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Monitoring and Managing Spatial-Temporal Variability on Farm: A
Crop Modelling Approach for Nitrogen Management

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Supervisor: Professor Stephen Hallett
Associate Supervisor: Professor Jacqueline Hannam
Associate Supervisor: Dr Elizabeth Stockdale (NIAB) Associate
Supervisor: Dr Benjamin Marchant (BGS)

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Abstract

Spatial variability in soil properties leads to significant differences in nitrogen use efficiency and crop response, creating challenges for optimising fertiliser management in wheat production. This research evaluates the feasibility of using the Sirius Crop Simulation Model to inform site-specific N management, integrating high-resolution soil sensing, long-term yield maps, and agronomic data. A systematic review identified key knowledge gaps, including the lack of crop simulation model applications for UK wheat at the sub-field scale and challenges in spatially parameterising soil properties. To address these, Sirius was validated using long-term agronomic data, accurately simulating spatial-temporal variability in grain N uptake (RRMSE = 19.5%), demonstrating its potential for spatial N management. A framework for cleaning, validating, and applying whole-farm yield map datasets was developed and applied to a 435 ha commercial farm. This enabled management zone delineation based on soil and economic performance and demonstrated how such techniques could be used to support precision agriculture, including crop modeling parametrisation. Sirius was then parameterised and applied across 30.5 ha using these management zones techniques, generating zone-specific N recommendations ranging from 160–216 kg N ha⁻¹, simulating potential for improvements in nitrogen use efficiency and reducing unutilised N, particularly in low available water capacity zones where current farm standard N application increased leaching risk by up to 31.1 kg N ha⁻¹. This research demonstrates a novel integration of crop simulation models into precision N management for UK wheat, combining validated models with refined spatial data techniques to improve farm-scale decision-making. While some model limitations remain, particularly in biomass simulations, the study highlights the potential for models to support economic and environmental sustainability in wheat production. Future work should validate model-derived recommendations in field trials, explore multi-model comparisons, and assess broader rotational impacts to enhance long-term farm management.

Keywords:

Cropping System Model, Sirius, Nitrogen, Management zones, Yield maps

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List of Abbreviations

AHDB	Agricultural and Horticultural Development Board
APSIM	Agricultural Production Systems Simulator
CSM	Crop Simulation Models
CSM	Cropping System Model (used interchangeably with crop simulation model)
CY	Combine yield
DEFRA	Department for Environment Farming and Rural Affairs
DSSAT	Decision Support System for Agrotechnology
DUL	Drained Upper Limit
ECa	Apparent Electrical Conductivity
GS	Growth Stage
HEC	High ECa
Kp	Percolation Coefficient
KSAT	Saturation Water Content
LAI	Leaf Area Index
LEC	Low ECa
LL	Lower Limit
MAE	Mean Absolute Error
MBE	Mean Bias Error
MME	Multi Model Ensemble
MZ	Management Zone
NFS-CE	New Farming Systems Cultivations Experiment
NFS-RE	New Farming Systems Rotations Experiment
NOpt	Economic optimal Nitrogen rate
NUE	Nitrogen Use Efficiency
PAWC	Plant Available Water Capacity
PRISMA	Preferred Reporting for Systematic Reviews and Meta Analysis
PTF	Pedotransfer functions

REfertN	Fertiliser Grain Nitrogen Recovery
RL	Recommended List
RMSE	Root Mean Square Error
RRMSE	Relative Root Mean Square Error
RUE	Radiation Use Efficiency
RY	Recorded yield
SAMS	Soil and Agronomic Monitoring Study
SD	Standard Deviation
SOC	Soil Organic Carbon
SOM	Soil Organic Matter
SPEI	Standardised Precipitation Evapotranspiration Index
TMAF	The Morley Agricultural Foundation
USDA	United States Department of Agriculture
WIGIN	Wheat Genetic Improvement Network

1 Introduction

1.1 Overview

This research investigates and develops the application of Cropping System Models as practical tools to manage spatial-temporal variation in Nitrogen (N) use efficiency in UK wheat. Experimental field trial data and on-farm datasets are utilised to develop a framework for the application of models in devising spatially appropriate nitrogen management strategies at the sub-field scale, considering the spatial variability in soil properties and environmental risk potential.

Chapter 1 introduces the research context and outlines the research question, aim, objectives, and contributions to the industry and knowledge. Additionally, a summary of the subsequent chapters and research structure is provided.

1.2 Background and context

1.2.1 UK wheat and nitrogen fertiliser use

Wheat (*Triticum aestivum* L.) is the UK's largest cultivated arable crop, encompassing 1.7 million ha⁻¹ in 2023 (DEFRA, 2023a). The soils, climate, and production efficiency within the UK allow for yields close to agroecological potential, averaging 8.2 t ha⁻¹ (2014-2023), while yields over 16 t ha⁻¹ are possible (Bruinsma, 2009; DEFRA, 2023a; Mitchell and Sheehy, 2018). With an increasing global population, and the challenges posed by climate change, maintaining productivity in main supplier and exporter regions such as the temperate European climates is important in maintaining and increasing national and global food security (Röder et al., 2014).

N is a major macronutrient essential for plant growth. Plants primarily absorb N from the soil as nitrate (NO₃⁻) and ammonium (NH₄⁺), although foliar uptake is also possible (Ferrari et al., 2021; Woolfolk et al., 1997). While the largest pool of soil N is in organic form, it is not directly available to plants and must first undergo mineralisation. Alternatively, plants can access N from mineral sources supplied through fertilisers and manures. N is a fundamental component of proteins, amino acids, nucleic acids, membrane lipids, and other essential compounds. Among

these, proteins are particularly important, as they include enzymes, transporters, and structural components of cells. As the central element of amino acids, N plays a crucial role in grain protein formation, a key quality trait in wheat for milling (Ohyama & Sueyoshi, 2010; Shewry, 2007). N fertiliser inputs substantially increase canopy biomass, allowing for better photosynthetic potential (Hawkesford, 2014). There are several studies describing the uptake, redistribution, and mechanisms of N plant interactions (Barracough et al., 2010a; Fradgley et al., 2021; Hawkesford, 2014; Hawkesford and Riche, 2020). High N fertiliser inputs are required to realise the high yield potentials, made possible through advances in plant breeding, and the efficacy of plant protection products (Sylvester-Bradley et al., 2008).

Optimum N fertiliser rates often increase yields by a factor of two compared to those relying on the soil N supply alone (Figure 1-1). On average, UK wheat receives 186 kg N ha⁻¹ in total N fertiliser (2013-2022) (DEFRA, 2023b), however fertiliser rates vary widely, ranging from 0-350 kg N ha⁻¹ at a field level (Baxter

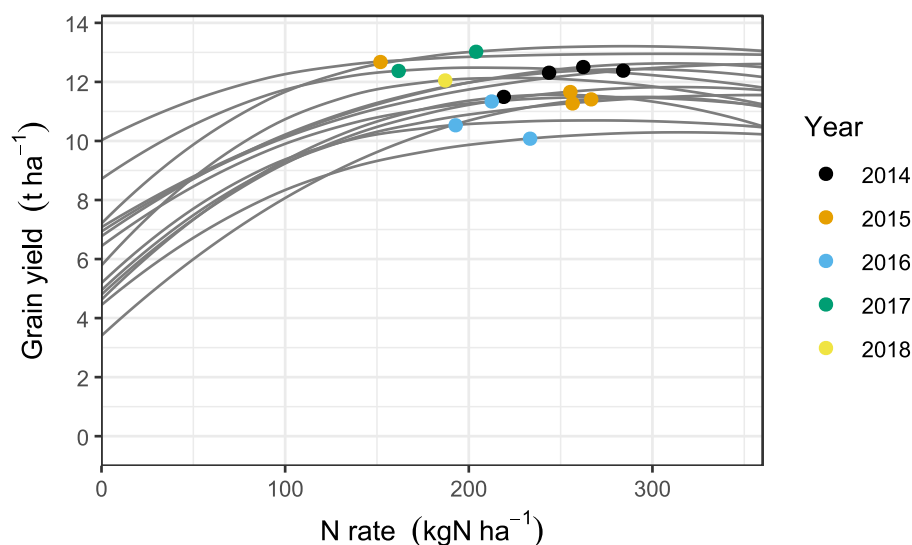


Figure 1-1 Nitrogen response trials (n=14) conducted at the Morley Agricultural Foundation (TMAF) between 2014 to 2018 across 9 fields. Trial data acquired via pers. comm. NIAB, 2023. Nitrogen response curve fitting, and determination of economic optimum nitrogen (coloured points) calculated following methodologies outlined in George (1984) and Kindred et al (2018a)

and Clarke, 2023). The efficiency with which a crop or system utilises applied N fertiliser and other N sources is known as Nitrogen Use Efficiency (NUE).

1.2.2 Nitrogen Use Efficiency (NUE)

There are many definitions and calculations for NUE, utilising different system components and stocks (Congreves et al., 2021). Most indices are based on the ratios of crop yield (utilisation efficiency), or crop N concentrations (uptake efficiency), as compared to that of soil and/or fertiliser N sources (Congreves et al., 2021; Hirel et al., 2007; Sylvester-Bradley and Kindred, 2009). Figure 1-2 illustrates the calculation and components for the NUE metric; Fertiliser Grain Nitrogen Recovery (REfertN). Over 30 years ago Hart et al. (1992) reported, using ^{15}N labelled fertiliser, that above-ground fertiliser recovery averaged 68% in Eastern England. In a recent study by Baxter and Clarke (2023) apparent N fertiliser recovery was calculated at 73% across a large multi-farm dataset across the UK. However, these findings were obtained on high-yielding crops, which will typically correlate to higher NUE (Barraclough et al., 2010a). Even within this dataset a proportion of the farms assessed demonstrated poor NUE. Overall NUE is likely to be lower nationally, estimated at between 50-75% (Mitchell and Sheehy, 2018).

The inefficient use of N can lead to losses out of the soil-crop system. This mainly occurs through three pathways: (i) Ammonia (NH_4^+) volatilisation, which can contribute to mass concentration of particulate fine matter with negative impacts on human health and that of the wider ecosystem (Marais et al., 2021; Misselbrook et al., 2000); (ii) The nitrification and denitrification of soil mineral N applied as fertiliser to nitrous oxide N_2O . This is estimated, with a large amount of uncertainty, to be around 0.46%-0.6% of applied N (Cowan et al., 2020; Sylvester-Bradley et al., 2009). N_2O is a greenhouse gas with a global warming potential 298 times that of CO_2 (Houghton et al., 2001); (iii) Nitrate (NO_3^-) anions that are not taken up by plants or microorganisms can be prone to leaching into freshwater. The amount of N lost through leaching varies based on soil type, weather, pest and disease pressures, and rotation. Goulding et al. (2000) reported mean annual losses of 30 kg N ha^{-1} , with losses as high as 60 kg N ha^{-1} .

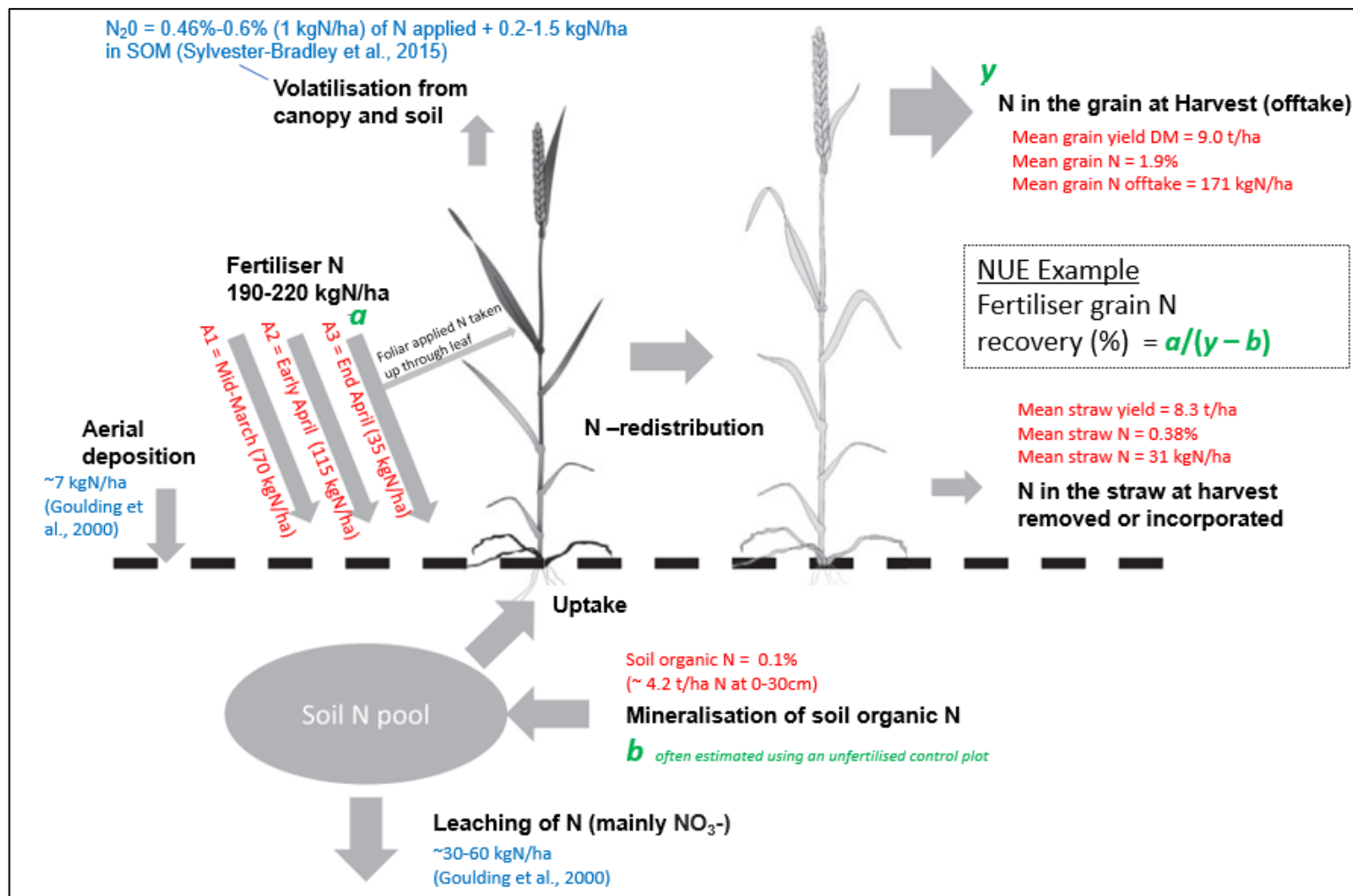


Figure 1-2 Schematic showing major fluxes of N in a UK wheat crop, adapted from Hawkesford (2014). Annotations in red represent example proportions from experiments at the Morley Agricultural Foundation, Norfolk, UK. Annotations in blue represent UK literature averages, green annotations provide example inputs into the calculation from fertiliser grain N recovery, a measure of NUE

¹ in wet years under economic optimum fertiliser for wheat on one long-term experiment. Losses can be higher when NUE is poor (Shepherd et al., 1993), or losses of post-harvest soil N are high (Cooper et al., 2017). Agricultural land is the main (70%) source of nitrates in ground and surface water in the UK, with groundwater and river concentrations generally being highest in the drier, arable dominated eastern England (Environment Agency, 2019), many areas have nitrate concentrations >50 mg NO₃ L⁻¹ (Burt et al., 2011a; Whelan et al., 2022). While some progress has been made (Burt et al., 2011a; Wang et al., 2016) future challenges of climate change (Dallison et al., 2022) and food security (Mitchell and Sheehy, 2018) will require greater improvements in NUE to meet water quality targets.

Nitrogen fertiliser production and N₂O emissions can account for over 70% of cereal crop greenhouse gas emissions (Kindred et al., 2021). As farmers endeavour to meet net zero commitments (NFU, 2020), lowering nitrogen fertiliser rates and/or enhancing NUE will likely be adopted as key strategies in meeting these targets. Recent supply issues coupled with high fertiliser prices brought about by geopolitical and market forces (Hassen and El Bilali, 2022) have also resulted in farmers looking to reduce N application rates and targeting its application where greatest returns are likely (DEFRA, 2022). These environmental, economic, and more recently geopolitical factors have made improving NUE a global priority (Udvardi et al., 2021).

1.2.3 Nitrogen management to improve NUE

There are generally two avenues for improvements in NUE, through the breeding and development of wheat varieties having improved N uptake and utilisation capabilities and through improved fertiliser and system management (Barracough et al., 2010a; Udvardi et al., 2021). Research interest in the development of varieties with enhanced crop nitrogen uptake capacity and efficiency is accelerating (Fradgley et al., 2021; Hawkesford, 2017; Hawkesford and Riche, 2020). This is evidenced by the recent commissioning of a scoping review looking at how variety interacts with nitrogen nutrition scenarios across the major UK crop groups (AHDB, 2024a). Despite the potential for varietal

differences in NUE, most of the on-farm variations within and between seasons are primarily an artefact of environmental factors such as soils and climate. Therefore despite some varietal influences, site and season appropriate, more targeted N management strategies can have the greatest impacts on NUE (Snyder, 2017). How this can be achieved is often summarised into '4 Rs' (Snyder, 2017; Venterea et al., 2016), thus:

Right source: using the right type and form of fertiliser including soil applied, foliar applied or organic N sources. Includes developing and using new enhanced efficiency fertilisers designed to slow solubilisation including urease, and nitrification inhibitors (Qiao et al., 2015; Thapa et al., 2016).

- i. *Right rate:* determining the appropriate rate that matches crop requirements, soil N supply and seasonal conditions. This rate should also consider non agronomic factors such as environmental risk and economics. Nitrogen rates are primarily determined using nitrogen response curves (Godard et al., 2008), while other considerations such as grain quality targets (Morris et al., 2022), and precision agriculture tools can be used to supplement this information (Diacono et al., 2012).
- ii. *Right time:* N is utilised most effectively when its presence in the soil coincides with the crop's requirements. Fertiliser (N) applications can be split across growth stages based on changes in crop demand, seasonal conditions and to meet end market quality characteristics (Efretuei et al., 2016; Morris et al., 2022).
- iii. *Right place:* addresses the importance of distributing applications within the crop's root zone to optimise nutrient uptake, as well as appropriate application method. However, it also has the potential to encompass precision agriculture methodologies, which account for the spatial diversity in crop nitrogen needs resulting from systemic heterogeneity in-field.

A fifth 'R' often discussed outside the "4 Rs" principles above encompasses practices that reduces fertiliser requirements through rotations, thus:

- iv. *Right rotational management*: Rotational management decisions such as residue management (Mary et al., 1996), cultivation practice (Powlson, 1980), incorporation of nitrogen fixing species into the rotation (Faligowska et al., 2019; Stobart and Morris, 2013) and a high level of agronomic best practice in managing pests and disease (Lammerts van Bueren and Struik, 2017).

This study is focused primarily on developing methods around two of these 'R's, namely 'right rate' and 'right place'. However, the methods and results are discussed within the full context of all 5 'Rs'.

1.2.4 Nitrogen management in the UK

Farmers in the UK decide what N fertiliser rate to apply, based on recommendations calculated using an industry standard reference book, 'RB209' (AHDB, 2023a). This allows registered trained advisors to consider, previous cropping, soil type, soil organic matter content, yield potential, historic grain N concentrations and overwinter rainfall to derive field specific N rates (Kindred and Sylvester-Bradley, 2014). These rates have been derived from N response experiments conducted over the last 85+ years, frequently re-assessed to account for temporal changes in agricultural systems (Crowther and Yates, 1941; George, 1984; Kindred et al., 2018a; Sylvester-Bradley et al., 2008). These experiments primarily determine the economically optimal nitrogen rate (NOpt), which is the fertiliser application rate that maximises economic return based on crop yield response.

The major limitations of the recommended methods in this are that they are based on averages and fail to capture the inherent variability in N response across experiments, driven by site and year. Data from N response trials conducted at The Morley Agricultural Foundation (TMAF) (Norfolk, UK) demonstrated that NOpt has ranged from 152-284 kg N ha⁻¹, influenced by field-season interactions (Figure 1-1). This indicates the current national average management guidelines are ineffective and limited (Kindred et al., 2012, 2015).

Potential mechanisms exist for spatially adjusting N rates across and within fields to accommodate temporally consistent variations in crop performance metrics. Growers have the flexibility to adjust N rates by ± 25 kg N per hectare for every 0.5% deviation in grain protein content from 11% for feed wheats (12% for milling wheats) (AHDB 2023b). Additionally, yield correlated with crop nitrogen demand can fine-tune N rates based on yield potential. In cases where yields consistently surpass 8 t ha^{-1} over multiple seasons, it is advised that N rates are augmented by 10 kg N ha^{-1} for every additional 0.5 t ha^{-1} of yield (AHDB, 2023b; Roques et al., 2016). Nevertheless, the relationship between yield or grain protein content and the economic N optimum remains inconclusive, while evidence of correlations across landscapes and fields exists, they tend to be weaker at the within-field scale (Kindred and Sylvester-Bradley, 2014; Kindred et al., 2018). These somewhat deterministic approaches fail to consider the dynamic factors influencing N uptake, overlooking other factors that likely influence N optimum, such as drilling date, establishment, and conditions leading up to N applications. They are also unable to consider the environmental consequences, such as leaching potential of a given management decision. Therefore, it is recognised that better recommendation methods accounting for spatial-temporal factors impacting crop N demand are required (Kindred et al., 2015).

1.2.5 Spatial variation in soils, productivity and NUE

Soils exhibit spatial variability between and within fields. This can be driven by physical factors, such as texture, stone content, and soil depth resulting from geological, pedologic and other earth system processes (Iqbal et al., 2005; Jenny, 1941). These physical differences can influence the spatial variation in other soil properties such as plant available water (Lawes et al., 2009) and chemical and nutrient dynamics (Baxter and Oliver, 2003). Topography can also influence soil chemical and water dynamics (Page et al., 2005; Silva and Alexandre, 2005). Other factors such as soil compaction (Wilcox et al., 2000), pest pressures (Archard et al., 2004) and weed populations (Metcalf et al., 2019, 2016) also exhibit spatial dependencies. These factors have direct and indirect impacts on nutrient use efficiency, crop growth and ultimately yield. The advent of yield

mapping and remote sensing technologies has enabled farms to measure the extent of spatial variability in both yield and crop growth temporally (Blackmore et al., 2003b; Maresma et al., 2020; Muhammed et al., 2016; Zamani-Noor and Feistkorn, 2022). Nonetheless, there persists a substantial challenge in effectively interpreting and analysing yield map datasets to guide spatially appropriate management decisions, including N (Blasch et al., 2020). Managing this variation at the sub-field scale, which is defined here as a spatial unit smaller than and within the field boundary, forms the basic principle of precision agriculture.

Some of the key factors impacting crop NUE vary spatially within fields including organic N, plant available water and mineral N content (Baxter and Oliver, 2003; Wetterlind et al., 2008). Studies utilising “chessboard” experiments have revealed significant variability in optimal N rates within fields. In one of the first such experiments, Lark and Wheeler (2003) illustrated how the economic optimum N rate for wheat ranged from 0 kg N ha⁻¹ to 200 kg N ha⁻¹ across different areas of a sandy clay loam field in Bedfordshire, UK. More recently, Kindred et al (2015) found that within fields with diverse soil types, soil N supply varied by 60-120 kg N ha⁻¹, with NOpt differing by up to 100 kgN/ha. Analysing a larger dataset spanning six fields, Kindred et al (2017) observed within field spatial variability in NOpt > 100 kg N ha⁻¹ in seven out of the nine years. Similar studies have demonstrated variations in optimal N rates for other crops (Kendall et al., 2019). The large variations in NOpt, possible within fields, has resulted in the development of techniques to manage this variation through variable rate technology .

