvester-Bradley, 2014) reported that within field grain protein at NOpt varied considerably, concluding that multiple N response experiments in every field and season would be required, although clearly impossible, for a precise assessments of site-specific N response. However, CSM can allow us to simulate virtual experiments, complementing 'real' experiments, but these need to be evaluated relative to the real system (Jones et al., 2017b).

4.2. *Crop simulation models as a precision agriculture tool for UK wheat*

4.2.1. *Model calibration and validation*

UK wheat cultivars exhibit large diversity and turnover (Curtis et al., 2018), including variation in phonological development (Sheehan and Bentley, 2021) and NUE (Barraclough et al., 2010). Therefore, accurate cultivar parameters, reflecting this diversity are essential for applied modeling on farm. In this study a calibration procedure updated parameters for *cv* Claire. These parameters demonstrated good model performance when modelling two of the varieties grown in this study including good simulation of maturity date, grain protein, yield and grain N offtake. Using parameters representative of wheat grown across a region is common practice (Delgado et al., 2005; Jin et al., 2017). However, cultivar specific parameters would likely improve model performance and improve relevance of modeling derived recommendations (Miao et al., 2018). Collecting additional experimental data, particularly around crop phenology following standardized protocols (Manschadi et al., 2021; Pasley et al., 2023) from LTE with high variety turnover or long running annual variety trial series could expand available cultivar parameters to support wider applications of CSM. This can identify varieties most suited to a hyper local environment or soil type (Paz et al., 2003).

For CSM to support spatially specific N management they must accurately simulate crop N dynamics and yield across expected ranges of N, soil, and weather (Morarl et al., 2021; Sadler et al., 2000; Sadler and Russell, 1997). The validation of the Sirius model against observed spatial variation in crop growth within the NFS-RE demonstrated it's suitability for inferring appropriate agronomic management decisions.

Across both soils representing the extremes of observed variation in the NFS-RE Sirius demonstrated good model performance, as evidenced by the RRMSE for yield (19.5%), grain protein (15.4%), and total grain nitrogen offtake (19.5%) over various nitrogen rates and years. The largest errors in yield simulation occurred in 2012, with a RRMSE of 23.4%. This year had higher than normal spring and summer rainfall (Kendon et al., 2013), creating favorable conditions for the foliar disease Septoria leaf blotch (*Zymoseptoria tritici*). Record levels of the disease were reported in the UK in 2012 (Gosling and Roberts, 2017), and on the NFS-RE trial, 15–28% infection was recorded on the 220 N plots, with smaller levels of infection on the 0 N and 110 N treatments (NIAB, personal communication, January 2024). It has been reported that for every 1% of leaf area infected, there is a potential yield loss of 0.67% (Gosling and Roberts, 2017). Since Sirius does not model the impact of disease on crop growth, it only simulated yields and response to N without accounting for this observed yield loss from disease. This underscores the need for the development of improved pest and disease modules for crop simulation models (Donatelli et al., 2017) particularly in high disease pressure areas. The only year in our dataset where significant disease pressure was recorded was in 2012. This suggests in most years (4 out of 5) good control was achieved through fungicide sprays, and therefore N management considerations could assume minimal losses from disease pressures. The overestimation in yield in 2017 cannot be explained by disease pressures. However, there was significant grass weed populations (*Fescuta*) recorded in the trial that would likely reduce yield potential (NIAB, personal communication, January 2024). Sirius appeared to effectively capture the impacts of water stress in 2010, the year with the lowest simulated and recorded yields at 110 N and 220 N, a year marked by a very dry spring in eastern England with recorded impacts on agriculture (DEFRA, 2010).

Sirius overestimated yield on average by a greater proportion on the LEC at 110 N and 220 N. This could be explained by the nature of the physical characteristics of these soils. Sandy and stoney soils with lower available water capacity have lower cation exchange capacities and can be potentially more prone to other nutrient limitations and yield limiting influences (Alfaro et al., 2004; Huang and Hartemink, 2020). Previous studies have demonstrated that model performance can vary spatially when soil properties influencing crop growth are unaccounted for in model structures (Paz et al., 1999; Thorp et al., 2007).