A survey conducted in 2012 found that 31% of English cereal farms were using some form of variable rate technology. By 2019, this number had only moderately increased to 42%, indicating a relatively slow pace of adoption over the past decade (DEFRA, 2020, 2012). Quantifying the utilisation and uptake of precision agriculture technologies for N management decisions is difficult. Data from 2014 indicates that more than 300 UK farms were using tractor/sprayer mounted Yara N sensor technologies, while over 500 were utilising satellite-based sensing

services for this purpose (Kindred and Sylvester-Bradley, 2014). While the numbers are likely to be higher today, with only 42% using all types of variable rate technology it is likely to be lower than this. Colaço and Bramley (2018) propose that the limited adoption of N management technologies stems from a failure to effectively demonstrate their efficacy and a lack of advances in their development. This aligns with commentary on the use of precision agriculture technologies for N management in the UK (Orson, 2016) and with recent research indicating that the full potential of digital agricultural technologies can only be unlocked when there is clearer evidence of improvements in management techniques (Ingram et al., 2022).

Satellite-based and tractor mounted N sensors (e.g. Yara N sensor ®) recommendations, provide an indication of canopy biomass and N content derived from indices such as Normalised Vegetation Index (NDVI) (Heiß et al., 2021, Pedersen et al., 2021). These technologies commonly assume that soil nitrogen supply is the major driver of variation in N requirements (Kindred and Sylvester-Bradley, 2014), applying more nutrients to areas of lower biomass and N content assuming additional N will promote canopy growth. There is the potential (although less common) for them to increase rates on the higher biomass areas assuming such areas have a higher yield potential, likely through higher soil available water or other nutrient supply (Colaço and Bramley, 2018). However, satellite and tractor mounted sensors do not provide recommendations of total N dose, but rather adjust the dose, based on an assumed optimal N supply rate for the entire field (Kindred et al., 2017). It is recognised that sensor-based N decision making tools fail to account for all the factors impacting crop N demand (Colaço and Bramley, 2018; Diacono et al., 2012; Pramod Pawase et al., 2023). They do not consider all the underlying factors influencing observed variation in crop N uptake or crop nutrient demand and how applying less, or more nutrients to an area might interact with soil properties and the potential losses to the wider environment.

1.2.6 Crop models as on farm management tools

Cropping system models (CSM) integrate soil and plant process models, describing changes in system states in response to external drivers such as weather or management, and determine the resulting impact on interacting components including crop, soil, and system losses (Jones et al., 2017a; Keating and Thorburn, 2018b). As discussed in the preceding section, traditional N management tools frequently examine components in isolation (e.g. crop N content using canopy sensors). Models enable the study of interactions among multiple system components (Jones et al., 2016). Stockdale and Gaunt, (1997) were early advocates of the potential for process-based nitrogen and cropping models to inform nitrogen management strategies. However, at the time the potential was limited by incomplete understanding of nitrogen dynamics in soil and crops, and the ability to accurately model them (Boote et al., 1996; Stockdale and Gaunt, 1997). While the understanding and capacity to describe and model these processes is not yet complete, there have been notable improvements over the last 25 years (Fradgley et al., 2021; Gärdenäs et al., 2011; Seidel et al., 2018; Udvardi et al., 2021).

Despite these advances, studies continue to describe process-based modelling used to inform N management as a desirable outcome in the future (Diacono et al., 2012; Snyder, 2017; Udvardi et al., 2021) and highlight that there is limited application in managing spatial and temporal variability in practice (Cammarano et al., 2020; Ma et al., 2016). There is little evidence of applications of CSM in a spatial-temporal context in the UK. This may be in part because perceptions of CSM are still *“too inaccurate and undecipherable to be communicated and trusted as guides for husbandry”* (Sylvester-Bradley et al., 2017, p.729). Some early attempts showed poor model performance at describing wheat growth and yield under different N management strategies (Sylvester-Bradley et al., 2005). This sub-optimal model performance was attributed to several factors including the accuracy of experimental data for model calibration and validation and reliance on qualitative soils data for parametrising soil profiles. The access to location-specific data collected following standardised protocols suitable for model parameterisation and calibration continues to be a challenge (Peng et al., 2020).

However, advancements in information systems, coupled with increased on-farm data collection and improved methods of handling, storing, and sharing field trial data, are facilitating more targeted and sophisticated analyses, and supporting crop modelling exercises (de los Campos et al., 2020; Raubach et al., 2021; van der Burg et al., 2021). Previously characterising spatial variability of soil for modelling and precision agriculture was expensive and labour intensive (Rossel and McBratney, 1998). Recently characterising soils at a greater resolution is possible through improved laboratory and infield measuring techniques (Castellini et al., 2021; Segal et al., 2009), remote sensing applications (Abdulraheem et al., 2023) and more accurate and updated pedotransfer functions (Hollis et al., 2015, 2012a). On-farm soil data collection is also increasing, with 47% of cereal farms having soil mapping and 22% of farms having examined soil profiles in multiple holes per field (DEFRA, 2020).

Models, such as the 'Sirius' model have continued to be developed since the early work of Sylvester-Bradley et al. (2005) in the UK (e.g. Crout et al., 2014; Martre et al., 2006). Therefore, there is a requirement to revisit and expand on existing research efforts to assess the effectiveness of current CSM in describing spatial variation in NUE and informing management within and across fields. This includes identifying where model development should be focused to create modelling tools better suited for informing on-farm N management. Additionally, there is a need to develop improved methods for application at a farm scale. Keating and Thorburn (2018b) described how previous research modelling cropping systems can be divided and explained by Oquist, (1978) "types" of research. Research describing system components and building dynamic system models relates to "how the world works" (*descriptive and nomothetic research*); *action research* uses models to guide practitioners and leads to improved cropping system management related to research on "how to change the world". There is limited evidence of models impacting real decisions and increasingly modelling studies should focus on *action research* demonstrating their ability to guide real world decision making (Keating and Thorburn, 2018b). The aim of this study therefore tackles this need and developed a framework for applying models to inform on-farm N management decisions for UK wheat crops.

1.3 Research aim and objectives

1.3.1 Aim

This research aims to evaluate the potential of cropping system models to inform economic and environmentally appropriate N management, accounting for within field spatial-temporal variations in soil properties for UK wheat crops.

1.3.2 Objectives

To accomplish this aim, five primary objectives were pursued. The first objective involved conducting a systematic review of the literature to evaluate the current state of development in utilising CSM to support precision agriculture. Subsequent objectives (2-5) were derived from the findings of this systematic literature review (see Appendix B). The five objectives together were to:

1. Undertake a systematic review of the use of cropping system models in supporting precision agriculture at the sub field scale.
2. Investigate the relationship between spatial variation in soil properties and NUE across a long-term farming system experiment.
3. Evaluate the performance of the Sirius crop model across observed variation in NUE and determine its suitability as a nitrogen management tool.
4. Develop a comprehensive framework for cleaning, validating, and applying whole-farm yield map datasets to effectively guide precision farming techniques including the application of cropping system models.
5. Assess the performance of a cropping system model to describe and manage spatial-temporal variation for N across farm.

1.4 Systematic review

1.4.1 Systematic review protocol

A systematic review was conducted to evaluate the application of CSMs in supporting precision agriculture. While CSMs have been widely used for various agricultural applications, including yield forecasting and climate impact assessments, their integration at the sub-field scale remains underexplored. Recent literature highlights a scarcity of studies applying CSMs to manage spatial variability in crop production (Cammarano et al., 2020; Ma et al., 2016; Pasquel et al., 2023). The review, therefore, aimed to synthesise current methodologies, data sources, and challenges associated with spatialising CSMs and their implementation for managing sub-field variation in arable cropping systems.

PRISMA guidelines were followed to ensure a transparent and replicable approach. Studies were retrieved from the Scopus database using predefined search terms, including "crop model," "crop simulation model," "precision agriculture," and "spatial variability." Inclusion criteria required studies to:

1. Apply CSMs for managing or explaining spatial variability.
2. Implement CSMs at a sub-field scale with multiple simulation points per field.
3. Focus on arable crops with integrated above-ground and below-ground process simulations.

Studies that were theoretical, lacked empirical data, or failed to incorporate soil modelling components were excluded. After screening 4,212 studies, a final selection of 71 articles met the criteria for review. Data extraction focused on the types of cropping system models used, calibration and validation procedures, parameterisation approaches, and how model outputs were utilised for precision management.

The review examined the evolution of CSMs in precision agriculture, identifying key applications and knowledge gaps. The spatialisation of CSMs was assessed by documenting:

- The range of models applied in different agroecological contexts.

- Data sources for parameterisation, including soil and cultivar parameters
- Evaluation methods and calibration strategies at the sub-field scale.
- The extent to which CSM outputs inform variable rate applications for nutrient and input management.

Findings were synthesised to determine the current limitations preventing widespread adoption of CSMs in precision agriculture, particularly in the UK. The review also explored broader global applications to derive insights relevant to UK wheat systems.

1.4.2 Summary of systematic review findings

A full description of the methods, results and discussion from the systematic review can be found in Appendix B. The knowledge gaps and research requirements identified are summarised in Table 1-1, along with documentation of how this thesis has addressed these requirements.

Table 1-1 Outcomes, research requirements of the Systematic Review with thesis contributions signposted

Knowledge Gap	Requirement	Addressed in this Thesis
Lack of Studies on Winter Wheat in the UK: No studies identified applying CSM to winter wheat in the UK at the sub-field scale	Conduct research focusing on CSM application at fine spatial resolutions for wheat in the UK, incorporating detailed calibration, parameterisation, and evaluation at the sub-field scale.	Chapter 2 evaluates the Sirius crop model at a fine spatial scale using data collected from on-farm experiments. Chapter 5 demonstrates this evaluation at a sub-field scale in a commercial setting.
Spatial parameterisation for soil properties at a sub-field scale is resource-intensive, limiting practical application.	Develop cost-effective methods for soil parameterisation. Investigate integration of management zone sampling with proximal sensing technologies to reduce sampling requirements.	Chapter 3 develops a whole-farm yield map analysis protocol to identify management zone delineation for model application. These methods are then applied in Chapter 4 across 7 management zones on a farm in Eastern England.

Lack of access to multi-cultivar calibration data sets limits accurate parametrisation of cultivar-specific traits within CSMs.	Create and maintain databases of cultivar-specific parameters using high-quality field trial data, including phenological stages, biomass, and yield components.	While the data required for parameterisation of new cultivars was not available, the parameters for cv Claire in the Sirius CSM were validated in Chapter 2 and shown to be suitable for modern UK wheat. Work has begun on developing parameters for modern cultivars in other CSMs (see Appendix F).
Few studies model across crop rotations with multiple crops, potentially limiting CSM accuracy by not tracking state variables over multiple years.	Develop rotational modelling approaches that track state variables such as nitrogen mineralisation and leaching over multiple years. Validate these models to reduce error accumulation.	This is not addressed directly in this thesis; however, the methods set out for wheat can now be used as a framework for application on other crops across rotations.
Limited comparative studies evaluate the spatial-temporal performance of different CSMs. Few studies incorporate multi-model ensembles to account for modelling structure uncertainty.	Conduct comparative studies using multiple CSMs to assess and quantify modelling uncertainty. Increase use of multi-model ensembles to provide robust CSM-derived management recommendations.	Not addressed in this study; however, work is ongoing to develop multiple parameterised models for modern UK wheat cultivars (see Appendix F).
Use of Remote Sensing for Model Calibration and Validation: Limited use of remote sensing data (e.g., satellite or UAV-derived LAI) for within-field CSM calibration and validation.	Expand integration of remote sensing technologies to monitor spatial-temporal crop growth variation. Use remote sensing data for CSM calibration and validation at the sub-field scale.	Not applied in this study and should be a focus of future research.
Insufficient long-term and high-resolution spatial data sets limit model calibration and evaluation. On-farm data sets often contain	Gather long-term, high-resolution spatial and temporal data sets, including multi-year yield maps. Assess and mitigate systematic	Chapter 3 addresses how on-farm yield maps should be analysed for use in CSM evaluations, accounting for errors. Additionally, data collected from the SAMS

systematic errors impacting their suitability for CSM applications.	errors in on-farm data to improve model reliability.	dataset used for model evaluation in Chapter 4 shows how targeted zonal sampling can also be used for model evaluation/parameterisation.
Validation of Economic, Environmental, and Practical Performance of CSM-derived Recommendations: Few studies validate the economic and environmental benefits of CSM-derived recommendations, such as nitrogen management strategies, at the field level.	Perform field-level validations of CSM-derived recommendations, assessing economic and environmental benefits. Compare these against conventional VRT methods to validate practical performance.	Within Chapter 4, the Sirius CSM is used to identify economic optimal N management strategies across management zones. The environmental benefit from reductions in unused N and carbon emissions savings from reduced fertiliser use can be compared. The NUE of the NOpt was also simulated, demonstrating how CSM can be used to associate environmental outcomes with N management strategies.

1.5 Methodological approach and contribution to knowledge

1.5.1 Thesis structure and approach

The research adopts a staged approach, consisting of 3 research chapters each written in manuscript form. Additionally, each chapter includes a section entitled “research context” providing a general overview of the chapter contribution to the overall aim and additional details about the characteristics and rationale of the datasets used. In the following paragraphs an overview of each chapter is provided including a breakdown of methodological approach, outcomes and contributions to knowledge; this is summarised in Figure 1-3.

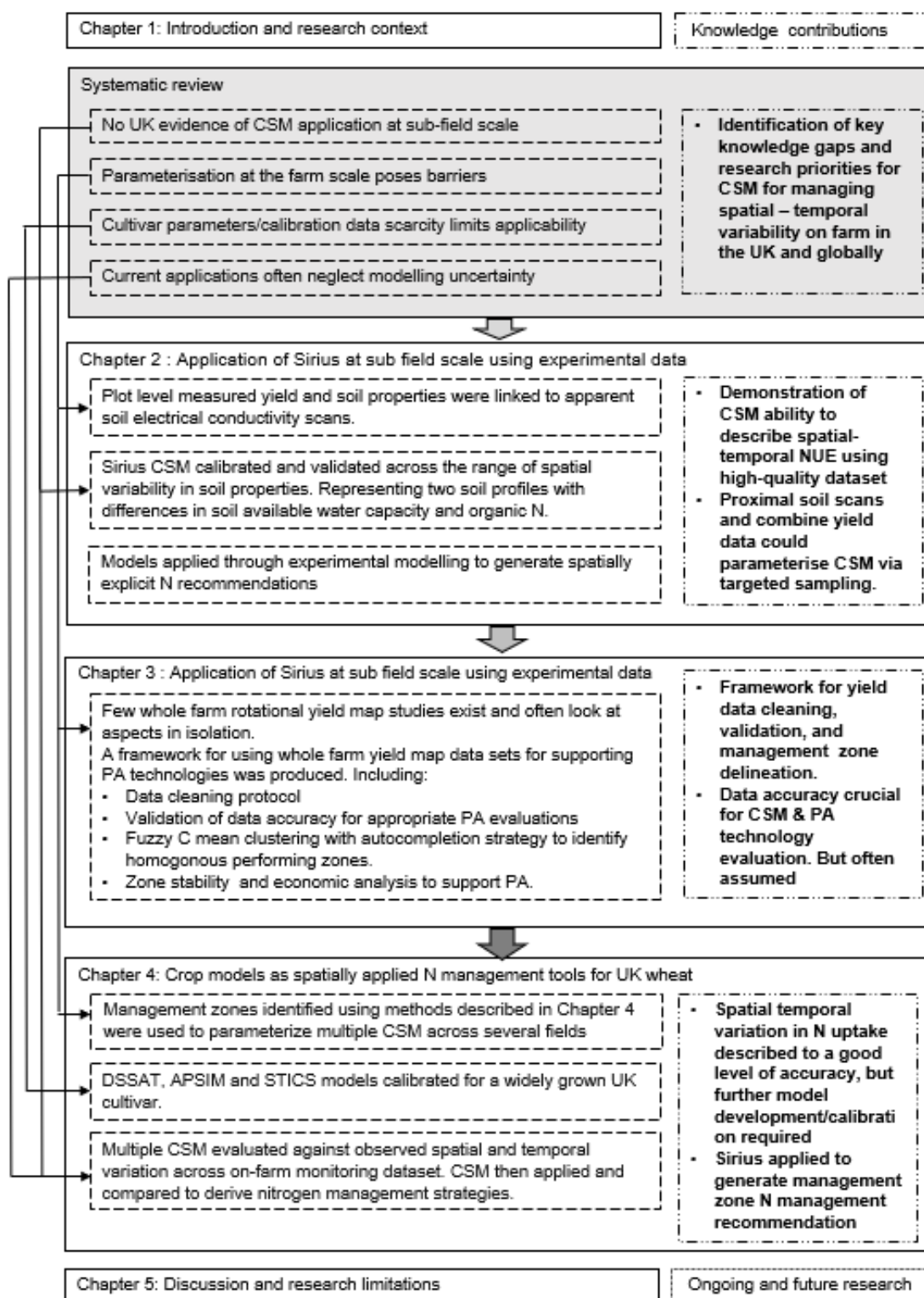


Figure 1-3 Research methodology, outcomes and contribution to knowledge

Chapter 2: Temporal variability in nitrogen use efficiency: insights from a long-term experiment and crop simulation modelling to support site specific nitrogen management (Objective 2 and 3)

Chapter 2 addresses specifically the lack of existing evidence for calibrating, parametrising, and evaluating crop simulation models to describe fine-scale spatial variability in UK wheat crops. In a three-step approach, the Sirius Crop model, widely utilised in other CSM applications (Clarke et al., 2020; Harkness et al., 2020; Jamieson et al., 1998), is evaluated against long-term experiment data from Morley, Norfolk, England. Firstly, the influence of spatial variation in soil properties (quantified using apparent soil electrical conductivity and measured plot-level soil physical and chemical properties), on crop properties, including grain yield, grain N content, and grain N fertiliser recovery is quantified. Secondly, the Sirius Crop model is validated using high-resolution plot-level experimental data across 5 years of wheat data for the extremes of the observed spatial variation in soil properties. Finally, an experimental modelling approach is used to infer optimal N management strategies across this spatial-temporal variation, demonstrating a key gap in how such models can be applied on farm. This chapter was presented at the Long-Term Experiments Conference Meeting Future Challenges (Rothamsted Research, June 2023) and has been published in the European Journal of Agronomy (Clarke et al., 2024a). Full reference described in Section 1.6.1.

Chapter 3: Whole-farm yield map datasets – data validation for exploring spatiotemporal yield and economic stability (Objective 4)

Chapter 3 addresses a key methodological limitation identified in the systematic review concerning the use of CSM on farms, emphasising the necessity for high-resolution soil data in accurately parametrising and validating these models spatially. While the delineation of relatively homogeneous management zones has been proposed to reduce sampling intensity, few studies to date have demonstrated the practical application of these methodologies across entire farms, nor addressed the accuracy of datasets. This chapter proposes a framework for leveraging whole-farm yield map datasets to guide precision

agriculture technologies, including cropping system modelling. The framework includes a data cleaning protocol and validation exercise, identifies homogeneous yield and economic management zones, and investigates zone temporal stability. The efficacy of this approach is demonstrated through a case-study utilising datasets and methodologies developed as part of an AHDB Strategic Farm Cereal Farm East work program. The findings of this research were disseminated through webinars and open days, practitioner technical events and has been published in the journal *Agricultural Systems* (Clarke et al., 2024b). Full reference described in Section 1.6.1.

Chapter 4 Assessing within-field nitrogen variability and optimised fertiliser use using the Sirius crop model

Chapter 4 applies the methods in Chapters 2 and 3 to demonstrate how, with appropriate spatial data sets and targeted soil samples, the CSM Sirius can be parameterised, evaluated and applied across management zones to inform spatially appropriate N management decisions for UK wheat. In this chapter, wheat yield map data from 2009-2023 from Morley Farms, Norfolk, UK, was used to identify a relationship between soil electrical conductivity and grain yield. Using the Standardised Precipitation Evapotranspiration Index (SPEI) derived from farm-specific weather data, the relationship demonstrated a consistent spatial variation in productivity attributable to spatially variable properties identifiable within a CSMS structure, such as plant available water. The yield map cleaning and clustering algorithms from Chapter 3 were applied to fields at Morley. Using the yield-based management zones data and ECa data, seven management zones were parameterised within the Sirius CSM. Sirius CSM was evaluated against historic yield map data, recognising the limitations of accuracy of such data sets. More detailed crop data sets collected in 2019 and 2022 were used for a more thorough model evaluation. The well-parameterised and evaluated model was then used to generate management zone-specific N rates, based on historical responses to observed weather and compared to the farm standard of between 200-220 kg N ha⁻¹ applied uniformly across a field .

1.5.2 Data sets

A summary of the datasets, crop models, and methods/algorithms utilised in this research, along with their respective types and ownership are presented in Table 1-2.

Table 1-2 Datasets, modelling software and computational scripts used in this research and details of ownership

Chapter	Item	Item type	Data ownership
1	N response trial data	Field trial data set (agronomic)	TMAF and AHDB, managed by NIAB
2	NFS Rotations and Cultivations Experiments	Field trial data set (agronomic and soil)	TMAF, managed by NIAB
	The Straw Incorporation Experiment	Field trial dataset (agronomic and soil)	TMAF, managed by NIAB
	Morley Farms soil ECa survey	Spatial data set (proximally sensed)	Collected as part of this research
	The Sirius crop model (Jamieson et al., 1998)	Crop model software	Rothamsted Research
	Weather data set 1990-2023	Rainfall, temperature, solar radiation, windspeed and vapour pressure data set compiled from onsite weather station data and synthetic sources	Compiled as part of this research
3	Yield Map data Set	Farm dataset (agronomic)	E J Barker & Sons
	Farm grain trailer weigh cell yield	Farm dataset (agronomic)	E J Barker & Sons
	Farm economic data	Farm dataset (economic)	E J Barker & Sons
	Fuzzy C-Means clustering with auto-completion strategy	Computation script (R language)	Hassal <i>et al.</i> , 2019
4	The Morley 'Soil and Agronomic Monitoring Study' (SAMS) data	Field trial data set (agronomic and soil)	TMAF, managed by NIAB
	Yield Map dataset	Farm data set (agronomic)	Morley Farms
	Morley Farms soil ECa survey	Spatial data set (remotely sensed)	Collected as part of this research

1.6 Research dissemination

Several forms of media have been used to disseminate the outcomes this research.

1.6.1 Papers in academic journals

1. Clarke, D.E., Stockdale, E.A., Hannam, J.A., Marchant, B.P. and Hallett, S.H., 2024. Whole-farm yield map datasets–Data validation for exploring spatiotemporal yield and economic stability. *Agricultural Systems*, 218, p.103972. <https://doi.org/10.1016/j.agry.2024.103972>.
2. Clarke, D.E., Stockdale, E.A., Hannam, J.A., Marchant, B.P. and Hallett, S.H., 2024. Spatial-temporal variability in nitrogen use efficiency: Insights from a long-term experiment and crop simulation modelling to support site specific nitrogen management. *European Journal of Agronomy*, 158, 127224, <https://doi.org/10.1016/j.eja.2024.127224>.

1.6.2 Academic conference proceedings

1. Clarke, DE., Stockdale, ES., Hannam, J., Marchant BP., Hallett, SH. 2022, *Spatial data to support management decisions on farm*. Constructing a Digital Environment [Conference presentation], 11-12 July 2022, University of Birmingham, Birmingham, UK.
2. Clarke, DE., Stockdale, ES., Hannam, J., Marchant BP., Hallett, SH. 2023, Spatial temporal variability in yield and nutrient use efficiency across a long-term farming systems experiment [Conference presentation], Long-Term Experiments: Meeting future challenges, 20-22 June 2023, Rothamsted Research, Harpenden, UK.
3. Clarke, DE., Martlew, J., Stockdale, ES. 2023, Incorporating yield data analysis to capture spatial soil carbon variation on farm [Poster presentation], Wageningen Soil Conference 2023, 28 August - 1 September 2023, Wageningen University & Research, Netherlands.
4. Clarke, DE., Stockdale, ES., Hannam, J., Marchant BP., Hallett, SH. 2023, Crop Simulation Modelling to Support Precision Nitrogen Management [Conference presentation], British Society of Soil Science and Soil Science

Society of Ireland Annual conference 2023, 4-5 December 2023, Belfast, UK

5. Clarke, DE., Stockdale, ES., Hannam, J., Marchant BP., Hallett, SH 2024, Crop Modelling to Support Spatial N Management in UK Wheat [Conference presentation], 19-21 May 2024, Florence, Italy.