In the 0 N plots, the lowest Sirius simulated grain protein was 8.6% (1.5% grain N), which was equivalent to the minimum grain N limit within Sirius (Jamieson and Semenov, 2000; Sinclair and Amir, 1992). This threshold is based on relatively old data sets (Spiertz and Ellen, 1978). On the NFS-RE the lowest recorded grain protein was 6.6% (1.1% grain N). This is comparable to minimum recorded in other data sets using modern UK wheat varieties without N fertilization (Hawkesford and Riche, 2020). Mechanistic models like Sirius should be continuously updated as our understanding of the system (i.e. new cultivars) changes (Keating, 2020; Stockdale and Gaunt, 1997). As demonstrated here LTE conducted under controlled and repeated conditions provide the platforms for updating model accuracy and relevance (Johnston and Poulton, 2018).

No comparable studies for wheat in the UK have been identified, highlighting the novelty of the application of CSM for managing spatial variability in UK wheat. Cammarano et al., (2020) found the DSSAT model explained 72% of the variation across spring barley yields from management zones in a field in Scotland, comparable to 77% in this study. The RMSE for yield of 1.3 t ha^{-1} (RRMSE=19.5%) is comparable to other spatial model evaluations in wheat outside of the UK (Basso et al., 2011a; Ward et al., 2018; Wong and Asseng, 2006). Basso et al., (2009a) reported a RMSE of 0.2 t ha^{-1} (r^2=0.91) using the DSSAT model across management zones for an Italian field, when the model was initialized with measured soil moisture contents at sowing. Initial soil moisture and mineral N content may have improved model performance across the NFS-RE (Cammarano et al., 2021). Model accuracy would also be improved using cultivar specific parameters for each growing season and recorded weather data instead of synthetic data for some variables. Although no significant difference across the NFS-RE was reported in the years in this study there are likely to be small differences in crop response to experimental treatments not currently accounted for in Sirius. For example, modeling approaches could include the impact of management practices such as tillage in future applications (Basso et al., 2011b; Bertocco et al., 2008).

4.2.2. Model application

The validated CSM was used to simulate 29 years of N response experiments on the extremes of variation recorded across the NFS-RE. The mean NOpt for both soils (HEC=234, LEC=222 kg N ha^{-1}) exceeded the current farm standard N rate of 220 kg N ha^{-1}. As previously described, Sirius tended to overestimate yields on both soils at 110 N and 220 N, as a result of being unable to simulate impacts on yield such as disease. This overestimation of yield potential is likely to have increased the simulated NOpt. Modeling derived recommendations should therefore be interpreted as recommendations at maximum potential yield and be altered based on season-specific conditions and influences (Cho et al., 2012). Modeling results suggest that the LEC have a lower NOpt compared to the higher yield potential HEC soils. This is in line with other studies using models to determine N management strategies in rainfed agricultural systems (Albarenque et al., 2016). Modelling N response over 29 years of recorded weather data provided a temporal data set that allows response probability to be evaluated so growers can incorporate risk management into their N management decision-making. Analysis shows there is a much greater chance (31%) of NOpt being below 200 kg N ha^{-1} on the LEC soil than HEC soil (10%). Farmers in the UK and across Europe are under pressure to meet greenhouse gas emissions reduction targets, which will likely require a reduction in overall N use (Squire et al., 2022). Recent geopolitical circumstances have also put pressure on N fertiliser availability resulting in some farms making decisions where best to reduce nitrogen applications (spatially and rotationally, i.e. which crops) (Ben Hassen and El Bilali, 2022). The modeling exercise here suggested significant N fertiliser reductions would be less economically detrimental on the LEC than the HEC soils.