1.6.3 Industry events/media

The research was disseminated through other industry webinars, events, podcasts and conferences. A full list and links to available media is available in Appendix C

1.7 References

- Abdulraheem, M. I., Zhang, W., Li, S., Moshayedi, A. J., Farooque, A. A., & Hu, J. (2023). Advancement of Remote Sensing for Soil Measurements and Applications: A Comprehensive Review. *Sustainability*, 15(21), 15444. <https://doi.org/10.3390/su152115444>
- AHDB. (2023a). *Nutrient Management Guide (RB209) Section 1 Principles of nutrient management and fertiliser use*. <https://ahdb.org.uk/nutrient-management-guide-rb209>
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2 Spatial-temporal variability in nitrogen use efficiency: insights from a long-term experiment and crop simulation modeling to support site specific nitrogen management.

2.1 Research context and Contribution Statement

The systematic review identified a significant research gap: Cropping System Models (CSMs) have not been evaluated for their ability to simulate observed spatial-temporal variation in UK wheat at the sub-field scale. A key limitation of many modeling exercises is the requirement for high-resolution soil data to parametrise CSMs and accurate, high-quality agronomic data to evaluate the model. Traditionally, agricultural field experiments have been used to demonstrate modeling capabilities in describing agronomic and soil responses to treatments such as nitrogen rate, irrigation, and seed rate (e.g. Salo et al., 2016). However, these applications assume that soil properties are spatially stable, apart from those influenced by experimental treatments.

Agricultural field trials are often influenced by underlying soil heterogeneity, which affects plant responses to imposed treatments. The New Farming Systems (NFS) Experiments, delivered by NIAB and supported by the Morley Agricultural Foundation, were established in 2007 at Morley, Norfolk. The NFS experiments explore the influence of primary cultivation techniques, cover cropping, companion crops, and nitrogen rates on soil, crop performance, and economics (NIAB, 2024a). Preliminary work has documented large underlying variation in soil properties, which appears to influence crop yields. This preliminary work was not particularly detailed but served as an initial exploration (Clarke, 2019), which in part led to the motivation behind this PhD project.

The NFS experiments, therefore, present a unique opportunity to evaluate CSMs in describing the influence of fine-scale (sub-field) spatial variation in soil properties on crop growth and nitrogen use efficiency (NUE). The primary investigator of this PhD project has been the lead field technician on the NFS experiments since 2017, ensuring a thorough understanding of the data sets,

methodologies, and experimental setup. This familiarity is valuable for reducing model input uncertainty and ensuring data sets are comparable and accurate. Additional data sets required for this PhD project, including additional proximal soil ECa scans and targeted soil sampling, were collected as part of this research.

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2.2 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 mean 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 parameterised 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 a 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 optimise the data requirements for model parameterisation to support site-specific N management.

2.3 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; Kindred et al., 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 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 minimising 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, 2018a). 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., 2017b; Keating and Thorburn, 2018a). 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 parameterisation (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 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., 2009) 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 long term experiments 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 long term experiments featured in this study. However, this spatial variation, combined with high spatial (plot) and temporal (multiyear) data sets, collected as part of long term experiments, 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 long term experiments in the East of England and to link this to the spatial-temporal variation in yield and NUE. The Sirius model (Jamieson et al., 1998) was calibrated for use at this site and cropping system. Sirius is a process-based simulation model which simulates wheat growth by modeling key physiological processes, including light interception, carbon assimilation, and water and nitrogen uptake, using site specific daily weather data, soil characteristics, and crop management inputs. Soil electrical conductivity (ECa) is a proximally sensed measure of soil resistance that has been strongly correlated with clay content and soil water holding capacity (Heil and Schmidhalter 2012). In this study, ECa is used to quantify the spatial heterogeneity of soil properties across the long term experiments and assess how crop response correlates with this observed variation, utilising five years of winter wheat data across three contrasting nitrogen fertiliser application rates. Measured data sets on soil and crop properties were used to parametrise and validate Sirius 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 crop simulation model as a tool for on-farm management decisions for UK wheat crops.

2.4 Materials and methods

2.4.1 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, 54m 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) (Figure 2-1A, Table 2-1).

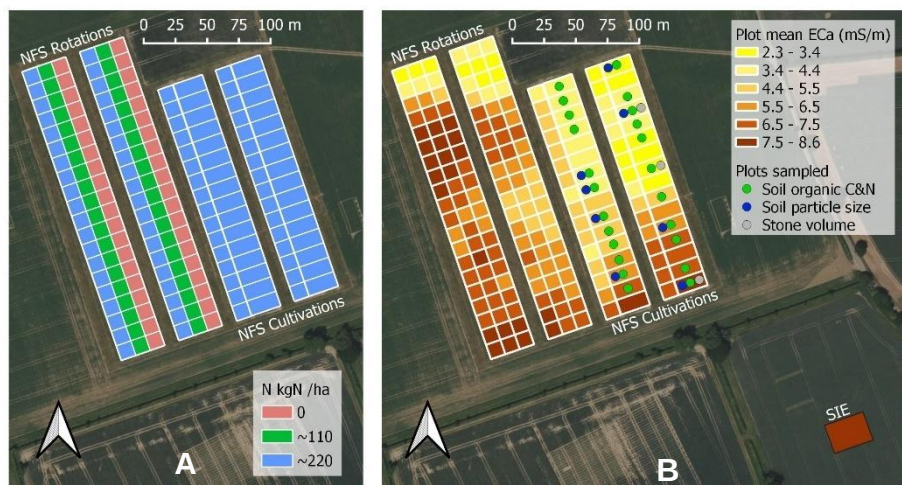


Figure 2-1 A, NFS Rotations (NFS-RE) and NFS Cultivations (NFS-CE) experiments with current N rates for winter wheat, B. Plot mean ECa across the NFS-CE and NFS-RE and Straw Incorporation Experiment

Table 2-1. NFS-RE wheat crop varieties, drilling date and the N rate at full farm standard N (220N)

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

These will be referred to as 0N, 110N and 220N 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 (Figure 2-1A). 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., 2018a). 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 12x24 and 12x12 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 minimise 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 the aim to maintain soil indices at levels that are not crop limiting. The Straw Incorporation Experiment 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 (0-250kg N ha⁻¹ in winter wheat). This experiment was located approximately 150m south of the NFS-CE (Figure 2-1B).

2.4.2 Data collection and analysis

2.4.2.1 Soil apparent electrical conductivity (ECa)

Soil 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 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 (Figure 2-1B). 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 Straw Incorporation Experiment with the mean ECa and measured data for soil organic matter across the experiment was comparable to the higher ECa and organic matter plot values recorded on the NFS experiments (7.5-8.5 mS/m).

2.4.2.2 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 (Figure 2-1A) 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 3 kg soil sample was taken at depths between 0-30 cm, 30-60 cm and 60-90 cm, soil was sieved through a 2 mm sieve and stone volume calculated by water displacement.

2.4.2.3 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 long term experiment. 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 analysed from a composite 500 g sample from each plot using FOSS INFRATECH NIR scanner annually calibrated using UK Grain Testing Network 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).

2.4.2.4 Spatial temporal variation in fertiliser grain N recovery efficiency

Fertiliser Grain N recovery efficiency (RE_{fertN}) is a metric of NUE (Equation 2.1), defined as the percentage of N applied as fertiliser within the grain at harvest, accounting for background soil N levels using the unfertilised (0N) control (Congreves et al., 2021):

$$RE_{fertN} = \frac{u - u_0}{n} \times 100 \quad (2-1)$$

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 220N plots. Linear regression equations for Plot ECa ~grain yield and ECa~grain protein (Appendix D.1) 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 0N and 220N. Therefore, mean values at 0N and 220N for plots ranging from 2.5-3.5 (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) were used to quantify the relationship between plot ECa and RE_{fertN} in each year.

2.4.3 Crop modeling

2.4.3.1 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 Straw Incorporation Experiment, 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.

2.4.3.2 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 mineralisation 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 (Figure 2-2). It is 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, 2012b). These were corrected for the volume of stones in each soil layer recorded in representative plots (Figure 2-3) (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, 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=0.5, LEC=0.8). 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.

2.4.3.3 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 1990-2022 (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).

2.4.3.4 Cultivar parameterisation and N response validation on the Straw Incorporation Experiment

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 (Gasó et al., 2021). Sirius has been calibrated and validated for cv Claire, which remained on the UK Recommended List (RL) until 2018 (AHDB, 2023c) 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 phenological parameters (e.g. start of stem extension (GS 31: BBCH Scale (Meier, 1997)) and maturity (GS 91) to cv Claire. Therefore, the previously calibrated phenological 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 Straw Incorporation Experiment (see appendix D.1). 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 to 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., 2019a).

The Straw Incorporation Experiment was cropped with cv JB Diego and cv Relay in 2014 and 2015 respectively, both varieties were grown on the NFS-RE (Table 2-1). 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 equation 2 2:

$$u = y \times ((p/5.7)/100) \quad (2-2)$$

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, 2023b).

The soil parameters for HEC soil were used for the Straw Incorporation Experiment 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 (0-90cm) prior to N fertiliser application in the spring.

2.4.3.5 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 using the model parameterised for measured soils data.

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 equation 2-3:

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

where y_i is the observed data, $\hat{y}_i$ 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).

2.4.3.6 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 equation 2 4:

$$y = a + b.rN + c.N \quad (2-4)$$

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 equation 2 5:

$$NO_{\text{opt}} = [\ln(k - c) - \ln(b(\ln(r)))] / \ln(r) \quad (2-5)$$

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 (2-4).

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

Unlike the modeling in 2.4.3.4 and 2.4.3.5, 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 programming language (R Core Team, 2023). Crop modeling was performed through the native MS Windows application for Sirius (Sirius, 2023).

2.5 Results

2.5.1 Spatial variation across a long term experiment

2.5.1.1 Spatial variation in soil properties

Plot mean soil ECa ranged from 2.3 mS/m to 8.6 mS/m across the NFS experiments (Figure 2-1A and Figure 2-2). Soil ECa was significantly correlated to both clay and sand content at 0-30 cm and 30-60 cm depths (Figure 2-2A) 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 to 68.9% respectively at 0-30 cm depth, and from 15.3 to 30.8% and 49.2 to 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 (Figure 2-2B&C). Stone content was higher on the lower ECa plots (Figure 2-3), 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 Appendix D). 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).

2.5.1.2 Spatial temporal variation in crop performance

The variation in soil properties across the NFS-RE quantified through EC_a showed significant relationships to key crop measures and their interactions with N rate (Figure 2-4). Except for 2012 at 220N, a significant correlation between

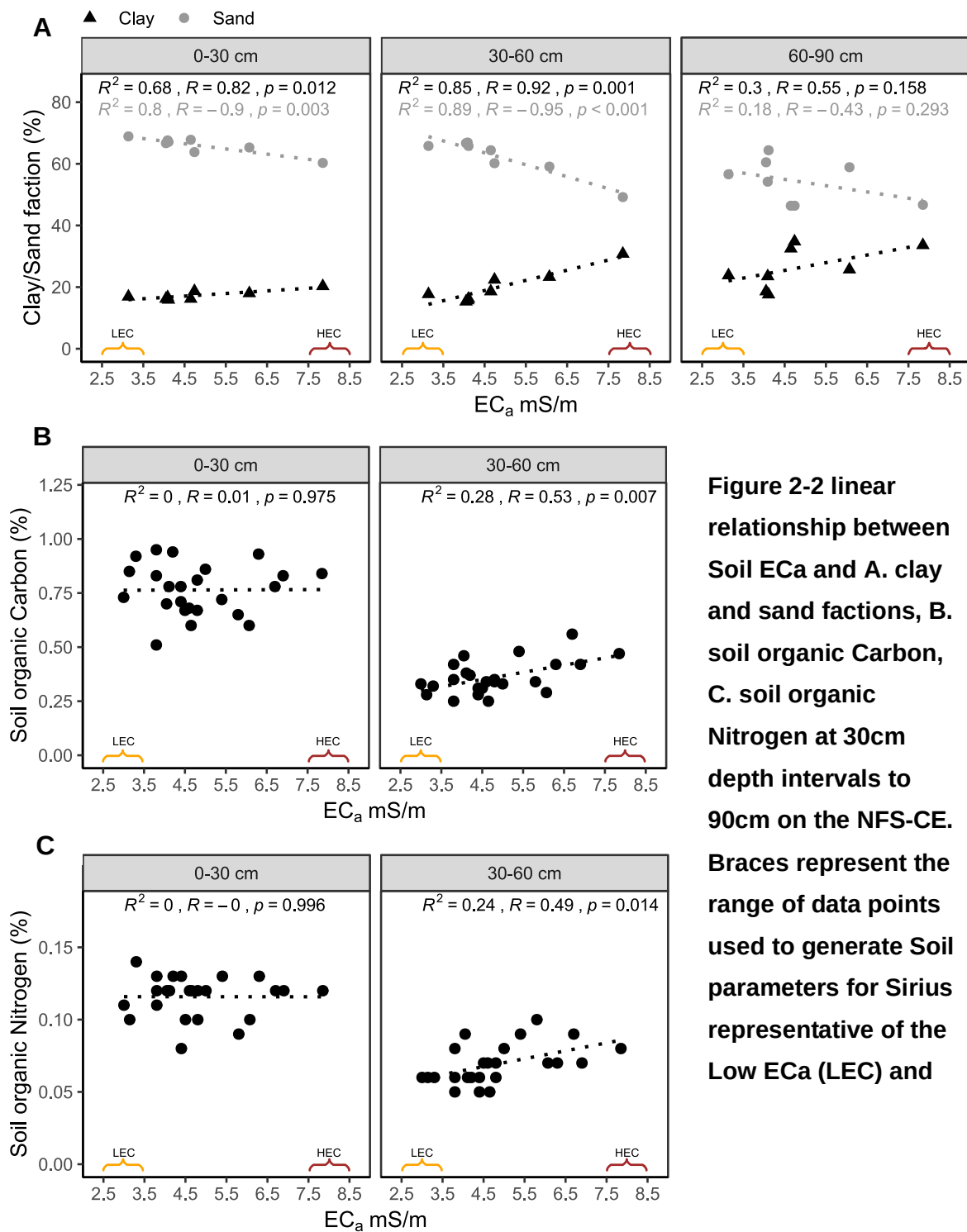


Figure 2-2 linear relationship between Soil EC_a and A. clay and sand factions, B. soil organic Carbon, C. soil organic Nitrogen at 30cm depth intervals to 90cm on the NFS-CE. Braces represent the range of data points used to generate Soil parameters for Sirius representative of the Low EC_a (LEC) and

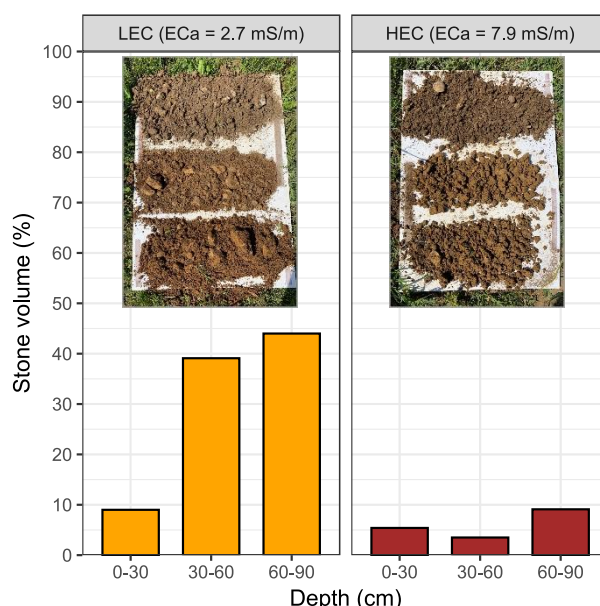


Figure 2-3 Stone volume by 30cm soil depth (0-90cm) and images of reconstructed profile excavation for HEC (7.5-8.5 mS/m) and LEC (2.5-3.5 mS/m)

ECa and grain yield was observed at all N rates in all years (Figure 2-4A). Across the five years, plot ECa accounted for 71%, 87%, and 79% of the variation in plot yield at 0N, 110N, and 220N, respectively.. The range of 5-year mean yield between the LEC and HEC plots was 9.0 to 10.7 t ha⁻¹ at 220N, 7.5 to 9.5 t ha⁻¹ for 110N and 4.2 and 5.5 t ha⁻¹ at 0N, respectively. In 2012, 110N and 220N yields were similar and 0N yields were similar to those of other years at 110N. In 2017 and 2020 the yield response at 220N compared to 110N 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 (Figure 2-4B). In 2010, 2017 and 2020 a significant negative correlation between ECa and grain protein was recorded at 220N. No significant correlation was recorded in 2012 and 2015. At 110N a significant negative correlation was recorded in 2010 and 2020, a significant positive correlation in 2012 and no correlation in 2015. At 0N a significant negative correlation was recorded in 2010, 2015, 2017, and 2020. Across the 5-year mean there was a

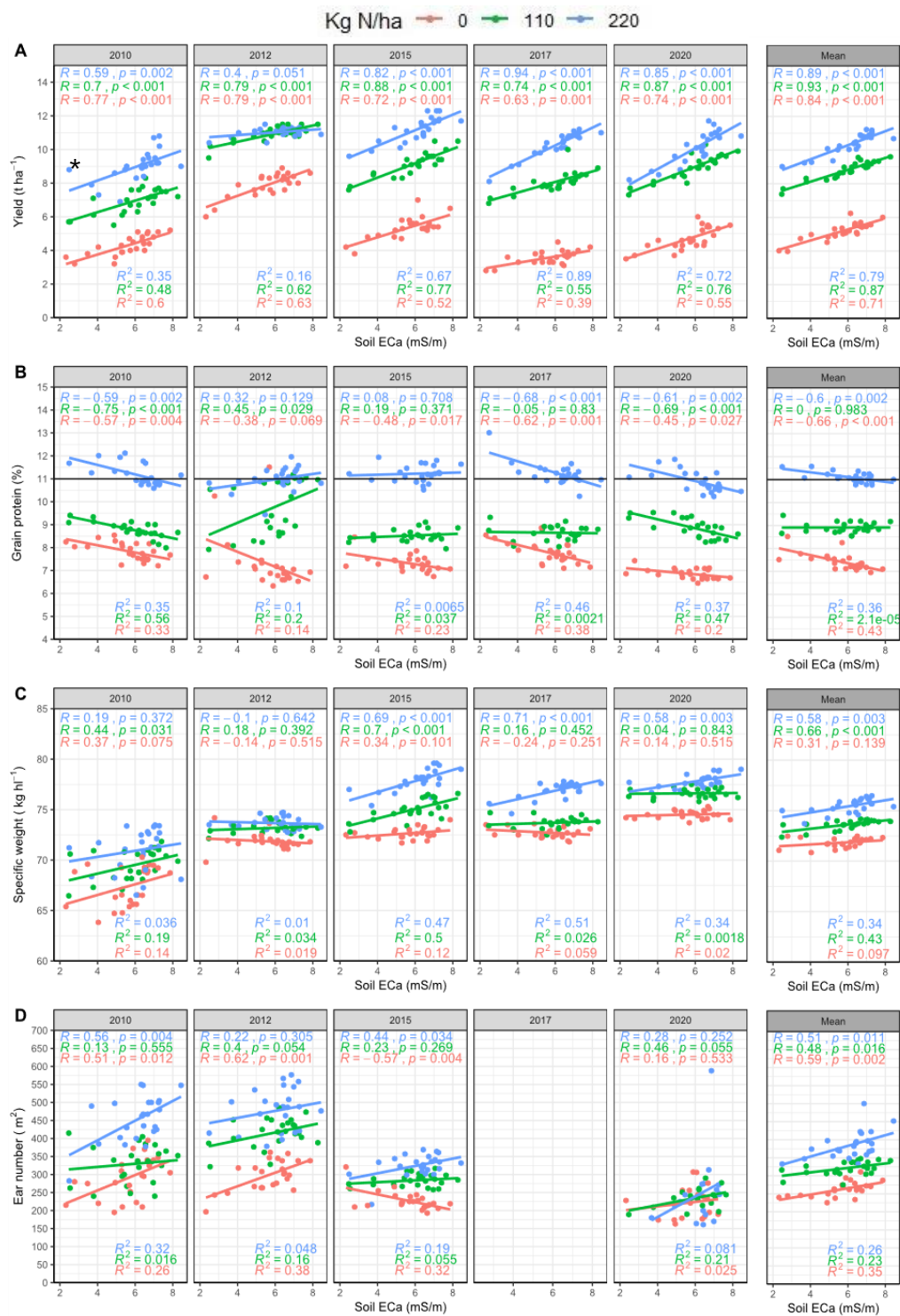


Figure 2-4 Linear relationship between plot ECa and wheat performance metrics (2010-2020) and their 5-year means, (A) grain yield, (B) grain protein, where the black line at 11% represents the optimal grain protein for yield, (C) grain specific weight and (D) ear numbers (no ear numbers were recorded 2017). The asterisk (*) in 2010 yield plot represents influential outlier when calculating grain N fertiliser recovery.

significant negative correlation between grain protein and plot ECa at 220N and 0N 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 220N and 7.8% and 7.2% at 0N ha. The plots defined as LEC on average exceed the 11% optimal grain protein for yield for feed wheats (AHDB, 2023a).

Plot mean ECa was significantly correlated to grain specific weight in 2015, 2017 and 2020 at 220N, in 2010 and 2015 at 110N and in no years at 0N (Figure 2-4C). Across the five years on average there was a significant correlation with ECa and specific weight at 220N and 110N explaining 34% and 43% of the variation, respectively. ECa was significantly correlated to ear numbers in 2010 and 2015, but not in 2020 at 220N (Figure 2-4D). No significant correlation was recorded in any years at 110N but was significantly positively correlated in 2010 and 2012 at 0N and negatively correlated in 2015. On average across the 5 years ECa was positively correlated to ear numbers at all N rates.

2.5.1.3 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 0N and 220N) ranged from 46.7% to 56.0% from low to high ECa (Figure 2-5). This equates to an average $19.7 \text{ kg N ha}^{-1}$ 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 (Figure 2-4A), resulting in higher RE_{fertN} , this observation contradicts the overall trend of lower yields on the low ECa plots in that year.

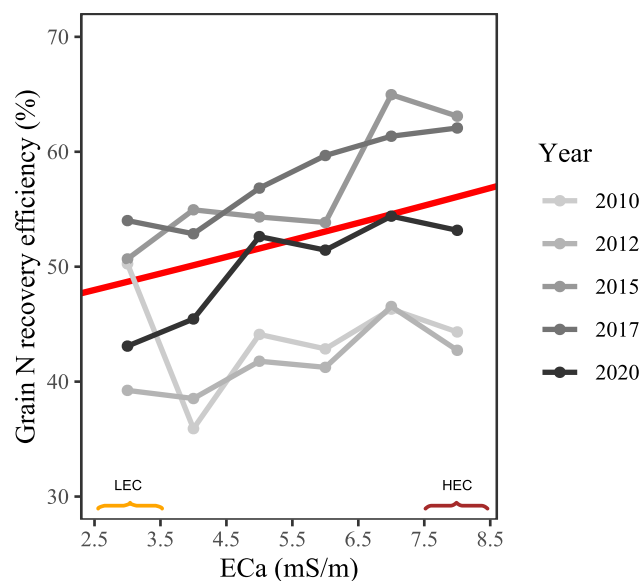


Figure 2-5 Grain N recovery efficiency (2010-2020) by plot ECa ranges 2.5-3.5 (LEC), 3.5-4.5 , 4.5-5.5, 5.5-6.5, 6.5-7.5 and 7.5-8.5 (HEC). Red line = Grain N recovery efficiency across range of ECa from regression equations for the five year mean grain yield and protein

2.5.2 Crop simulation modeling

2.5.2.1 Sirius validation Straw Incorporation Experiment

The updated parameters for Winter Wheat 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 simulated the longer growing season in 2015 (Figure 2-6A). The calibrated parameters explained 82% of the variation in yield across the two years (Figure 2-6B). 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 (Figure 2-6B, C and D).