An advantage of CSM is their ability to infer system responses to management decisions. Here we used Sirius CSM to simulate in-season nitrate leaching and N surplus from model derived NOpt. The LEC soil had higher in season N losses, with Sirius simulating the effects of the free draining properties of the lower AWC soil. The majority of N loss was from available soil mineral N at sowing (assumed to be 30 kg N ha^{-1}), and a simple modeling exercise of running the model without any N applications confirmed this. These results are in line with measured quantities of overwinter leaching in wheat crops (Webb et al., 2000). The calculated simulated N surplus was higher on the HEC soils, despite the higher simulated yields. This is likely a result of a combination of higher NOpt resulting in higher fertiliser rates, lower levels of N losses through leaching, and higher soil organic N levels resulting increased soil mineralized N. The relatively high post-harvest N surplus is in line with other studies demonstrating that NOpt can still result in large quantities of surplus N (Thorp et al., 2006). N surplus and leaching risk potential should be considered together, as a soil with high surplus N and lower leaching risk may not pose the same environmental risk as a soil with lower surplus N and greater potential for over winter leaching. This poses interesting policy and management considerations as well as identifying limitations with this modeling exercise. In this study modeling was performed on 29 independent seasons, with model being reset for each simulation. The LTE, and most farming systems follow a rotation of multiple crops and crop types. Therefore, using the model over a single crop and season we fail to track model variables across multiple years (Thorp et al., 2007), to account for how the soil type, simulated N surplus and leaching risk interact across a rotation. This would allow for management techniques i.e., rotation/cropping as well as N rates to be designed to minimize environmental risk associated with these modeled states. Such approaches are possible with multi-crop models such as DSSAT and APSIM (Jones et al., 2003; Keating et al., 2003). However, such rotational modeling is intrinsically more complex requiring multiple crop specific cultivar parameters and modelling errors are prone to accumulate over seasons (McNunn et al., 2019). Whilst the Sirus model was validated for yield and grain protein, it would be beneficial to validate of other simulated responses such as post-harvest soil N, or N lost over winter. These data sets are harder to obtain and less frequently monitored in LTE but would greatly improve the validation of models as spatial management tools. CSM vary in their simulations when using the same spatial data sets as inputs. Future work should compare the results of multiple models in model ensembles for spatial applications in UK wheat crops (Wallor et al., 2018). There is also the need to develop appropriate mechanisms to appropriately identify economic and environmental impacts of management options. Some studies have used a risk-based approach such as setting appropriate thresholds for modeled N losses (e.g. < 30 or 40 kg N ha^{-1} in 80% of simulated seasons (Basso et al., 2007; Thorp et al., 2006)). However, such targets will likely need to be site specific based on the associated local environmental risk factors (Burt et al., 2011).

Crop models enable exploration of system responses to multiple iterations. In this study, we demonstrated the capability of simulating spatial variations within an LTE using soil specific NOpt and typical drilling dates, N timings, and splits. Future research should employ experimental modeling techniques to analyze NOpt variation response to within-field spatial properties and determine the effects of N application timing, drilling date, and plant populations on management and system responses. Moreover, findings can guide optimal management decisions for specific weather events and climate change scenarios could be incorporated to investigate high-resolution on-farm impact of future weather patterns.

Keating and Thorburn, (2018) express concern that models are not being used to make positive differences in real world situations. Here we demonstrated an application of modeling to inform on farm management using LTE data sets. The next logical steps are to take these methodologies to inform management decisions on farm. It is our aim to do this using a new type of long-term monitoring study at Morley that records spatially explicit data sets across rotations suitable for model validation (TMAF, 2023).

5. Conclusion

Results showed large spatial variation in soil properties across a LTE. Soil ECa was strongly correlated to both the variation in soil properties and temporal and spatial patterns in crop growth and performance quantified using LTE data sets. This demonstrated how proximal soil sensing and targeted farm-specific soil measurements can be used to generate soil maps that can be used to explain the variation in yield across farms and fields. Furthermore, we demonstrated how such data sets could be used to calibrate and validate crop simulation models to guide spatial management of N in UK wheat crops. The Sirius CSM performed to a good level of accuracy in simulating yield and grain N offtake. Simulations can be improved with more complete data sets suitable for model validation, particularly initial parameterisation and environmental risk such as N loses and post-harvest N. We demonstrated that spatially explicit, economic optimum N management plans and risk-based N management decisions can be made from experimental modeling and CSM outputs. Further work is needed to demonstrate CSM spatial accuracy on a wider range of soil types, and testing the reliability of different models for management recommendations. LTE with high spatial-temporal data sets and quantified spatial variation are suitable places to test this.

Declaration of Competing Interest

The authors have no relevant financial or non-financial interests to disclose.

Data Availability

Data will be made available on request.

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Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.eja.2024.127224.

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