2.5.2.2 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 available water capacity

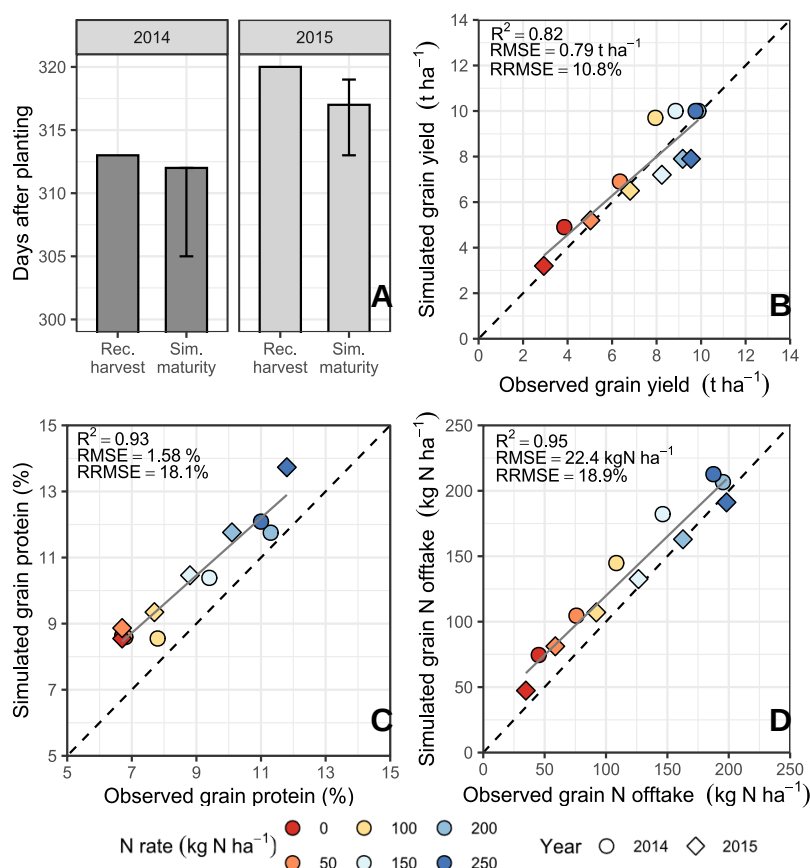


Figure 2-6 Comparison of observed and simulated data for wheat performance. (A) Recorded date of harvest compared to simulated maturity date at 200 kg N ha⁻¹, with error bars representing the maximum and minimum across N rates. (B) Observed yield compared to simulated yield. (C) Simulated grain protein compared to observed grain protein. (D) Observed grain N offtake compared to simulated grain N offtake (Equation 2.2).

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 2-2).

At 110N and 220N Sirius overestimated yields on both soils, primarily because of higher simulated yields in 2012 and 2017 (Figure 2-7A). 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

Table 2-2 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).

		0 (kgN ha ⁻¹)		110 (kgN ha ⁻¹)		220 (kgN ha ⁻¹)		
	Soil	HEC	LEC	HEC	LEC	HEC	LEC	Mean
Yield (t ha ⁻¹)	Observed	5.0	3.7	7.9	6.5	9.2	7.7	6.7
	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 (kgN ha ⁻¹)	Observed	62	54	128	109	178	155	114.2
	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

(Figure 2-7A). At 220N across all years Sirius simulated 1.2 t ha⁻¹ lower yields, 0.6 % higher grain protein and 18 kgN ha⁻¹ 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 110N than 220N 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 110N on the HEC, surpassing the 8.1 t ha⁻¹ simulated yields on LEC plots at 220N (Table 2-2).

Sirius overestimated grain protein at all N rates and on average by 0.7% at 220N 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 0N in the observed data set (Figure 2-7B). The errors in grain yield and grain protein did not seem to propagate to total grain N offtake which showed comparable RRMSE (Figure 2-7C).

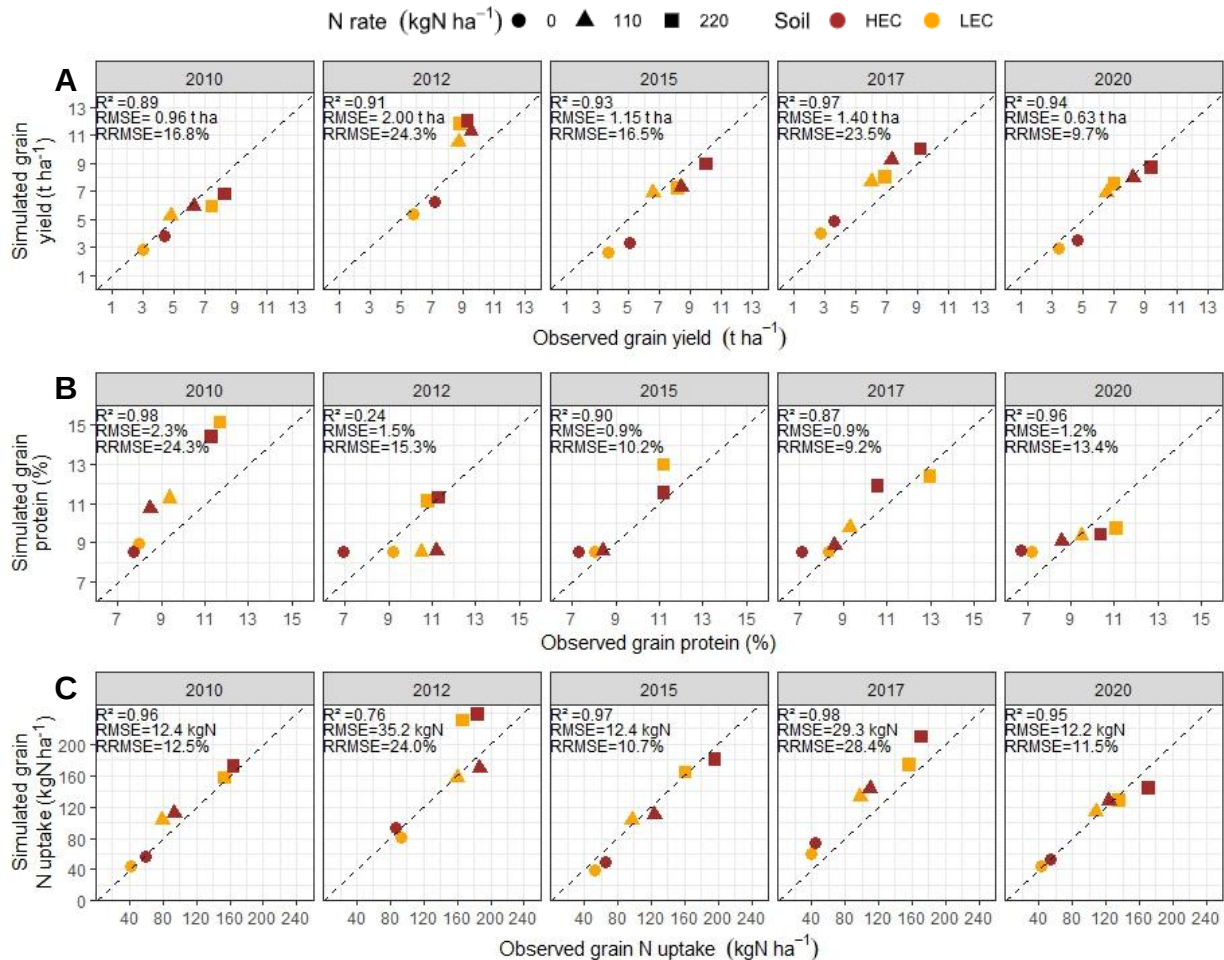


Figure 2-7 Sirius validation for the NFS-RE at 0N, 110N and 220N on the Low ECa (LEC=plots 2.5-3.5 mS/m) and High ECa (HEC=plots 7.5-8.5 mS/m) plots for A; grain yield, B; grain protein, C: grain N uptake.

2.5.3 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) (Figure 2-8A). 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,

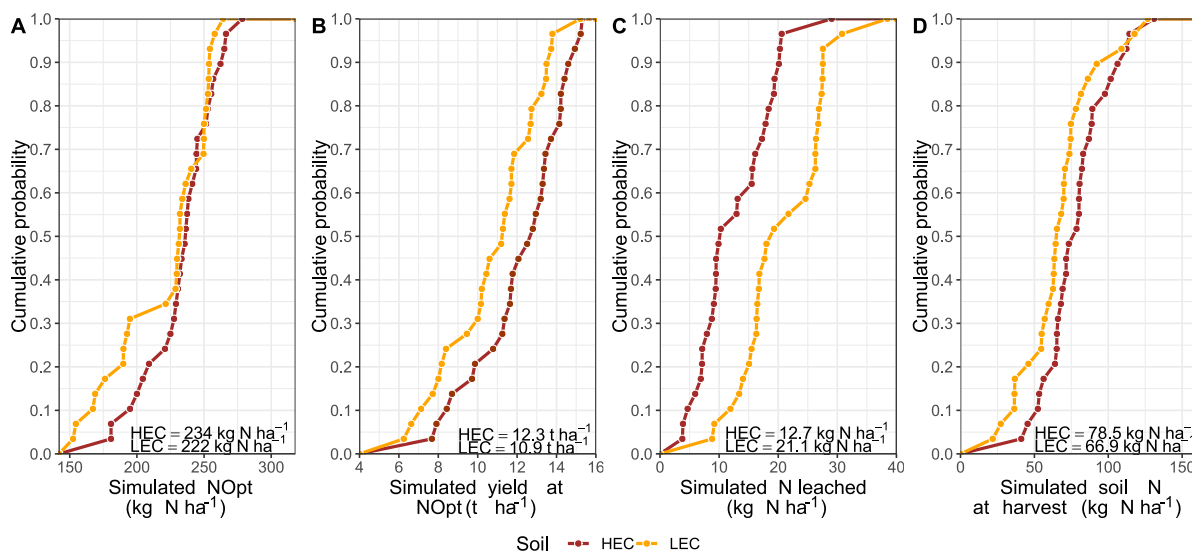


Figure 2-8. Sirius simulation results for HEC (brown) and LEC (yellow) soils displayed as cumulative probability using 29 years of weather data. (A) simulated NOpt, (B) simulated yield at NOpt, (C) simulated within growing season N leached, (D) simulated surplus N.

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 (Figure 2-8B). 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 (Figure 2-8C). 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) (Figure 2-8D).

2.6 Discussion

2.6.1 Potential of crop simulation models to optimise nitrogen management

This study demonstrates how the Sirius crop simulation model can be used to optimise N management by simulating spatial and temporal variations in wheat yield, grain protein, and nitrogen uptake. The model was validated against observed spatial variation in crop growth within the NFS-RE and demonstrated

good performance, supporting its application for site-specific nitrogen management.

2.6.1.1 Model evaluation

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 220N plots, with smaller levels of infection on the 0N and 110N 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 110N and 220N, 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 110N and 220N. 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 0N 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 fertilisation (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 long term experiment 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., 2011b; Ward et al., 2018; Wong and Asseng, 2006). Basso et al, (2009) 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 initialised 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., 2011c; Bertocco et al., 2008).

2.6.1.2 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 110N and 220N, as a result of it 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) (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 arose 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 mineralised 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 long term experiment, 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 minimise environmental risk associated with these modeled states. While this study focuses on economic optimal N and nitrate leaching, surplus nitrogen also contributes to nitrous oxide (N₂O) emissions, a potent greenhouse gas. By using models to determine appropriate N rates, both leaching and N₂O emissions can be minimized, as excess N availability drives

these losses. Expanding modeling frameworks to include gaseous losses should be considered in future modeling exercises. Both rotational modeling and N₂O emissions can be simulated using multi-crop models such as DSSAT and APSIM (Jones et al., 2003; Keating et al., 2003). However, 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 Sirius 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 long term experiment 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., 2018a). 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., 2011b).

Crop models enable exploration of system responses to multiple iterations. In this study, we demonstrated the capability of simulating spatial variations within an long term experiment using soil specific NOpt and typical drilling dates, N timings, and splits. Future research should employ experimental modeling techniques to analyse 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 & 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 long term experiment 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).

2.6.2 Spatial variation in soil properties and influence on grain yield and NUE

In this study, Sirius was validated and applied within an long term experiment, integrating proximal soil scans and agronomic data to demonstrate how spatial datasets can identify variation in NUE and enhance model parameterisation and application on farms. Variations in ECa measured across the NFS-RE exhibited a strong correlation with sand and clay fractions 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 & 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 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 observed variation could be used to parametrise 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 150kg 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 0N. The relationship between NUE and water uptake efficiency is understood to be co-limiting (Quemada and Gabriel, 2016; Sadras, 2004) with N fertilisation shown to improve water uptake efficiency 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 110N and 0N. 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 long term

experiment 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, 2023b). Using the 5 year mean linear 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, the yield increase from 110N to 220N was small in plots with the lowest ECa, and a similar but less pronounced trend was observed in 2017. In these years the smaller response to 220N on the low ECa soils suggests NOpt rates might be below the farm standard 220N 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, Cropping system models can allow us to simulate virtual experiments, complementing 'real' experiments, but these need to be evaluated relative to the real system (Jones et al., 2017).

2.7 Conclusion

Results showed large spatial variation in soil properties across a long term experiment. Soil ECa was strongly correlated to both the variation in soil properties and temporal and spatial patterns in crop growth and performance quantified using long term experiment 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 losses 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 test the reliability of different models for management recommendations. long term experiments with high spatial-temporal data sets and quantified spatial variation are suitable places to test this.

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3 Whole-farm yield map datasets – data validation for exploring spatiotemporal yield and economic stability

3.1 Research context and contribution statement

Over the past three decades, farms have increasingly adopted yield mapping technologies, such as mass flow sensors on combine harvesters (Blackmore and Marshall, 1996; Blackmore, 1999). By 2019, more than a third of UK cereal farms were using these technologies (DEFRA, 2020), resulting in extensive spatial yield data across multiple years, fields, and crops. This data enables spatial-temporal yield performance analysis to be conducted (Muhammed et al., 2016).

The systematic review showed, yield maps are frequently utilised in two primary ways: (1) to statistically appraise spatial-temporal yield data for identifying sampling sites (i.e., management zones), grouping gridded soil profiles, and creating spatially structured model outputs, such as nitrogen (N) rates for yield-driven management zones; and (2) to evaluate models by comparing simulated yields with observed yields from yield maps, thereby validating model calibration and/or parameterisation processes.

Yield-based management zone delineation, has typically been applied to individual fields or small groups of fields. However, these approaches often lack sufficient spatial resolution, are rarely implemented across entire farms, and frequently overlook economic considerations. Addressing these gaps is crucial, as sampling within spatially coherent management zones has been identified as a potential method to reduce the data requirements for crop CSM parameterisation at scale. Additionally, the benefits of precision agriculture, such as spatially explicit nitrogen management, can vary widely between fields—some fields may experience substantial gains, while others may show limited benefits (Jin et al., 2019). Therefore, whole-farm appraisals are essential to identify where PA, including CSMs, can be most effectively deployed to deliver both economic and environmental benefits. This study addresses these limitations by analysing a whole-farm, ten-year yield map

dataset to identify spatially and temporally stable management zones that could yield the greatest economic benefits from PA technologies.

The accuracy of yield map data collected on farms is often assumed and used to evaluate precision agriculture technologies, such as CSM. However, significant inaccuracies in these datasets have been shown to hinder the evaluation of CSM performance in simulating observed spatial and temporal variations (e.g. Jégo et al., 2012; Kersebaum et al., 2005). While controlled experimental studies have quantified the accuracy of calibrated combine yield mapping technologies (Grisso et al., 2002; Morgan, 2020), there remains a lack of real-world appraisals regarding the accuracy of multiyear yield map datasets collected on farms. This gap is crucial because it is these on-farm datasets that will be required for wide scale evaluation of precision agriculture technologies, including validating CSM approaches.

Chapter 3 develops a comprehensive framework for utilizing whole-farm yield map datasets to support spatial-temporal economic appraisals on farms, as well as for validating and, where possible, correcting errors in these datasets. This chapter utilises datasets provided through the AHDB Strategic Cereal Farm East initiative. While the primary aim of this study was to identify areas of the farm most suitable for Environmental Land Management Schemes (ELMs) using yield maps and farm economic data, the framework developed for cleaning, validating, and analysing multi-year, whole-farm yield map datasets also hold significant relevance for the application of crop models on the farm. While the least productive areas of farms that are suitable for environmental schemes may be taken out of production, there will likely still be areas with reduced economic and productive potential. These areas could improve their economic performance through the targeted application of nutrients based on site-specific demand. Additionally, these same areas are likely to benefit from improvements in nitrogen use efficiency, as they tend to be the most affected by inefficiencies in nutrient utilisation.

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3.2 Abstract

Statistical methods used for delineation of field management zones are frequently only applied to relatively small areas, with few studies performing rotational, whole-farm economic spatiotemporal appraisals. To enable accurate economic analysis, yield map datasets must contain minimal errors while cleaning procedures are often used to remove errors, it is rare that cleaned data is validated before its application. The objective of this study was to process, validate and combine spatial statistical approaches for a rotational yield map dataset from a whole farm, across 7 crops in a winter wheat-based rotation. Developing a framework for using validated yield map datasets to support precision agriculture techniques that are applicable for farm-level decision making. The rotational completeness of a 10 year combine yield map dataset for a 435 ha farm in Eastern England was assessed. The dataset was cleaned statistically, and its accuracy assessed by comparison with recorded yields from trailer weigh cells. The cleaned, validated, and corrected yield map dataset was used to identify management zones across the whole farm using fuzzy clustering. The temporal stability of management zones and economic performance across the rotation was also assessed. Data cleaning methods removed 16% of data points, improving the degree of spatial correlation within the individual yield maps. Independent validation demonstrated varied accuracy of yield maps from combine harvester data and errors in wheat ranged from 0.53 – 1.53 t/ha RMSE. These errors have implications for researchers using combine yield data to develop and validate precision agriculture technologies. This data set required correction before yield data can be applied with confidence for on-farm decision making. Compared to the zones with the highest margin in each field, 34% of zones had an average annual margin loss of >£100 ha. The temporal stability of the resulting management zones also varied. Areas with the lowest economic performance and greatest yield stability across years will potentially see the greatest economic and environmental benefits from precision agriculture techniques. The accuracy of combine yield map data should not be assumed. The application of these datasets, including for the identification of management

zones or in developing precision agriculture techniques should attempt to address this through data cleaning and validation procedures. Only then should it be used for on farm decision making, such as identifying areas with the most economic benefit by applying precision agriculture tools such as variable rate nutrient applications.

3.3 Introduction

The influence of soil properties on agricultural productivity usually shows structured or periodic temporal and spatial variation (Shaddad et al., 2016). It is therefore practical for farmers to divide fields into management zones (MZ) to account for this variation, potentially adjusting fertiliser, pesticide inputs or field operations to better suit the soil or potential yield of the zone (Milne et al., 2012). Identifying MZ can be achieved through measuring spatial variation in soil properties and adjusting inputs, based on known crop responses to the quantified properties (Lark et al., 2020). Soil sampling in a random or grid scheme that is subsequently interpolated using geostatistical methods to provide spatial information about soil properties is one way to achieve this (Marchant et al., 2012). ‘On the go’ sensors such as those recording soil electrical conductivity (James et al., 2003; Moral et al., 2010) and gamma ray spectrometry (Dierke and Werban, 2013; Kassim et al., 2021) offer increased sampling density at relatively low cost and are therefore being increasingly used to delineate MZ. A limitation of these techniques is that it is assumed they sufficiently reflect those soil properties that are responsible for variation in crop yield and that therefore farmers would benefit economically from site specific management through either increased yields or reduced inputs. For MZ to be advantageous there should be a strong and consistent relationship between soil properties and the spatial and temporal patterns in yield (Guastaferro et al., 2010b). These patterns in yield may also be impacted by other factors outside soil-climate interactions, for example spatial pattern in agronomic factors such as weed, and pest pressures (Metcalf et al., 2019).

Yield maps have been used to interpret spatial and temporal yield trends since their early adoption (Blackmore, 1999). More recently, farmers have compiled

datasets having sufficient yield observations to allow spatial yield variability and temporal yield stability to be captured across rotations (Maestrini and Basso, 2021). Geostatistical methods for identifying spatially coherent MZ from combine harvester yield data often use non-hierarchical fuzzy clustering and spatial smoothing approaches to ensure that zones are spatially coherent and are of practical use in farm management (Milne et al., 2012). The identification of MZ through clustering identifies homogenous yield zones that are significantly distinct from others. However, this provides little context for variation in the magnitude, scale or stability of yield without further investigation (Maestrini and Basso, 2021); this being a key influence on MZ-specific operations (Khosla et al., 2010; Muhammed et al., 2016). Identifying MZs where yield is consistently temporally higher or lower can allow for strategic soil and/or agronomic management that is proportional to the yield and economic trend (Basso et al., 2011). Management zones with unstable yield trends over time may need more reactionary approaches that consider seasonal influences using remote sensing or crop and soil modeling (Maestrini and Basso, 2018).

Statistical criteria used to assess the yield stability and/or management zone identification using yield maps are frequently applied at a sub-farm spatial scale (Cammarano et al., 2020, Bazzi et al., 2015) and over a large selection of fields across many farms (Maestrini and Basso, 2018). Applying the zoning across whole farms and rotations are less common. Studies of spatial-temporal yield patterns across whole farms commonly only focus on a single crop (Filippi et al., 2019; Kharel et al., 2019; Oliver et al., 2012) offering little context to the overall rotational productivity and stability of an area.

More recently field level economic information such as fixed and variable costs and grain market price has been incorporated to produce multi-field economic appraisals, identifying economically optimal areas for delivering ecosystem services and precision agriculture techniques (Adhikari et al., 2023; Capmourteres et al., 2018). In addition to economic appraisals researchers and farmers are increasingly relying on combine harvester yield data to support more complex processes such as the spatial calibration and validation of crop

simulation models at a management zone level (Cammarano et al., 2020; Wallor et al., 2018), conducting on-farm field experiments (Marchant et al., 2019) or validating remote sensing technologies (Maresma et al., 2020).

Systematic and operator error can lead to inaccuracies within combine yield data (Arslan and Colvin, 2002; Blackmore and Marshall, 1996; Robinson and Metternicht, 2005). This can be addressed using a range of methods to remove outliers and erroneous points and has led to the development of data cleaning protocols (Sun et al., 2013; Vega et al., 2019) and software (Sudduth and Drummond, 2007). It is often assumed that after cleaning procedures this represents a true reflection of the yield. However, systematic errors within the data sets can occur (Morgan, 2020; Simbahan et al., 2004) in some cases deviating by 5-10% (Grisso et al., 2002; Morgan, 2020). Studies validating combine yield data with independent yield data are scarce. In the few cases where validation occurs this has been performed under controlled conditions on small data sets collected under optimum use and calibration (Arslan and Colvin, 2002; Grisso et al., 2002; Morgan, 2020). These conditions are unlikely to represent inaccuracies resulting from commercial combine yield data typically used in research and for decision making on farm. For greater levels of accuracy appropriate calibration using specific manufacturer recommendations is crucial. In most studies using combine yield data it is rare for details of calibration procedures to be described. However, calibration procedures are often skipped or not possible during harvest under time and resource pressures. Previous studies have concentrated on each aspect in isolation such as data cleaning or management zone formation/stability analysis or economic mapping or accuracy validations. Our work integrated all these components into a comprehensive framework. This framework considered these different sources of error so that accurate yield data is used in spatio-economic appraisals or for supporting precision agriculture technology such as validating crop model outcomes. Accounting for all these errors avoids erroneous outputs or misguided management decisions. Specifically, the framework demonstrated how long-term, rotational yield map datasets can effectively underpin the application, development, and monitoring of precision agriculture techniques. The framework

used a long-term yield map dataset for an entire farm in Eastern England. The dataset was cleaned statistically and evaluated by comparison with recorded field yields. Management zones were identified across the whole farm using the corrected dataset and their temporal stability was assessed along with the economic margins across rotation.

3.4 Materials and methods

3.4.1 Study site and data sets

The study was conducted across 35 fields at Lodge Farm, Westthorpe, Suffolk, UK (Lat: 52.262837, Lon: 1.005092), with a total farm area of 435 ha. The soils range from a clay loam to sandy clay loam (Ashley and Beccles 1 associations, Cranfield University 2022). The farm operates a twelve-year rotation comprised of first and second wheats (*Triticum aestivum*) with spring barley (*Hordeum vulgare*), spring beans (*Phaseolus vulgaris*), winter oilseed rape (*Brassica napus*), and a two-year grass seed crop (*Lolium perenne*) as break crops, in this context these are defined as non-cereal crops. In addition, spring oats (*Avena sativa*), spring linseed (*Linum usitatissimum*) and spring wheat (*Triticum aestivum*) have also been grown intermittently. For each field, operations, fertiliser and pesticide inputs and management costs were recorded by the farm. The mean market value (grain price) that outputs were sold for, by year was also recorded. This enabled the profitability (net margin (£ ha⁻¹)) for each location within a yield map to be calculated. Over a ten-year period (2011-2020) 258 yield maps were collected using a combine harvester equipped with yield monitoring capabilities. Two combine harvesters were used, a CLAAS 570+ from 2011-2014 and a CLAAS 760tt from 2015-2020. The yield monitoring equipment was calibrated at intervals throughout the seasons, primarily when switching between varieties within crops or between different crop types and is likely representative of typical on-farm use. At each yield point the combine harvester records a time stamp and grain moisture content. In addition to yield maps, total grain offtake was recorded for each field using an RDS Liftlog weighing system fitted to the grain trailers. These were calibrated using a public weighbridge and provide an accurate record of total field crop offtake (tonnes) at harvest grain moisture. The

spatial and temporal completeness of the dataset was assessed in two ways: i) the number of yield maps were recorded for each crop for the harvestable crops grown, and ii) the proportion of spatially mapped farm margin was recorded from arable operations for the ten-year period.

3.4.2 Yield data cleaning

Yield data cleaning is required to identify and remove points that are unlikely to hold an accurate representation of yield and will therefore lower the accuracy of the yield map and any subsequent analysis. These points are most easily denoted through identifying points recorded outside optimal combine harvester operation or expected yield values. The time stamp recorded for each field yield point was used to provide the combining sequence for each yield map. The sequence was split at data points recording a change of direction that exceeds 0.6 radian (34.4°) (Kindred et al., 2016). These points are recorded as the combine harvester turns out of, or into, each transect (swath) and were removed. The point preceding and succeeding these points were also removed to exclude points with yield values obtained as the combine harvester fills and empties at the beginning and end of a respective transect (Sudduth and Drummond, 2007). Points recorded at combining speeds in excess of 10 km/h were also deleted as these are considered outside realistic optimal working speeds. Very short swaths (< 3 yield points) were also removed as the combine harvester has likely not reached optimal grain flow operation over a short distance. The distance to the closest parallel swath was further calculated for each point. The mean yield and distance to adjacent swath was also calculated for each swath. Any such transect with a mean distance less than 5.5m (2m less than header width) to the closest adjacent transect was identified as a potential partially filled swath. Then, to avoid the closest full swaths to the partial swaths being also identified, only swaths with a yield 10% below or above the field average swath yield for the field were removed. The final cleaning stage was to remove data outliers. Firstly, all points lying well outside expected yield values (<0.1 or >18 t/ha) were removed. Secondly, all points that were greater or less than the mean field yield, plus or minus 2.5 standard deviations respectively were also removed. This is threshold

is often applied for outlier identification in yield maps data sets (Córdoba et al., 2016; Muhammed et al., 2016; Sun et al., 2013).

The success of the cleaning process was then assessed by comparing the points removed for each step, and the effect that this had on the mean field yield. An experimental semi-variogram was also used to quantify the spatial correlation evident within each yield map, prior to and after the cleaning process. Spherical, exponential and gaussian models were used to fit the semi-variogram, and the model with the best fit selected and recorded for each field year. The relative structural variability has been used to determine the success of data cleaning in other studies (Vega et al., 2019). However, this method fails to include the range of spatial correlation, which might only be a few meters, implying little spatial correlation between nearby yield points regardless of the nugget to sill ratio used in the calculation (Schabenberger and Pierce, 2001). Here, we measure the degree of spatial correlation by considering the ratio of the area under the variogram to the area of the pure nugget model with the same sill variance up to 40m. The 40m threshold was used for all yield maps as some degree of spatial correlation is expected but is also of adequate distance to feature sufficient yield points. It is also the same threshold that other spatial variation statistics for yield maps have used (Peralta et al., 2013). The values reported are 1 minus the ratio, so a higher value indicates a higher degree of spatial correlation at a distance of 40m.

3.4.3 Yield data validation

To create co-located yield measurements across years, a 10 m x 10 m grid was imposed over each field area. Cleaned yield and corresponding moisture content in each year were assigned to their nearest grid cell, and if more than one measurement was found within a grid cell the mean of all points within that grid cell was calculated. Applying data to a grid prevents areas having a potentially greater density of yield points, for example if combine speeds were slower in certain areas of the field (e.g. due to lodging), having a disproportionate impact on the mean yield for that combine yield map. A Combine Yield (CY) mean for each field was calculated using the mean of all grid cell yields. Yields were not

adjusted for moisture at this stage so they could be compared to yields recorded by the grain trailer weigh cells which recorded weights at the actual moisture content at harvest. Some yield maps displayed areas of fields with gaps (no yield points). Field years were discarded from the analysis if large areas of missing data were found to be due to recording error, for example if the yield monitoring software was not engaged or a field trial had taken up a large area of the field. Also, gaps in the data identified through consultation with the farmer as having been a result of 'failed' or 'unharvestable' crop were treated as zero yields, these gaps often arose as a result of crop destruction prior to harvest to minimise grass weed return. In these maps a field average CY would likely overestimate yield as these zero yields do not feature in the mean. To mitigate this, the CY average for these fields was calculated by dividing the total offtake (the combine yield map average yield, multiplied by the total area of the yield map) by the true field area. Trailer Weigh cell Recorded Yield (RY) was then calculated by dividing total crop offtake (t) by the recorded sown crop area (ha). The accuracy of CY compared to RY was assessed for each crop. For winter wheat, which had the greatest number of fields in each year (>10), the accuracy over time was also assessed. The Root Mean Square Error (RMSE), Mean Bias Error (MBE) and Mean Absolute Error (MAE) were used to evaluate combine yield monitor accuracy compared to recorded yields. These were calculated by equation 3-1-3-3:

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^n (X_{RY,i} - X_{CY,i})^2}{n}} \quad (3-1)$$

$$\text{MBE} = \frac{1}{n} \sum_{i=1}^n (X_{RY,i} - X_{CY,i}) \quad (3-2)$$

$$\text{MAE} = \frac{1}{n} \sum_{i=1}^n |X_{RY,i} - X_{CY,i}| \quad (3-3)$$

Where, n is the number of yield maps, X_{RY} is the recorded field average yield (t ha^{-1}), and X_{CY} is the combine field average yield (t ha^{-1}). The mean percent error was also calculated from the MAE and the RY.

3.4.4 Yield correction and gridded net margin

To account for large errors in the dataset, gridded yields were adjusted so the mean of the CY equaled the mean of the RY for that field. Corrected points were then adjusted to an industry standard of 15% moisture for cereals and pulses, and 9% moisture for oilseeds. This adjustment used the corresponding gridded moisture content recorded by the combine. For each yield value, moisture adjusted yields were standardised to have a mean unit variance ($\mu=0$, $\sigma=1$) to allow for comparison between years and different crops.

Net margin (NM) (£) for each grid cell in each year was calculated using the equation 3-4:

$$NM = (Y_{CY}Gp) - (Fc + Vc) \quad (3-4)$$

where Y_{CY} is the grid cell corrected and moisture adjusted yield recorded by the combine yield monitor ($t\ ha^{-1}$), Gp is the grain price (£) for that crop achieved on farm that year, Fc is the fixed costs (£) (including machinery depreciation, and land rent) and Vc is the variable costs (£) (seed, pesticides, fertilisers and machinery operations). All Fc and Vc are actual costs incurred on the farm for inputs and machinery costs for a given season, not values derived from an industry standard reference material such as the John Nix Farm Management Pocket Book (e.g., Redman, 2015).

3.4.5 Clustering and yield stability analysis

Spatially coherent zones of homogenous yield performance for each field were identified using the Fuzzy c-means clustering algorithm with optimal completion strategy as outlined by Hassall et al. (2019). The Fuzzy c-means algorithm was used to identify clusters within the standardised yield dataset, the auto completion strategy of which allows for the algorithm to be run on locations (grid cells) when a complete set of yield observation is not available. In long term datasets such as this study this can be a high proportion. Normalised classification entropy was used to identify the appropriate number of clusters. The number of clusters was restricted to between 2 and 6 to avoid a high number of clusters having only

subtle yield variations, with cluster entropy used to distinguish the optimal number clusters. Clusters were then smoothed using a coherence index and variogram.

The temporal yield stability for each grid cell was identified using the methods set out by Maestrini and Basso (2018) and thresholds reported by Maestrini and Basso (2021). The mean and standard deviation of the normalised yields across all available years for every grid cell was calculated. A grid cell was classed as stable if the mean SD of all grid cells within that cluster was <0.8 , and unstable if $SD > 0.8$. The stable grid cells were classified as high yielding if the standardised mean yield was >0.2 , or low yielding if the standardised mean yield was <-0.2 , and those falling between these boundaries classed as medium. These thresholds were identified by Maestrini and Basso, (2021) using a simplex search procedure to ensure repeatability regardless of which year's yield map data was used in the analysis. No thresholds for categorizing cluster, rather than grid cell, stability have been previously reported. Therefore, to provide context to cluster stability, the standard deviation of the mean standardised yield across seasons for each cluster is reported.

3.5 Results and Discussion

3.5.1 Spatial data availability across rotations

Between 2011-2020 harvestable crops were grown in 345 fields, and the yields spatially mapped in 258 (75%) (Table 3-1). A large proportion of the fields missing yield maps were found to occur when fields were cropped with herbage grass seed. Combine yield monitors do not currently reliably measure yields for this crop as combining takes place at high seed moisture content and lodging is often widespread. The 258 yield maps accounted for 65% of the total farm margin (2011-2020), with over one third of the total farm net margin (2011-2020) unable to be spatially allocated. In this study herbage grass accounted for just 16% of crops grown but 25% of the total farm margin. These data gaps, place limitations on the confidence in spatially mapping productivity for rotational management decisions, particularly if, as is the case in this study, a high value, rotationally valuable crop is not spatially mapped. This will likely be representative of the situation on many UK farms. In 2020, 15% of the total cropped area was in crops

not widely spatially mapped (DEFRA, 2021a), a large proportion of these were high value potato and vegetable crops (El Chami and Daccache, 2015). The reason for areas having relatively poor economic performance in a combinable crop might not follow the same patterns of spatial variability in crops that are biologically very different, such as root or horticultural crops (Boubou, 2018). The true rotational value of these area/zones could therefore be undervalued.

For precision agriculture the spatial patterns identified in combinable crops are likely to provide sufficient contextual information to enable management decisions for that crop alone. However, land managers are now being incentivised to take areas of land out of production across rotations to support environmental schemes. Under a re-design of the European Union's Common Agricultural Policy, farmers will be encouraged to devote between 3-7% of their land to non-productive schemes (European Commission, 2023). In England under the Sustainable Farming Incentive as currently outlined, this area will be between 5-10% of land entered (DEFRA, 2021b). Yield maps, and the economic productivity maps derived from them, can be used to undertake cost/benefit analysis by growers to identify areas that are economically likely to obtain the best returns from these schemes (Capmourteres et al., 2018). However, gaps in spatial productivity data as described here will limit the applicability of these "precision conservation" approaches.

An incomplete record of spatial productivity across a rotation also imposes limitations of some precision agriculture techniques. Crop-soil nutrient cycling models developed using experimental plot data could be extrapolated to guide precision management decisions. These models often require a complete across-season record of crop offtake (yield) in order to perform correctly (Shan et al., 2021). Even simpler nutrient removal calculations based on grain analysis or standard figures (Inman et al., 2005) will have significant limitations with large gaps in the data set (Longchamps et al., 2022). The limitations of rotational data sparsity will need to be addressed for complete nutrient budgeting to be achievable, either through yield mapping of all crops across the rotation or using

other sources of information to fill in the data gaps, such as remote sensing and crop modelling techniques (Jeffries et al., 2020; Pasquel et al., 2022).

Table 3-1 Number of field years and number of yield maps for each crop across the 35 fields (2011-2020). Margins are reported as a % of the total farm net margin for each crop (2011-2020). Financial (£) data not presented for data protection. Margin contribution is the total contribution that the crop has made to total farm profits. Margin mapped is the percent of which this has been spatially mapped through yield maps.

Crop	Field years (n)	Yield mapped (n)	Margin contribution (%)	Margin mapped (%)
Winter Wheat	186	172	54	48
Spring Barley	31	30	7	7
Spring Beans	22	19	3	2
Winter OSR	21	19	7	6
Spring Linseed	21	12	3	1
Spring Oats	5	4	1	1
Spring Wheat	2	2	1	1
Herbage Grass	55	0	25	0
Other crops	2	0	1	0
Total	345	258	100	65

3.5.2 Data cleaning

Across the 10-year period, the farm collected 912,485 individual yield data points. Across all crops, 16% of points were identified as erroneous through the cleaning procedures and were removed (Table 3-2), an example field prior to and after cleaning is shown in Figure 3-1. Spring linseed, winter oilseed rape and spring oats had a higher proportion of errors (22% and 28% respectively). The cleaning process increased the yields on average in all crops; for winter wheat, field mean yields increased by 0.72 t/ha after cleaning. Across all yield maps the degree of spatial correlation was found to improve following data cleaning,

Table 3-2 Yield map cleaning results including data points removed in each cleaning step, valid points retained, mean yields before and after cleaning (t ha⁻¹) and the degree of spatial correlation (DSC) for all raw (unprocessed) and cleaned yield maps by crop

Crop	Raw points	Swath spacing	Turning	Yield outliers	Distance	Total removed	Valid	Raw yield	Clean yield	Raw DSC	Clean DSC
Winter Wheat	586742	5788	55186	23963	915	85852	500890	9.80	10.52	0.07	0.24
Spring Barley	128631	1617	11150	5395	150	18312	110319	7.92	8.57	0.06	0.25
Winter OSR	62580	3602	8240	2107	74	14023	48557	4.75	5.29	0.07	0.25
Spring Linseed	57298	2319	7813	2026	267	12425	44873	3.35	3.79	0.12	0.26
Spring Beans	49246	132	4895	2389	31	7447	41799	3.93	4.26	0.07	0.24
Spring Oats	17702	992	3318	597	58	4965	12737	6.94	7.80	0.05	0.22
Spring Wheat	10286	37	1129	480	5	1651	8635	5.28	5.89	0.17	0.36
All (n258)	912485	14487	91731	36957	1500	144675	767810	-	-	0.09	0.26

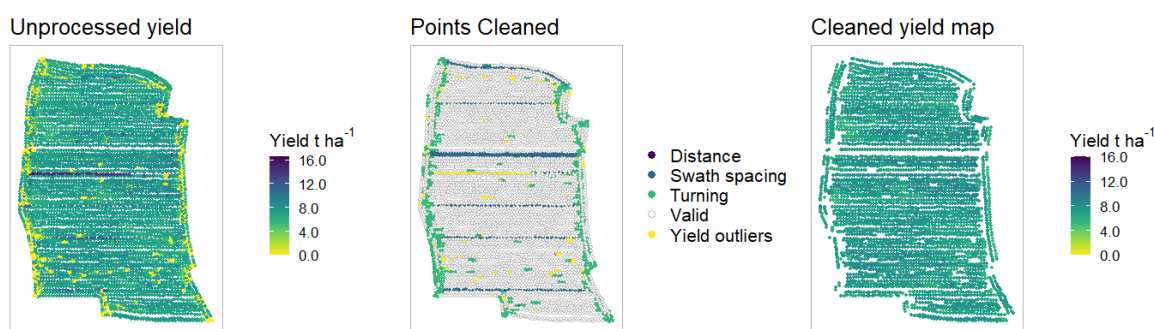


Figure 3-1 Yield map cleaning example, Field 4, 2015 winter wheat

increasing from 0.09 to 0.26 across all crops. Spring wheat presented the greatest degree of spatial correlation after data cleaning (0.36), although from a relatively small sample size ($n=2$). The degree of spatial correlation at 40m was found to be relatively consistent across all other crops, ranging from 0.22 to 0.26.

Previous studies have shown that large errors in yield maps can occur, and cleaning is advantageous (Blackmore and Marshall, 1996; Sudduth and Drummond, 2007; Vega et al., 2019). The identification of areas of similarity (management zones) relies on the data having a certain level of spatial correlation, the larger degree of spatial correlation achieved through cleaning indicates that geostatistical prediction (in this study this was conducted through clustering) is likely to be more accurate than if performed with raw yield map data (Schabenberger and Pierce, 2001).

3.5.3 Yield map accuracy

All crops except for spring barley had CY mean yields higher than RY, with an MBE of 0.46 t/ha for all winter wheat crops (Figure 3-2 and Table 3-3). The accuracy of the combine yield maps varied depending on crop. The MAE as a percent of mean recorded yield (%E) was 8.1% for winter wheat and 6.0% for spring barley, representing 63% of crops grown across the rotation. The reported accuracy of yield monitor data by manufacturers has been found to vary between 1% and 6% (Arslan and Colvin, 2002; Blackmore and Marshall, 1996; Blackmore, 1999; Blackmore et al., 2003b; Larscheid and Blackmore, 1996). The mean

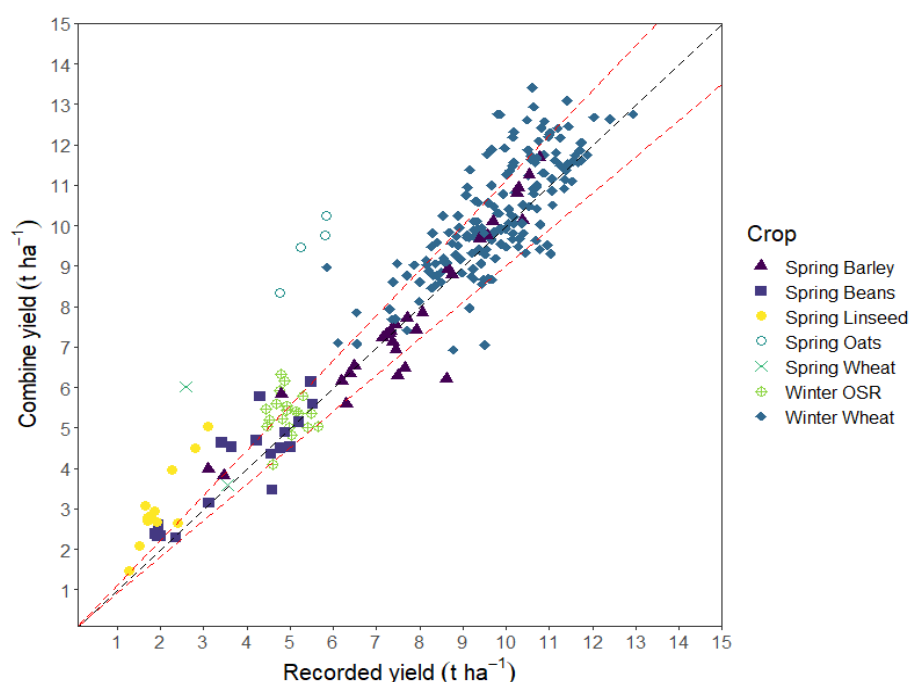


Figure 3-2 Average field yield from recorded and. Combine harvester yield monitor (t/ha), grey line is $y=x$, red line is $y=x$ plus and minus 10% error

percent errors for winter wheat and spring barley of 8.1% and 6.0% respectively, are comparable to errors reported in previous, smaller validation studies. (Grisso et al., 2002) reported errors of 10%, while (McNaull and Darr, 2020) found mean field yield errors of around 5% for a single cropping season calibration study in corn (maize) and (Morgan, 2020) reported a 5.7% mean error over two seasons for wheat. Accuracy decreased to 12.3% and 12.8% for winter oilseed rape and spring beans respectively. The greater inaccuracies in these two crop types are likely to be a result of larger variations within the field due to agronomic and external (pest damage) pressures experienced in these crops (Ortega-Ramos et al., 2022; Wright, 2008). The accuracy of spring linseed, spring oats and spring wheat was very poor, with differences between RY and CY of 52.2%, 74.4% and 56.4% respectively. These crops are not part of the main rotation, the farmer in this study acknowledged that it is possible that yield monitoring equipment calibration was not as rigorous prior to the harvesting of these crops as they were not considered of long-term importance to the farm, this may explain the much

Table 3-3 Summary statistics for combine harvester mapped yield and recorded yield

Crop	Year	n	Recorded mean yield	Combine mean yield	r	MBE	MAE	%E	RMSE
Spring Barley	All	30	7.79	7.77	0.94	-0.02	0.47	6.0	0.69
Spring Beans	All	19	3.73	3.98	0.90	0.25	0.48	12.9	0.63
Spring Linseed	All	12	2.01	3.06	0.90	1.05	1.05	52.2	1.18
Spring Oats	All	4	5.42	9.45	0.95	4.03	4.03	74.4	4.04
Spring Wheat	All	2	3.07	4.80	-	1.73	1.73	56.4	2.43
Winter OSR	All	19	4.95	5.36	0.02	0.41	0.61	12.3	0.73
Winter Wheat	All	171	9.78	10.25	0.77	0.46	0.79	8.1	1.03
	2011	20	9.54	10.39	0.54	0.85	1.30	13.6	1.53
	2012	20	9.67	10.44	0.26	0.77	0.96	9.9	1.21
	2013	11	9.74	9.81	0.65	0.08	0.69	7.1	0.93
	2014	13	11.30	11.47	0.64	0.17	0.43	3.8	0.60
	2015	17	11.05	11.81	0.03	0.76	1.20	10.9	1.39
	2016	21	8.68	8.76	0.88	0.08	0.51	5.9	0.64
	2017	18	10.34	10.16	0.84	-0.18	0.37	3.6	0.53
	2018	16	8.40	9.20	0.56	0.80	0.92	11.0	1.16
	2019	20	10.58	11.22	0.91	0.64	0.71	6.7	0.84
	2020	15	8.85	9.28	0.76	0.44	0.66	7.5	0.80

n = number of fields, r= correlation coefficient, MBE = mean bias error, MAE = mean absolute error, %E = mean percent error, RMSE = root mean square error

larger errors in these crops. It is not possible to provide evidence of the calibration steps taken for each yield map across the ten-year dataset, nor would it be for most studies using yield map data. It is likely that during harvest, a time-pressured operation, with work rates optimised to maintain efficiency, that occasionally yield monitor calibration procedures can be missed, or operational errors occur. This study presents a real-world data set, that is likely to be comparable to those collected under commercial farms in the UK and globally. Generally, in the main combinable crops (wheat and barley), yield map accuracy was good, however with potential for large errors, with 29 out of the 171 wheat fields (17%) presenting errors greater than 15% (Figure 3-2). These large errors will have significant limitations for their use on farm, reducing the accuracy and effectiveness of the methods discussed previously including spatial economic analysis and nutrient budgeting. These reported errors would also have implications for the use of yield

map data for implementing PA technologies. It is common to use combine yield data to calibrate and validate modelling and remote sensing techniques. For a model/technique to be appropriately assessed, high quality “observed” data that is free from errors is required (Boote et al., 2016), particularly when identifying the best performing from a selection of models/methods. For remote sensing applications (Zhao et al., 2020) reported an RMSE of 0.88 to 1.44 t ha⁻¹ when comparing 6 canopy indices derived from Sentinel 2 data with yield monitor data. (Wallor et al., 2018a) used yield monitor data to assess the accuracy of 11 crop simulation models for modeling within-field variation in yield, reporting a RMSE ranging from 0.5 to 3.5 t ha⁻¹ for a field in Germany. There is nothing to suggest that the yield map data in those studies has the same level of errors as the dataset reported in this study. However, the errors in modeling techniques reported in these studies are of a similar magnitude to the average errors reported in this study between yield map data and weighed recorded yields for winter wheat across years (0.53 to 1.53 t ha⁻¹ RMSE). If similar exercises were performed on this data set, there is potential to not identify the best model, but that which is closest to the errors in the validation data set. (Kersebaum et al., 2005) found that when spatially validating the HERMES crop model, results agreed well with

hand-harvested yield data, but poorly with combine harvester yield map data, demonstrating the limitations that inaccurate yield map data can pose in modeling exercises.

Researchers and farmers should make use of, and where currently not available commence collecting, data sets to validate combine harvester yield data, including field level yields recorded over weighbridges or grain trailer weigh cells. Studies using combine yield data would also benefit from reporting the specific calibration methods employed, an exact record of calibration timings would have also strengthened this study. Further development and testing of automatic methods of identifying erroneous yield maps is also required (Blasch et al., 2020). These additional data sources will provide validation of yield map data and where possible allow for some level of correction for large errors, strengthening the applicability of yield maps on farm and in the development of precision agriculture techniques.

To minimise the impact of potential yield map errors in subsequent management zone and yield stability analysis in this study, the field combine yields were adjusted to the mean RY for a given field. This correction assumed that the errors in the yield maps were relative, i.e., consistent across the whole field. The majority (158/258) of CY are within 10% of RY, so adjustments required for these maps were small. The main purpose of this correction is to reduce the influence large errors will have on interpreting temporal trends in yield stability or the accuracy of long-term margin analysis.

3.5.4 Clustering and yield stability

In this study 159 clusters (MZ) were identified across an entire 35 field, 435ha arable farm in eastern England using a fuzzy-c means clustering algorithm with an optimal completion strategy (Figure 3-3). The optimal number of clusters in each field varied. With limits set between 2 and 6 clusters, no fields had just two clusters, 6 fields had 3 clusters, 12 fields had 4 clusters, 9 fields had 5 clusters, and 8 fields had 6 clusters. The mean cluster area was 2.87 ha. It is recognised that the number of zones and the size of these zones needs to be manageable

for a farmer. While its recognised managing 159 individual zones is more complex than 35 individual fields it is by no means infeasible. Recent estimates indicate 31% of UK farms, 36% of farms in the United States and 49% of Australian farms are already using variable rate technology (Lowenberg-deboer and Erickson, 2019). At a fundamental level, yield-based management could be employed using the validated and corrected management zone yield performance (Rodriguez et al., 2019), for which there are UK specific nitrogen recommendations (AHDB, 2023). Sampling management zones either at a single composite sample from within each zone (Oliver et al., 2010) or multiple points within each zone to provide some context of homogeneity within the identified zones (Tagarakis et al., 2019). Both methods would also require fewer samples compared to commercial grid sampling services, typically surveying at one sample per ha (Marchant et al., 2012). In the past, farmers bore the financial burden of adopting precision agriculture technologies. However, in the UK, there has been a notable shift, with farmers now having the opportunity to receive payments for implementing precision agriculture technologies (DEFRA, 2024a). This incentivises the adoption of these technologies, offering financial support to manage the increased complexity associated with transitioning from a whole-field approach to a more nuanced management zone strategy.

Across the rotation, all clusters were profitable, but large variation in cluster performance was recorded with the least profitable cluster recording a mean annual margin of £10/ha, the most profitable with a mean annual margin of £781/ha (Figure 3-5A). Caution should be exercised when comparing cluster performance across fields. Margins within a field are impacted by the number of data years available for each field, ranging from 4 to 10 years (Figure 3-4). Other compounding factors such as different cropping histories, drilling dates, inputs and crop varieties make it difficult to compare cluster margins across fields. Capmourteres et al. (2018) claim to be the first study estimating economic feasibility of set-aside to deliver ecosystem services, using a small sample size of 3 farms across 140ha in Ontario Canada. More recently Adhikari et al. (2023) produced spatial margin data and stability across 3 fields (56.3 ha) in Texas from 3 years of yield data. In this study a whole farm ten-year rotational margin map

across 435 ha in the UK is created, where farmers have the potential to be paid for actions that protect and improve the environment (DEFRA, 2023). There are areas that are clearly underperforming compared to the margin potential for a given field and therefore might be suitable candidates for environmental land management schemes. For example, the most productive zone in field 19 (Figure 3-5A) has a mean annual margin of £654 (top 5th percentile of all clusters) compared to the worst performing cluster which had a mean margin of £275 (85th percentile of all clusters). This can be compared with the actions that support farmland and wildlife, paying between £590 - £732 ha/per year under the Sustainable Farming Incentive (DEFRA, 2023c). Although calculations on the cost of establishment and management of these actions would need to be subtracted and fixed costs accounted for these areas have the potential to be more profitable under agri-environmental schemes. In a high yielding system, with mean wheat yields of 10t ha (Table 3-3), however, the profitability appraisal of cropping against environmental schemes is likely to be close and therefore having accurate data that has been under appropriate cleaning and validation to generate such analysis is vital, and to our knowledge this validation applied here is a novel step in the analysis. There is also potential for environmental schemes to improve the profitability of areas that remain in agricultural production. Recent research has shown that environmental schemes, such as flowering strips, can enhance pest control services by providing habitat for beneficial fauna, thereby reducing pest pressure. While yield benefits are more variable, there is evidence supporting their effectiveness. Additionally, extended leys (lasting more than one year) can increase soil carbon concentrations, which has been shown to enhance soil function and productivity when these areas are returned to arable cropping. As well as identifying areas most suitable for environmental land management schemes whole farm economic assessments such as this provide information to guide more targeted management. All though rotational history make it difficult to compare across zones, it is possible to compare economic performance of zones within the same field (Figure 3-5B). Across the farm the highest margin MZ within each field account for 30% of the total farm area (135.0 ha). Over 34% (155.5 ha) of total farm area had a margin loss > £100 ha compared to the most productive

(economically) performing MZ within each field, 13% (58.2ha) had a margin loss > £200 ha and 6% (25.9ha) had a margin loss >£300 ha.

Across the farm 31% (140.5 ha) of grid cell yields are classified as high yielding and stable, 15% (66.2 ha) as medium yielding and stable, 17% (79.0 ha) as low yielding and stable, and 35% (159.0 ha) of grid cells as unstable (Figure 3-6A). When averaged across clusters mean standardised yield standard deviation is below 0.8t/ha in all clusters (Figure 3-6B). Visually, the rank order of cluster yields tends to be fixed with only a few clusters exhibiting large inter-annual variation in standardised yield performance (Figure 3-4 Standardised (mean unit variance $\mu=0$, $\sigma=1$) yields for each cluster by field number. Field number can be identified in Fig 3.3.). The highest yielding and most stable grid cells are notably concentrated away from field edges (Figure 3-6A). The lower yields and greater yield instability close the field edges is likely attributed to the presence of headlands where wheeled traffic is more intensive and greater levels of soil compaction are expected (Sunoj et al., 2021), possible shading from trees, and greater weed competition (Robinson et al., 2022) . However, yields can sometimes be higher close to field boundaries as a result of helpful ecosystem services (Duelli and Obrist, 2003).

It is recognised that there will always be a certain level of subjectivity to interpreting stability (Maestrini and Basso, 2021). This allows the stability of a MZ performance to be compared with the long-term economic performance. As all management has historically been uniform within a field (no precision agriculture technologies used), net margin maps change proportionally with yield, however it highlights the range of income within fields across the rotation, not just across a single crop or year providing an economic justification for precision agriculture technologies. This rotational validated spatial economic data set is vital for monitoring the success of precision agricultural techniques that might be employed on farm. The benefit of precision agriculture is often inconclusive and further ground truthing is required on many technologies (Ingram et al., 2022; Jin et al., 2019). This need for “validation research” has been recognised in recent perception studies analyzing digital agriculture/smart farming technologies

(Ingram et al., 2022; Regan, 2019). Accurate measurements of crop yield are crucial for the science of crop production at the field and farm scale (Sylvester-Bradley et al., 2017). The validated management zone yield performance, stability maps along with spatial economic data provides a framework for the farm to measure the economic success of any precision agriculture or environmental scheme adopted against relative historic economic performance. Precision agriculture techniques might reduce input costs (i.e., fertiliser application) to account for lower yield potential and demand, therefore, yield map patterns will remain unchanged in subsequent years, but the relative economic performance of the zone, in theory will improve.

3.6 Conclusion

This study has demonstrated how the accuracy of yield map data from a combine harvester after data cleaning steps cannot be assumed, and that any application of yield map datasets, including the identification of management zones in developing and validating precision agriculture techniques should attempt to address this through careful data cleaning and accuracy validation procedures, ideally with the potential to correct for errors. Once the data has been validated and corrected only then the real value can be obtained from geostatistical analysis at the farm level. We advocate for a proactive approach, encouraging farmers to not only conduct proper calibration but also collect data sets for suitable data validation. Allowing for more reliable and robust results in precision agriculture applications and economic assessments. The fuzzy clustering with an autocompletion strategy identified management zones and allowed for yield stability assessed at the farm scale. The data validation and correction allowed for an accurate whole farm, rotational spatial economic appraisal. Such data sets will be key in performing economic cost benefit (compared to continued cropping) analysis of environmental schemes for which farmers will be paid for delivering ecosystem services.

The accurate management zone yield, yield stability, and economic performance data should be used to develop, and assess the success of precision agriculture

management strategies, particularly those that require the calibration and validation of crop, soil, or nutrient budgeting models.

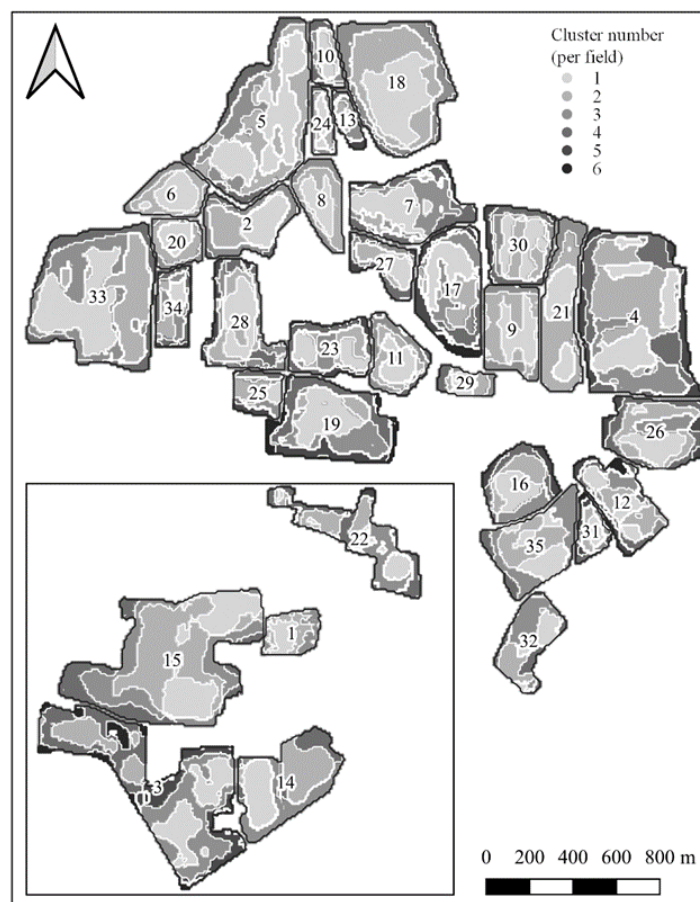


Figure 3-3 Clustering results for each field, with field number, grey scale is used as no significance in cluster number between fields.

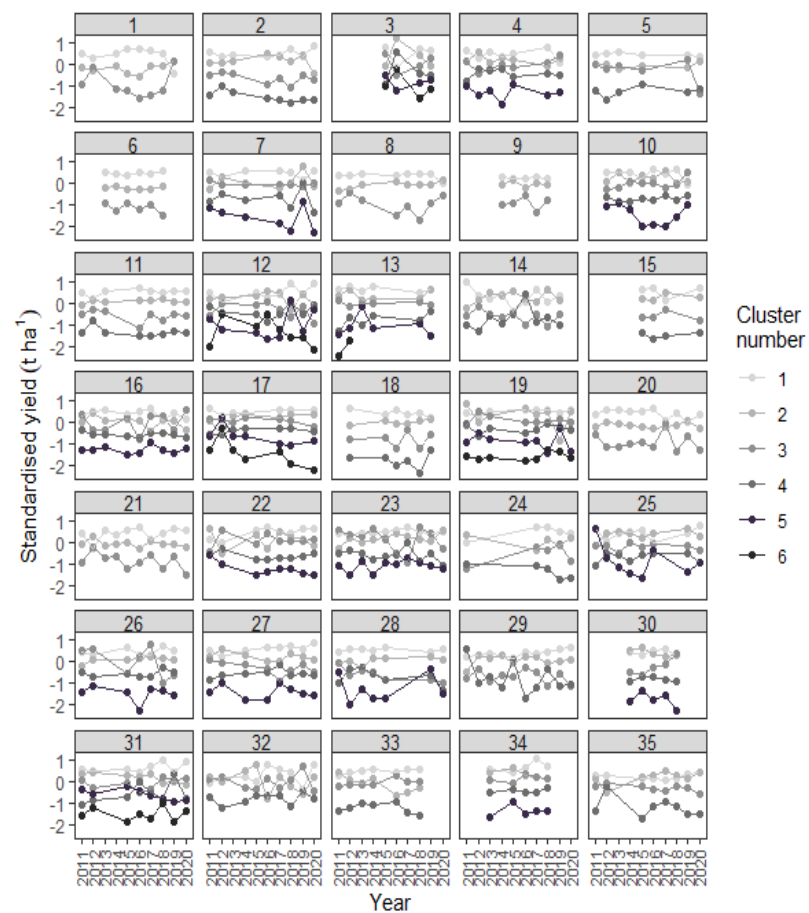


Figure 3-4 Standardised (mean unit variance $\mu=0$, $\sigma=1$) yields for each cluster by field number. Field number can be identified in Fig 3.3.

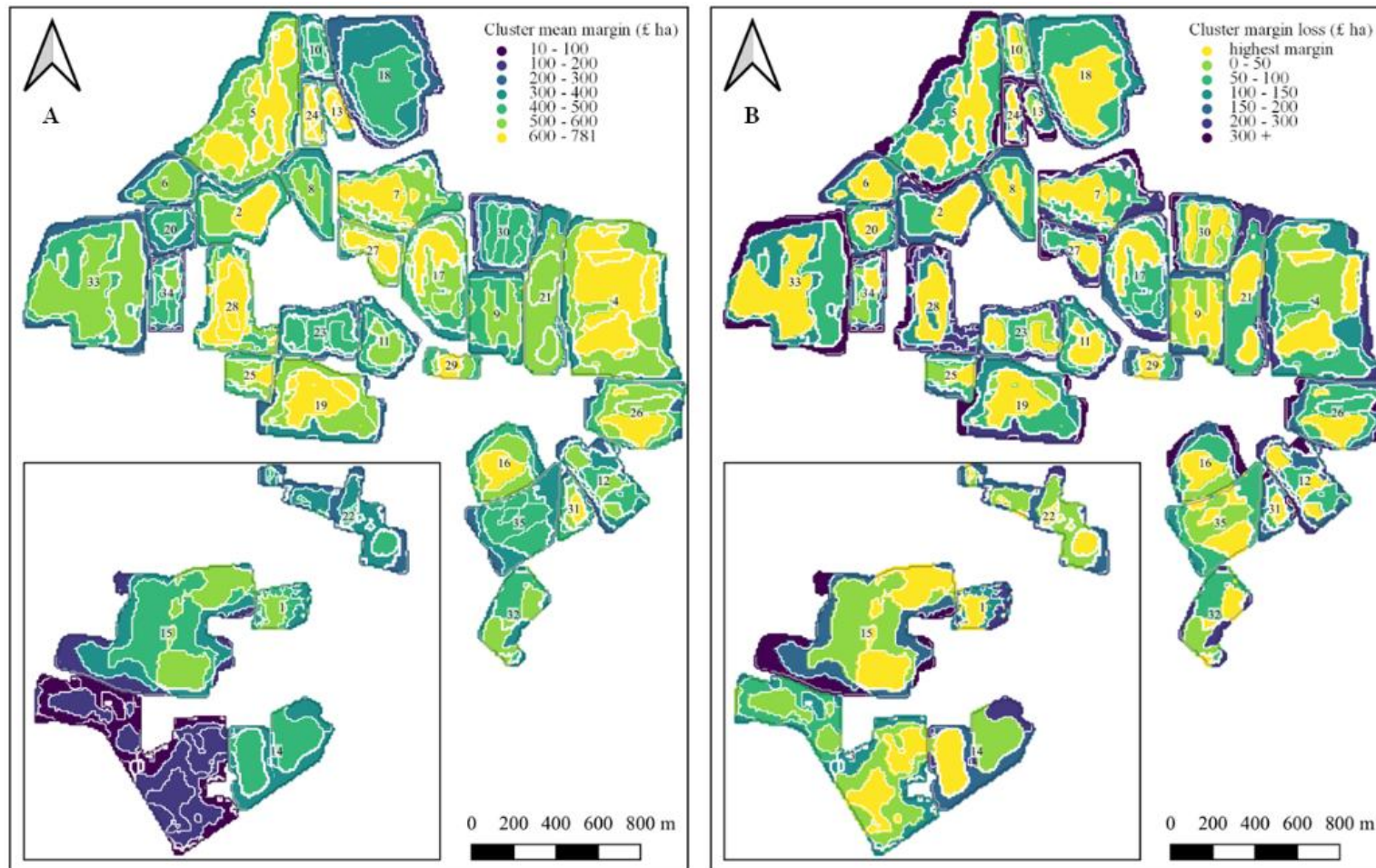


Figure 3-5A: Mean cluster margin across rotation (£ ha, 2011-2020), B: Mean annual cluster net margin loss compared to the cluster with the highest net margin within each field (£ ha, 2011-2020).

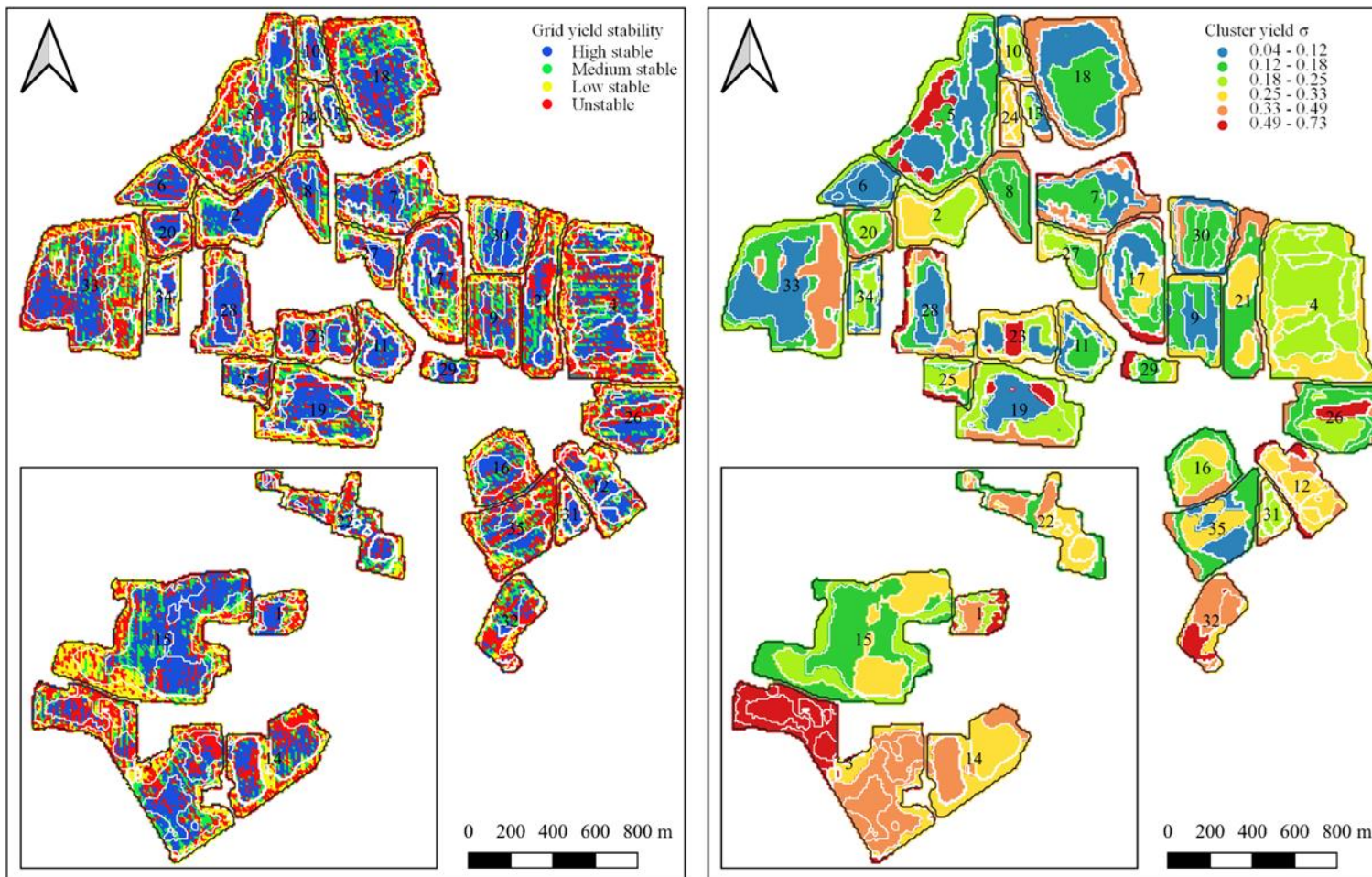


Figure 3-6A: Grid cell yield stability across available years yield data for all fields, B: Standard deviation of cluster mean yields across available years (2011-2021) for each field.

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4 Assessing within-field nitrogen variability and optimised fertiliser use using the Sirius crop model

4.1 Research context and contribution statement

Chapter 4 integrates the methods from Chapters 2 and 3 to apply the Sirius CSM across commercial fields at Morley Farms, Norfolk. Using 15 years of yield map data, spatially coherent yield performance zones were identified. Additional data from the Morley SAMS dataset—a long-term monitoring project supported by The Morley Agricultural Foundation and delivered by NIAB—was used to parameterise seven management zones in Sirius.

Unlike many studies that rely on small trial plots or short-term datasets, this research applies a commercial farm dataset, enabling a more realistic evaluation of spatial and temporal variability in nitrogen response. Sirius was chosen because it has been extensively calibrated for UK wheat systems and was demonstrated in Chapter 2 to accurately simulate fine-scale responses to variation in soil properties. This makes it a suitable model for assessing nitrogen uptake and yield variability at a fine spatial scale.

Building on the validation of Sirius in Chapter 2, Chapter 4 evaluates the model using two years of agronomic data from targeted site-specific samples and yield maps to assess its ability to simulate spatial and temporal variation in yield, yield components, and nitrogen uptake. While the dataset in Chapter 2 had higher temporal and spatial resolution, the methods in Chapter 4 represent a more applied approach, aligning more closely with what is feasible on commercial farms.

The validated model was then used to generate zone-specific nitrogen management recommendations, evaluating simulated nitrogen use efficiency and potential reductions in nitrogen leaching compared to a standard farm-wide N rate. This study demonstrates how CSMs can be integrated into real-world precision agriculture, helping to refine nitrogen management strategies and improve on-farm decision-making.

CRedit authorship contribution statement: David E. Clarke: Conceptualization, Data curation, Formal analysis, Funding acquisition, Investigation, Methodology, Visualization, Writing – original draft, Writing – review & editing. Elizabeth A. Stockdale: Funding acquisition, Methodology, Project administration, Supervision, Writing – review & editing. Jacqueline A. Hannam: Funding acquisition, Methodology, Project administration, Supervision, Writing – review & editing. Benjamin P. Marchant: Funding acquisition, Methodology, Project administration, Supervision, Writing – review & editing. Stephen H. Hallett: Supervision, Writing – review & editing, Funding acquisition, Methodology

4.2 Abstract

Achieving high wheat yields in the UK requires substantial nitrogen fertiliser inputs, yet nitrogen use efficiency remains variable, leading to environmental losses through volatilisation, leaching, and greenhouse gas emissions. Traditional farm-wide N management strategies often fail to account for within-field variability in soil properties and crop response. This study applies the Sirius Crop Simulation Model across three commercial wheat fields at Morley Farms, Norfolk, integrating on-farm yield map data and agronomic observations to assess the potential for spatially targeted N management strategies. Yield performance zones were identified using historical yield maps and soil electrical conductivity measurements, representing key soil-driven variations in plant-available water capacity. Seven management zones, covering 30.5 ha, were parameterised in Sirius to simulate spatial and temporal variation in wheat yield, yield components, and nitrogen uptake. The validated model was then used to generate zone-specific N recommendations, compared to a standard farm-wide N rate of 218 kg N ha⁻¹. Sirius effectively simulated management zone yield (RRMSE = 14.7%) and N uptake (RRMSE = 13.6%) across 11 site-years. The model captured grain number variation better than individual grain weight and showed poor performance in simulating straw biomass (RRMSE = 58.9%). Simulations using a long-term weather dataset identified optimal N rates for each zone, improving NUE and reducing unutilised nitrogen, particularly in low PAWC zones, where excessive N application increases leaching risk by up to 31.1 kg N ha⁻¹ compared to the farm's standard practice. This study demonstrates how crop simulation models can be integrated into precision agriculture workflows, using yield maps, soil sensing, and long-term datasets to refine nitrogen management. By incorporating realistic spatial variability in soil and crop responses, this work provides a framework for improving farm-level NUE, reducing environmental impact, and supporting sustainable intensification in UK wheat production.

4.3 Introduction

Winter-sown wheat (*Triticum aestivum* L.) is the UK's most widely cultivated arable crop (DEFRA, 2023a). Favourable soils, climate, and efficient production practices enable yields close to their agroecological potential (Bruinsma, 2009; Mitchell and Sheehy, 2018). Achieving these yields often requires substantial nitrogen (N) fertiliser inputs (Sylvester-Bradley et al., 2008), averaging 186 kg N ha⁻¹ (DEFRA, 2023b). To determine how efficiently this nitrogen is used, Nitrogen Use Efficiency (NUE) metrics can be applied (Congreves et al., 2021). Based on recent calculations, the average apparent NUE of applied N fertiliser is 73% across a large dataset across multiple farms in the UK, but there is considerable variation, with some farms displaying low NUE (Baxter and Clarke, 2023). Inefficient N use can lead to losses from the soil-crop system, including ammonia (NH₄⁺) volatilisation, which negatively impacts human health (Marais et al., 2021; Misselbrook et al., 2000); Additionally, the nitrification and denitrification of N to nitrous oxide (N₂O) account for about 0.46%-0.6% of applied N (Cowan et al., 2020; Sylvester-Bradley et al., 2009). Nitrous oxide emissions, along with emissions from N fertiliser production, represent over 70% of the crop's greenhouse gas emissions (Kindred et al., 2021). Nitrate (NO₃⁻) that is not utilised by crops or microorganisms can leach out of the soil system, with agriculture being the main source (70%) of nitrates in the UK's ground and surface water, with the drier, arable-dominated regions of eastern England particularly vulnerable to such losses (Environment Agency, 2019). Given the challenges of climate change and a growing global population, the UK's high agricultural productivity will be vital for sustaining and enhancing food security both nationally and globally (Röder et al., 2014). Therefore, where NUE is below the target threshold of 90% (Hutchings et al., 2020) improvements are needed to meet water quality and agricultural emissions targets. Additionally, recent supply disruptions and high fertiliser prices due to geopolitical and market forces have led to renewed interest in reducing N application rates on farms and focusing on more targeted fertiliser use for better returns (Ben Hassen and El Bilali, 2022; DEFRA, 2022).

For the majority of the UK, the 'RB209' reference book (AHDB, 2023a) is used to determine N fertiliser rates (Kindred and Sylvester-Bradley, 2014). While these guidelines are regularly updated and are grounded in over 85 years of nitrogen response experiments (Crowther and Yates, 1941; George, 1984; Kindred et al., 2018), they do not fully capture site-specific and temporal variability in N response due to changing soil and weather conditions. "Chessboard" experiments have shown significant variability in optimal N rates within fields, differing by up to 100-200 kg N ha⁻¹ (Kindred et al., 2017; Kindred et al., 2015; Lark and Wheeler, 2003). Canopy sensors can detect spatial variation in crop N uptake, but they often fail to account for all factors influencing crop N demand and typically adjust doses, based on predefined optimal rates for the entire field (Colaço and Bramley, 2018; Kindred et al., 2017). Thus, more precise, location-specific methods for N management are required (Kindred et al., 2012, 2015).

Rainfall and plant-available water significantly influence crops' N response, and water limitations can drastically reduce NUE if N rates are not optimised (Quemada and Gabriel, 2016). Wheat in the UK is predominantly rain-fed, making it susceptible to drought. About 30% of wheat is grown on drought-prone soils, leading to an estimated 10% yield loss annually, with greater losses in dry years (Clarke et al., 2020; Ober et al., 2013). Plant available water capacity (PAWC) can vary considerably within fields (Daccache et al., 2015; Iqbal et al., 2005). The impact of water and nitrogen limitations on crop growth and yield is known to be co-limiting (Sadras, 2004), where the crop's response to water and N is greater than its response to each factor in isolation (Sadras, 2005). Therefore, the availability of both should be considered when determining the requirement of the other. This is a challenge as the interaction between N and water limitations can produce confounding effects when using the spectral reflectance from canopy sensors to determine N status (Pancorbo et al., 2021). This is complicated further by the fact that drought stress can often impact N uptake from N fertiliser applications, preventing a reactive N management approach (Sjulgård et al., 2024). Proximally sensed apparent electrical conductivity (ECa) can map spatial variations in soil properties that affect water holding capacity (Domsch and Giebel, 2004; Mcbratney et al., 2005; Waine, 1999). However, these datasets are

underutilised in managing spatial variation in plant-available water, being likely due to a lack of tools to interpret how location-specific plant available water interacts with nutrient demands and local climate.

Cropping system models (CSMs) integrate soil and plant process models to simulate soil-specific changes in system states influenced by external factors including climate variation and management practices. CSMs evaluate interactions among various components, including crops, soil, and system losses (Jones et al., 2017; Keating and Thorburn, 2018). Although the potential value of CSMs for supporting on-farm N management in the UK was recognised early (Stockdale and Gaunt, 1997), initial attempts to use these approaches showed limited applicability due to poor parameterisation of available data sets and the need for improved model structures (Sylvester-Bradley et al., 2005). Despite continuing development of CSMs (Crout et al., 2014; Martre et al., 2006), they are viewed by some as “too inaccurate and undecipherable” to be trusted for practical use (Sylvester-Bradley et al., 2017, p.729). Despite this, they are increasingly seen as valuable potential tools for future decision support in N management (Powlson, 2021). This is further been supported by studies demonstrating their applicability across various agro-ecological conditions (Basso et al., 2011b; Morari et al., 2021; Thorp and Bronson, 2013) and a recent UK field study using the DSSAT CSM for nitrogen management in spring barley demonstrated the potential for managing N in UK field crops (Cammarano et al., 2020).

The Sirius CSM (Jamieson et al., 1998), the most extensively developed CSM for UK wheat, has shown potential as an on-farm management tool by accurately simulating fine-resolution spatial-temporal responses in crop nitrogen uptake (see section 2.6.1). It has also been integrated into an N management tool for New Zealand wheat, though it requires users to select generic soil profiles, limiting the fine-tuning of soil-specific parameters (Armour et al., 2002). Accurate spatialisation of crop models at the within-field scale remains a significant challenge. However, using targeted samples within spatially coherent management zones is often considered the most plausible approach for

balancing the need for detailed soil data with reducing the complexity and intensity of sampling for model application (Pasquel et al., 2023). However, there are few studies parametrising and evaluating CSMs as on-farm management tools, and to our knowledge, no studies have yet evaluated CSMs for simulating spatial variability in wheat within and across fields on UK farms.

Before investing in the calibration, parameterisation, and evaluation of a CSM on a farm, it is essential to establish sufficient evidence that significant spatial variation exists, and that this variation is driven by mechanisms accounted for in the chosen model, such as spatial variation in plant available water capacity (PAWC) or organic N supply. In this study, we demonstrate how on-farm yield map data, soil ECa, and weather data can be used to quantify the extent of spatial variation in PAWC and its impact on yield variability. Following this, clustering (see section 3.4.5) was used to delineate spatially coherent management zones, which were then used to parameterise the Sirius CSM across seven zones representing broader on-farm variation. The model was evaluated using on-farm yield map data and data from an on-farm monitoring study. The evaluated model was subsequently used to identify spatially appropriate N management strategies based on historical weather data.

4.4 Material and methods

4.4.1 Study site and data

4.4.1.1 Study site description

This study is situated on a commercial farm in Morley, Eastern England, owned and managed by The Morley Agricultural Foundation (52°33'35"N, 01°01'39"E, 54m altitude). The soil is classified as an Endostagnic Luvisol (World Reference Base)/Ashley association, with a sandy loam topsoil (Cranfield University, 2023). Glaciofluvial and glaciolacustrine processes have created heterogeneous soils with variable sand and gravel contents. The arable land in the region is characterised by gentle slopes, which limits runoff and makes subsurface leaching the primary pollution pathway (Cooper et al., 2020). The climate is temperate maritime, with an average rainfall of 676 mm and a mean annual

temperature of 10.3 °C. A weather dataset from 1990 to 2022 is available for the site (Clarke et al., 2024b). Winter wheat is the primary cereal crop, grown on average once every 3 to 4 years.

4.4.1.2 Management Zones from Yield Map Data

From 2009 to 2023, cereal crop yields across the farm were mapped spatially using the yield mapping features on a CLAAS Lexion combine harvester. While exact calibration records are unavailable, calibration was reported by the farm to have been conducted for each crop within a season. Systematic errors within the dataset were removed using a cleaning protocol (see section 3.4.2). Spatially coherent yield performance-based management zones were identified using a fuzzy c-means clustering algorithm with an auto-completion strategy on all wheat crops (Hassall et al., 2019). In summary, the cleaned yield data was aligned to a 15 m x 15 m resolution grid for each field to ensure co-location between years. If multiple yield values were present within a grid cell within a year, the mean yield value was calculated. Yield values for each field were standardised to have zero mean and unit variance. This data set was retained for comparison with ECa data as well as used for the delineation of management zones. The fuzzy c-means clustering algorithm was applied to each field independently. The advantage of this method is that it can account for co-location sparsity. Therefore, if a grid is missing yield values within a given year, it need not be excluded from analysis - as with conventional clustering algorithms. Cluster numbers were limited to between 2 and 6, with the exact number of clusters (management zones) within a field being chosen based on the cluster entropy. Finally, the cluster membership was smoothed to ensure coherent management zones.

4.4.1.3 Soil electrical conductivity (ECa)

Apparent Soil Electrical Conductivity (ECa) was measured across 15 fields (124 ha) using a Dualem-1S scanner (Dualem Inc., Canada). A Trimble (Trimble Inc, USA) GPS unit recorded the location of individual ECa measurements (<0.2m accuracy) (Figure 4-1A). Scanning took place in January 2023 (20/01/2023 to 23/01/2023), an on-farm cosmic-ray soil moisture sensor recorded topsoil moisture between 30.1 and 31.2% and soil temperature between 1.3 and 2.8°C

(Cooper et al., 2021) at the time of sampling. The maximum topsoil moisture recorded between May 2015 and January 2023 was 35.83%, indicating scanning occurred near field capacity. Scanning was conducted at 12-meter intervals, and interpolation was performed using ordinary kriging with a spherical variogram model, selected for its effective representation of spatial correlation. The variogram parameters were estimated using a nonlinear weighted least squares method.

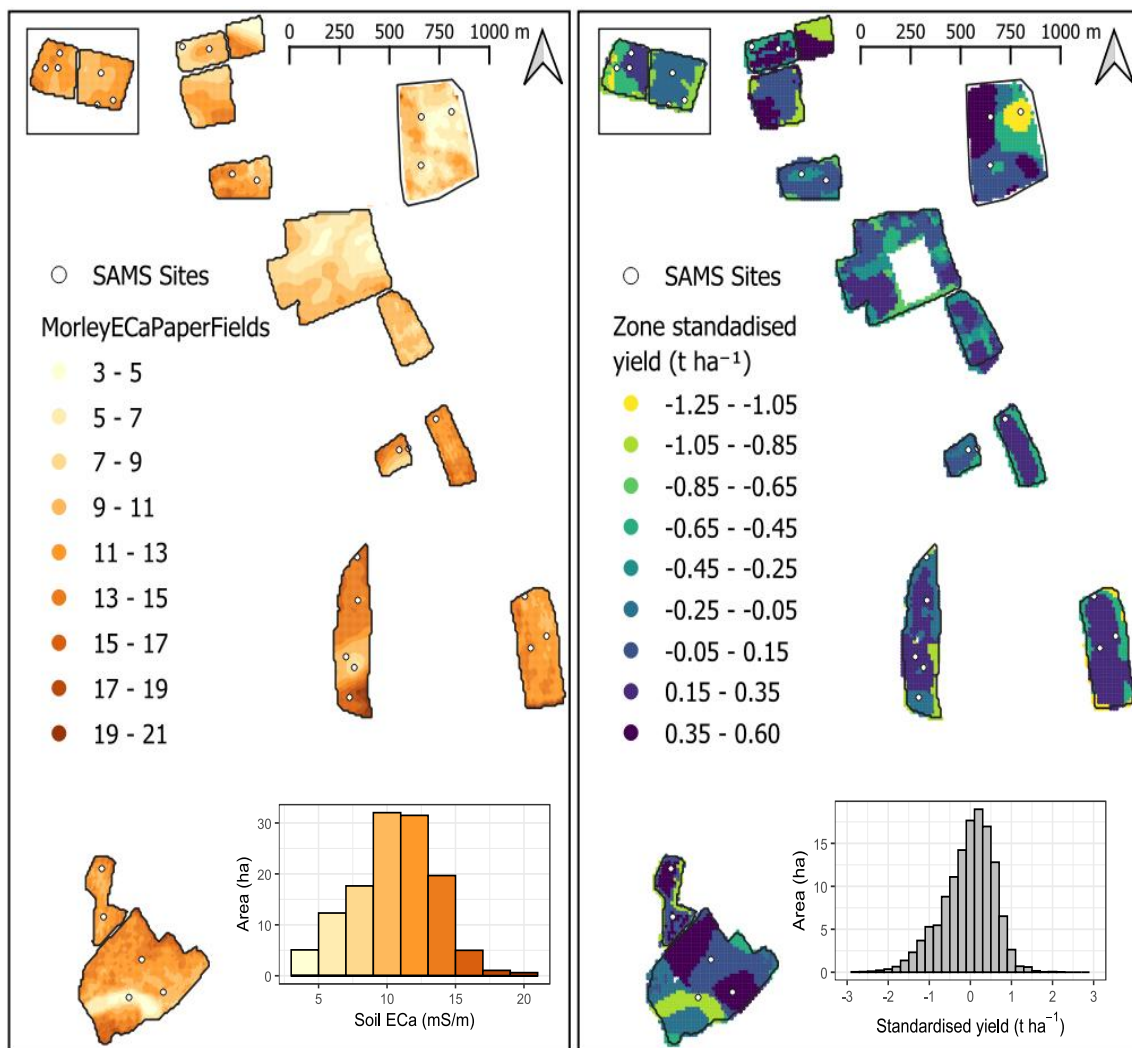


Figure 4-1 A: Kriged apparent soil electrical conductivity (ECa) and B: management zone mean standardised winter wheat yield performance (2009-2023) for smoothed clusters. Histogram insets represent distributions of the datasets. SAMS site locations are also identified on both maps.

4.4.1.4 Soil and agronomic monitoring sites

The Morley Soil and Agronomic Monitoring Study (SAMS) (TMAF, 2023) has conducted detailed monitoring of soil and crop properties at 29 spatially consistent sites annually since autumn 2018 (Figure 4-1A and B). SAMS sites were originally selected based on preliminary yield map data analysis, although this lacked the complexity or rigour of the described clustering performed in this study. Sites were situated across the range in historic yield variation within fields and across farm. Crop properties measured annually include ear populations, grain yield, mean individual grain weight, grain numbers, grain N content, straw (stem, chaff and leaf) weight and straw N content at harvest from three harvested 1m² quadrats. Each site's soil has been characterised in detail including soil particle size distribution (0-90 cm, at 30 cm intervals), determined by sedimentation, using the pipette sampling technique (Rowell, 2014). Topsoil (0-23 cm) soil organic matter has been determined annually through loss on ignition. Water retention characteristics and soil bulk density of the fine earth material (adjusted for stone content) were assessed using intact soil cores, sampled using a horizon-based sampling scheme (Zhang and Hartemink, 2017). Typically, three horizons were present and were sampled at three depths: typically, 5-10 cm (representing the historic cultivation zone of 0-30 cm), 35-40 cm (representing a 30-60 cm horizon), and 60-65 cm (representing 60-90 cm). Water contents at pressure heads between 0 kPa and -1500 kPa were measured from three replicates at each depth. Water retention curves were fitted using the Van Genuchten-Mualem model with the '*soilhyphi*' package in R. The drained lower limit (DLL, -1500 kPa) and the drained upper limit (DUL, -33 kPa) for each site was determined from these curves. Plant available water capacity (PAWC) can be interpreted as the difference between these water contents as a function of depth (Ritchie, 1981). Deeper profile sampling on farm has confirmed the rooting zone is widely >1.5m therefore the 60-90 cm profile was assumed to be representative of the deep subsoil (60-150 cm). The soils across the farm have previously been reported to contain stone content exceeding 40% of the total volume in certain areas (Clarke et al., 2024b). The high stone content makes it difficult to obtain intact soil cores, as a result some sites lack water release data

for the deep subsoil. At these sites the water release characteristics for 30-60 cm layer were considered to apply for the whole subsoil. This data extrapolation is common where data is not available for deep subsoil (Wallor et al., 2018a). The total PAWC of the three layers is the total PAWC to 1.5m (PAWC_{1.5m}).

4.4.2 Relationship between soil ECa, soil properties and spatial variation in wheat yield in response to weather

To identify the site-specific relationship between soil ECa and soil physical characteristics, the ECa from the grid cell for each SAMS site was compared to the measured soil particle size distribution and PAWC_{1.5m} using linear regression. The influence of spatial variation in ECa (the properties it is inferring) upon crop yield was assessed by comparing the gridded, standardised yield data for each year with the respective ECa value of that grid cell extracted from the ECa maps. The analysis included years with a minimum of 2 ha of grid squares for each quintile of the principal range in ECa (3-17 mS/m): 2009, 2011, 2013, 2016, 2018, 2019 and 2022. The approximate variation explained by a third-order polynomial model was used to quantify the influence of soil properties inferred through ECa on yield. This metric is calculated as 1 minus the ratio of the variance of the residuals from the third-order polynomial model to the sample variance of the yield. Specifically, it measures the proportion of the yield variance that can be explained by the polynomial relationship with soil ECa. To demonstrate the influence of weather on the response to ECa, the Standardised Precipitation Evapotranspiration Index (SPEI) (Beguería et al., 2014) was calculated from the long-term weather data set. Previous research has shown that for UK wheat crops, the SPEI correlates most strongly with drought impacts on wheat yields from April to July, with correlation strengthening as droughts extend over these months (Clarke et al., 2020). Therefore, the approximate variation explained in each year was compared with the SPEI-1 for April (the number refers to the number of previous months weather data is taken into account/accumulated i.e. SPEI-1 in April is April weather only), SPEI-2 for May and SPEI-3 for June and SPEI-4 for July (i.e. SPEI-4 for July accounts for weather for April, May, June and July).

4.4.3 Crop modelling

4.4.3.1 Fields

Previous work has shown that economic losses arising from inappropriate N rates can be modest, therefore efforts should be focused on identifying and managing fields where responses are likely to be greatest (Kindred et al., 2018). The modeling aspect of this study was situated across 3 fields (Manns, Hacketts and Perownes) (Figure 4-2). These fields were selected as they displayed some of the largest variations in both ECa and mean management zone standardised wheat yield (Table 4-1). These fields also had SAMS sites situated within defined management zones to allow for zone specific parameterisation of soil properties they have also grown winter wheat at least once since SAMS sampling

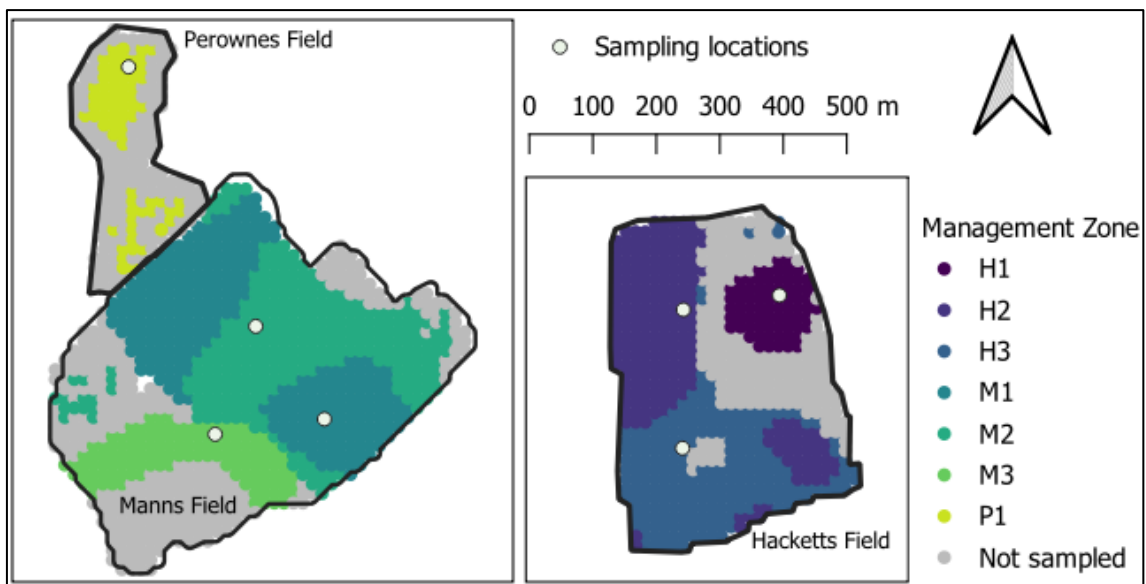


Figure 4-2 Management zones for Manns, Perownes, and Hacketts fields. Sampling (SAMS) sites, indicated by white dots, were used to parameterise Sirius for each zone. Grey areas represent management zones without a SAMS site, and therefore could not be parameterised.

commenced in 2018, therefore allow for high-level model evaluation using agronomic data collected through the SAMS study.

Table 4-1 SAMS Site corresponding management zone area, Site and management zone ECa, Site and management zone mean standardised wheat yield (2009-2022). Plant available water capacity for 150cm profile (PAWC), soil organic N (0-30cm) and percolation coefficient (Kq).

Site	MZ area (ha)	Site ECa (mS/m)	MZ ECa (mS/m)	Site yield (t ha ⁻¹)	MZ yield (t ha ⁻¹)	PAWC (mm)	N _{org} (t ha ⁻¹)	PMN (kgN ha ⁻¹)	Kq
M1	7.1	11.3	11.9	0.9	0.4	131	7.2	58	0.86
M2	7.0	13.4	12.1	0.2	0.0	111	7.1	84	0.73
M3	2.9	4.6	6.4	-1.2	-0.9	86	5.6	47	0.95
H1	1.6	4.9	5.1	-1.7	-1.1	104	4.6	32	0.95
H2	5.0	7.6	8.1	0.4	0.6	128	5.3	43	0.90
H3	5.3	6.9	9.6	0.3	0.1	126	5.6	49	0.91
P1	1.6	10.6	11.6	0.7	0.6	137	9.2	96	0.83

4.4.3.2 Sirius parameterisation

Sirius (2023) is a process-based model consisting of various sub-models describing soil and crop processes for wheat crops on a daily time step (Jamieson et al., 1998). Sirius has undergone significant development within the UK context, particularly in simulating nitrogen effects (Sylvester-Bradley et al., 2005). Phenological development is modelled with photosynthesis and biomass production derived from photosynthetically active radiation and radiation use efficiency. N levels, water limitations and heat stress all accelerate leaf senescence, reducing photosynthesis and grain yield, while stresses occurring during sensitive growth stages such as flowering can reduce primary grain number while grain size can be limited by stresses during endosperm development and grain filling (Senapati et al., 2019b, 2019a; Stratonovitch and Semenov, 2015).

Sirius requires detailed descriptions of soil parameters to simulate nitrogen and water processes effectively. Given the high stone content in soils at Morley, as indicated by previous studies (Clarke et al., 2024b), more detailed measurements were necessary since the small diameter cores fail to capture this variability accurately and can only be used to interpret water release characteristics of the fine earth material. At each site, soil was extracted to 90cm using a post hole borer. Large (5kg) bulk soil samples were collected at 30 cm intervals containing both fine earth and stones. Stone volume was measured by water displacement after 2 mm sieving. The DUL and DLL, of the fine earth material for each layer were derived from water release characteristic curves of intact soil cores. Saturation moisture content (SAT) was derived from the fine earth soil bulk density of the intact soil cores (Sylvester-Bradley et al., 2005). Organic N stocks were calculated using the topsoil organic matter adjusted for soil bulk density. Soil organic N was assumed to be 5.38% of soil organic matter (Heming, 2021). The volumetric water contents of the fine earth DUL, DLL and SAT and topsoil organic N were adjusted based on stone volume measurements from the pit excavations. A percolation coefficient (K) for each soil was estimated using the nonlinear relationship with profile average clay content (Addiscott and Whitmore, 1991) with a maximum of 0.95.

4.4.3.3 Sirius evaluation

The Sirius model was evaluated in two stages. Firstly, the simulated site yields were compared with the observed management zone mean yield from the combine yield maps. This high-level evaluation tested the accuracy of the Sirius model's parameterisation using soil properties measured at individual sampling points within each zone to accurately represent the mean yield of the entire management zone. For sites in Mann's Field (M1, M2 and M3) this included five years of data (2009, 2013, 2014, 2016, and 2019). For Hackett's Field, four years of data (2011, 2016, 2019, and 2022). In Perownes Field, five years of data was available (2009, 2011, 2014, 2016, and 2019). Across these years, five Group 4 feed winter wheat cultivars were grown: cv. Oakley, cv. JB Diego, cv. Relay, cv. Evolution, and cv. Saki. The Sirius model has previously been calibrated and validated for cv. Claire (Clarke et al., 2020; Senapati et al., 2019b). Since this

calibration has been demonstrated to be representative of modern elite UK wheat cultivars, including those mentioned above (see appendix D.1), they were used without further calibration. The effectiveness of yield map data for evaluation is limited by its accuracy and to a single measure, but it is representative of the data available for model evaluation across commercial farms. In this stage, Sirius was parameterised only with observed drilling date, N rate, and N fertiliser application timings. Plant populations and ear numbers were set to the Sirius defaults: 300 plants and 500 heads per m².

In the second stage, a more detailed and thorough evaluation was conducted using data collected as part of the SAMS study. This involved data collected from sampling sites in Mann's Field and Perownes Field in 2019, and Hackett's Field in 2019 and 2022. The combine yield map value for the 15 m² grid cell at each site was extracted. At harvest, the three 1m² quadrats yields were used to validate the combine yield map data. This comparison indicated the absence of major errors, and therefore the combine yield map values for each site were used for evaluation. The threshed grain samples were analysed for grain N content and mean individual grain weight. Grain number was calculated from grain yield and individual grain weight. Plant populations were counted in the autumn, and ear numbers were recorded prior to harvest; these parameters were then used to parameterise Sirius (see appendix E.1). We recognise that such data may frequently not be available for evaluation purposes, and therefore to quantify their importance for accurate modeling within Sirius, the evaluation was also run with Sirius default plant populations and ear numbers.

Data on soil moisture content and soil mineral N content at sowing were not available for either evaluation procedure. However, dry periods in the autumn have been shown to have little effect on simulated wheat yields in Eastern England, as a positive water balance generally occurs during the winter (Clarke et al., 2020). Therefore, simulations were run assuming no soil moisture deficit at sowing. A realistic estimate of 50 kg N ha⁻¹ was used for autumn soil mineral N content at sowing (Clarke et al., 2024a). Atmospheric CO₂ concentrations were set according to recorded levels for each year (NOAA, 2024). Model performance

was evaluated using linear regression, with the coefficient of determination (r^2), root mean square error (RMSE), and relative root mean square error (RRMSE) as evaluation metrics (See equation 2.3) .

4.4.3.4 Application of Sirius to support N management

To determine the simulated NOpt for each of the seven management zones, nitrogen application rates ranging from 0 to 360 kg N ha⁻¹ were simulated at 1 kg N ha⁻¹ intervals for each year of the 29-year weather dataset, resulting in a total of 80,864 simulations. Sirius requires the user to define ear numbers when they are expected to fall below the threshold of 500 ears m⁻². Previous work at Morley has shown that soils with lower ECa soils typically support lower ear populations on average (see section 2.5.1.2). This trend was also observed in ear counts from the 2019 and 2022 SAMS sites, where sites H1 and M3 had the lowest tiller numbers within their respective fields (Appendix E1). However, the SAMS dataset lacks the temporal length to generate representative long-term averages, therefore ear numbers for each site were set based on those recorded in the 2019 season. Since 2019 was a high-yielding year with good establishment and tiller survival, these values were used to represent a best-case scenario for each site. The ear numbers for H1 in 2019 were impacted by grass weed pressure; therefore, these were adjusted to 400 plants m⁻² to align more closely with the numbers on M3, with a similar ECa and PAWC.

A margin over N application was calculated for each simulation using the 2024 average feed wheat grain price and Nitram (34.5%N) fertiliser price (AHDB, 2024b). Environmental implications were quantified through the Fertiliser-N recovery Efficiency (RE_{fertN}) metric (Dobermann, 2007) using equation 4-1:

$$RE_{fertN} = \frac{(\text{Plant } N_N - \text{Plant } N_0)}{\text{Fertiliser N}} \times 100 \quad (4-1)$$

Where; Fertiliser N is the amount of N fertiliser applied (kg N ha⁻¹), Plant N_N is the total N uptake at harvest with the given N fertiliser rate, Plant N_0 is the total N uptake at harvest with zero fertiliser, representing soil N supply alone. Additionally, the Unutilised N (N_{un}) was calculated using equation 4-2:

$$N_{un} = (N_{min} + N_{fert} - N_{leach}) - \text{Plant } N_N \quad (4-2)$$

Where; in kg N ha⁻¹, N_{min} is the mean simulated mineralised N, N_{fert} is the N applied as fertiliser, N_{leach} is the simulated N lost through in season leaching and Plant N_N is the total plant N uptake at harvest.

Additionally, the greenhouse gas (GHG_N) emissions (CO₂e) per tonne of grain associated with N fertiliser use were estimated using the simulated NOpt and its respective yield. It was assumed that 3.3 kg CO₂e emissions are associated with each kg of applied N as a result of nitrous oxide emissions (Kindred et al., 2021; Sylvester-Bradley et al., 2009). A figure of 3.5 kg CO₂e per kg of applied N was used for the manufacturing emissions of ammonium nitrate fertiliser (Kindred et al., 2021).

The greenhouse gas emissions associated with nitrogen fertilisation were calculated using the following equation 4-3:

$$GHG_N \left(\frac{CO_2e}{t} \text{ of grain} \right) = (N_{fert} \times 6.8) \div y \quad (4-3)$$

Simulated margin over N, RE_{fertN}, N_{un} and ... derived from model derived NOpt were compared to the simulated values for the historic farm standard uniform N rate of 218 kg N ha⁻¹ across all zones (StdN₂₁₈), based on the mean NOpt identified through randomly distributed N response experiments on site (Kindred et al., 2018). Additionally, this was compared to the mean simulated NOpt of all sites, weighted by the size of the management zone as proportion of the whole study area (StdN₁₉₄), this represents a uniform model derived rate for comparison

4.5 Results

4.5.1 Spatial variation in soil ECa and soil physical properties

Soil ECa across the 126ha ranged between 3.2 ms/m and 20.9 ms/m, exhibiting a broadly unimodal distribution with a large proportion of the surveyed area falling between 10-15ms/m (Figure 4-3). While some fields display relatively

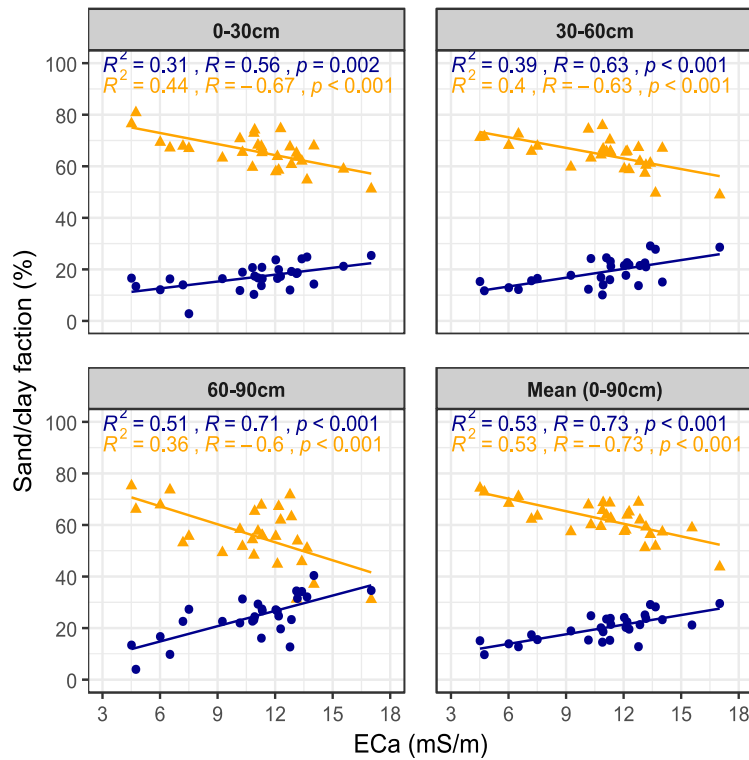


Figure 4-3 Relationship between soil electrical conductivity (ECa) and sand/clay faction at different soil depths (— Clay — Sand).

homogenous distribution in ECa others display more heterogeneity, with clear structural variation in ECa within fields. Using the SAMS sites data, soil electrical conductivity (ECa) is shown to correlate significantly with variations in clay and sand content (Figure 4-3). The strongest correlations occur for the mean clay and sand content over the 0-90 cm profile ($r^2 = 0.53$ and $r=0.73$). Generally, as ECa increases, clay content increases from 9.7 % to 29.5%, while sand content decreases from 43.7% to 74.3%. There is a moderate, but significant positive correlation between $PAWC_{150}$ and soil ECa (Figure 4-4). This indicates that as soil ECa increases it can be expected that PAWC will also increase. However, the relationship between soil ECa and PAWC is weaker than those for texture.

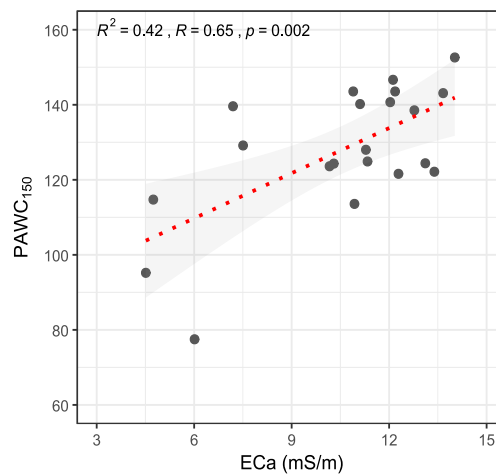


Figure 4-4 Relationship between plant available water capacity and soil ECa for 22 SAMS sites. Headland sites removed from analysis due to high levels of compaction

4.5.2 Relationship between soil ECa and spatio-temporal variability in yield

The relationship between soil ECa and standardised yield is positive in most years, with higher ECa values often associated with higher yields within fields (Figure 4-5). This positive correlation is observed up to approximately 9 mS/m. The strongest responses quantified using a third order polynomial regression are observed in 2011 and 2013 with 0.33 and 0.35 of the approximate variance explained, respectively. The years 2009, 2019 and 2022 show a similar trend, with slightly lower variance explained (0.24 to 0.29). In 2016 and 2018, the response to ECa was much weaker.

The relationship between the SPEI for April-1, May-2, June-3, and July-4, and the variance explained in the relationship between soil ECa and yield indicates that the yield response to soil properties associated with ECa is influenced by seasonal variation in weather conditions (Figure 4-6). Of the years analysed the April-1 SPEI value has the strongest correlation with the response of yield to ECa. However, these correlations are strongly influenced by the wet Aprils (April-1

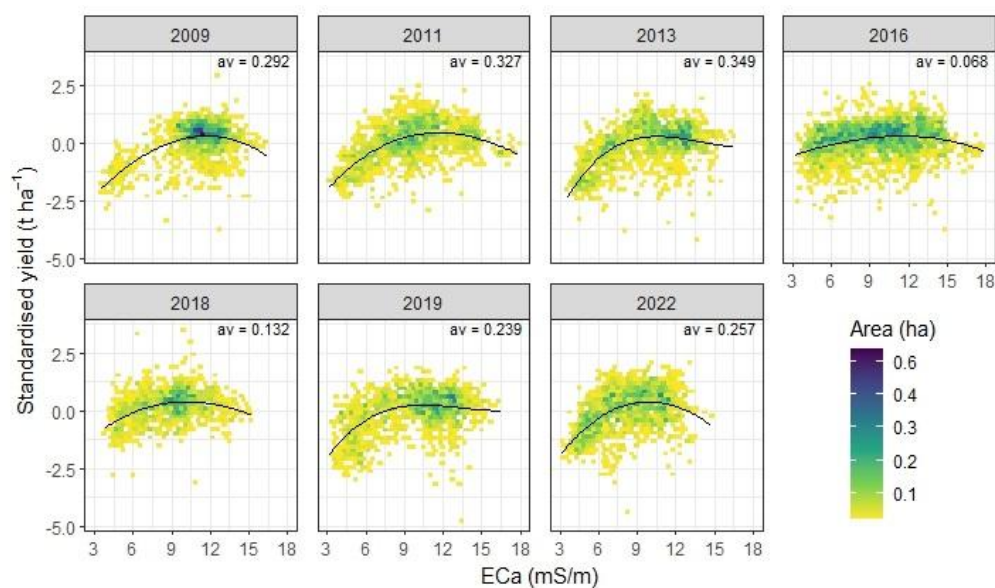


Figure 4-5 Hexagonal plots of 15 x 15m grid standardised yield vs. grid soil ECa for years with sufficient wheat area across observed variation in ECa

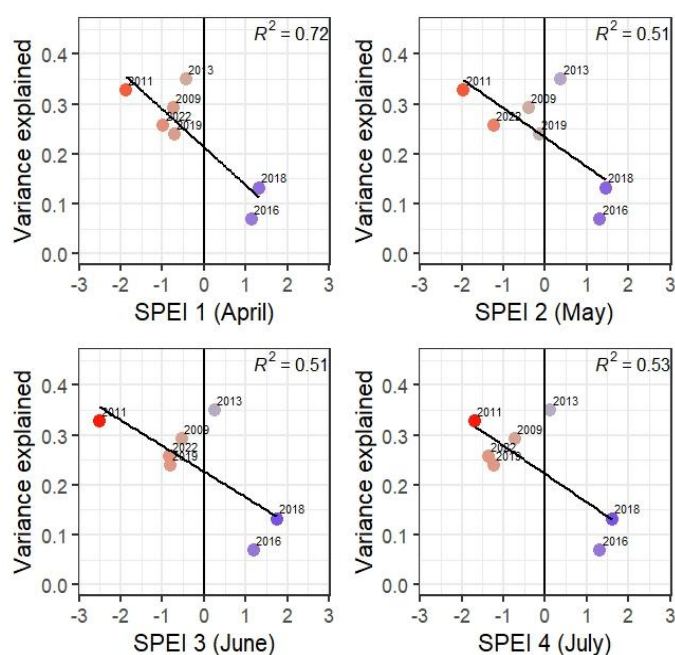


Figure 4-6 relationship between SPEI across key winter wheat growth (clockwise: SPEI 1 (April), SPEI 2 (May), SPEI 3 (June) and SPEI 4 (July)) and the approximate variation explained by the polynomial regressions for Soil ECa against combine yield maps

SPEI >1) of 2016 and 2018 following which the relationships between soil ECa and standardised yield are weakest. These years also maintained overly wet conditions over following months with the SPEI remaining < 1 in all lags. Above an SPEI of 0 at all lags there appears to be limited correlation to variance explained.

4.5.3 Sirius model evaluation

4.5.3.1 Management zone yield map data

Sirius simulated yield, as compared to observed management zone mean yield, was derived from combine yield map data, with an accuracy of 1.59 t ha⁻¹, equivalent to an RRMSE of 17.21% (Figure 4-7A). Simulated yields were closely aligned with observed management zone mean yields in 2009, 2014, and 2019, which were years with some of the highest observed yields. Sirius also accurately simulated the lower yields observed in 2022 and 2011, although there was a slight underestimation in these years. In 2013, the simulated yields were lower than those recorded using the combine harvester yield map data. The largest discrepancies were noted in 2016, where simulated yields were significantly higher than the management zone mean yield at all sites.

The mean across all years showed very close agreement with observed yields, particularly for the sites in Manns Field (Figure 4-7B). The highest simulated yields on average were in M1, while the lowest simulated yields were in M3, consistent with the observed management zone yields for those sites. The yields in P1, although slightly underestimated by Sirius, were in good agreement with observed data. Sirius simulated the mean average yield for H2 well, while the simulated yields for H1 were higher than observed but remained lower than those for H2, as recorded in the yield map data. Yields for H3 were slightly underestimated by Sirius.

4.5.3.2 SAMS Site data evaluation

The analysis of crop properties collected in 2019 and 2022 enabled a detailed evaluation of the performance of Sirius in simulating spatial-temporal variability in yield and plant N components with parameterisation for observed plant and ear

populations (Figure 4-8). Sirius demonstrated limited ability to simulate variations in individual grain weight, with an r^2 value of 0.22. The model notably simulated lower grain weights in 2022 compared to 2019. Despite this limitation, the simulated errors were within an acceptable range, with an RRMSE of 19.26% (Figure 4-8A). Sirius simulated the spatial-temporal variability in grain numbers across sites with a greater degree of accuracy, with an RRMSE of 8.52%, indicative of excellent model performance. The spatial-temporal variations in grain numbers were generally well captured, with an r^2 value of 0.50. The largest errors occurred at the M2 site in 2019 and the H2 site in 2022 (Figure 4-8B).

When the two yield components were combined for overall grain yield, Sirius demonstrated a good level of yield prediction accuracy, with the spatial-temporal variation in yield well captured, reflected by an r^2 value of 0.65 and an RRMSE of 14.71% (RMSE = 1.34 t ha⁻¹) (Figure 4-8C). The H2 and H3 sites in 2022 had the

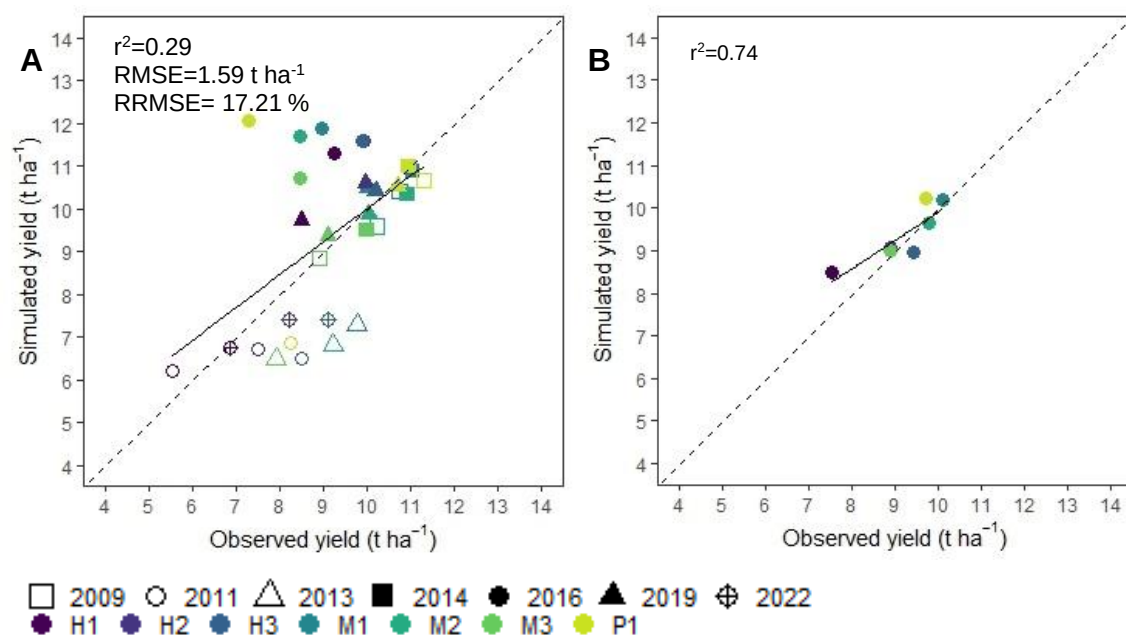


Figure 4-7 A: Observed mean management zone yield from combine yield maps compared to Sirius simulated yield for the respective sampling sites within this zone. **B:** The overall mean observed and simulated yields for each management zone and site, respectively. Colours in and B represent the management zone (H = zones in Hacketts field, M = zones Manns field and P = zone Perownes field), while the shapes in A represent year

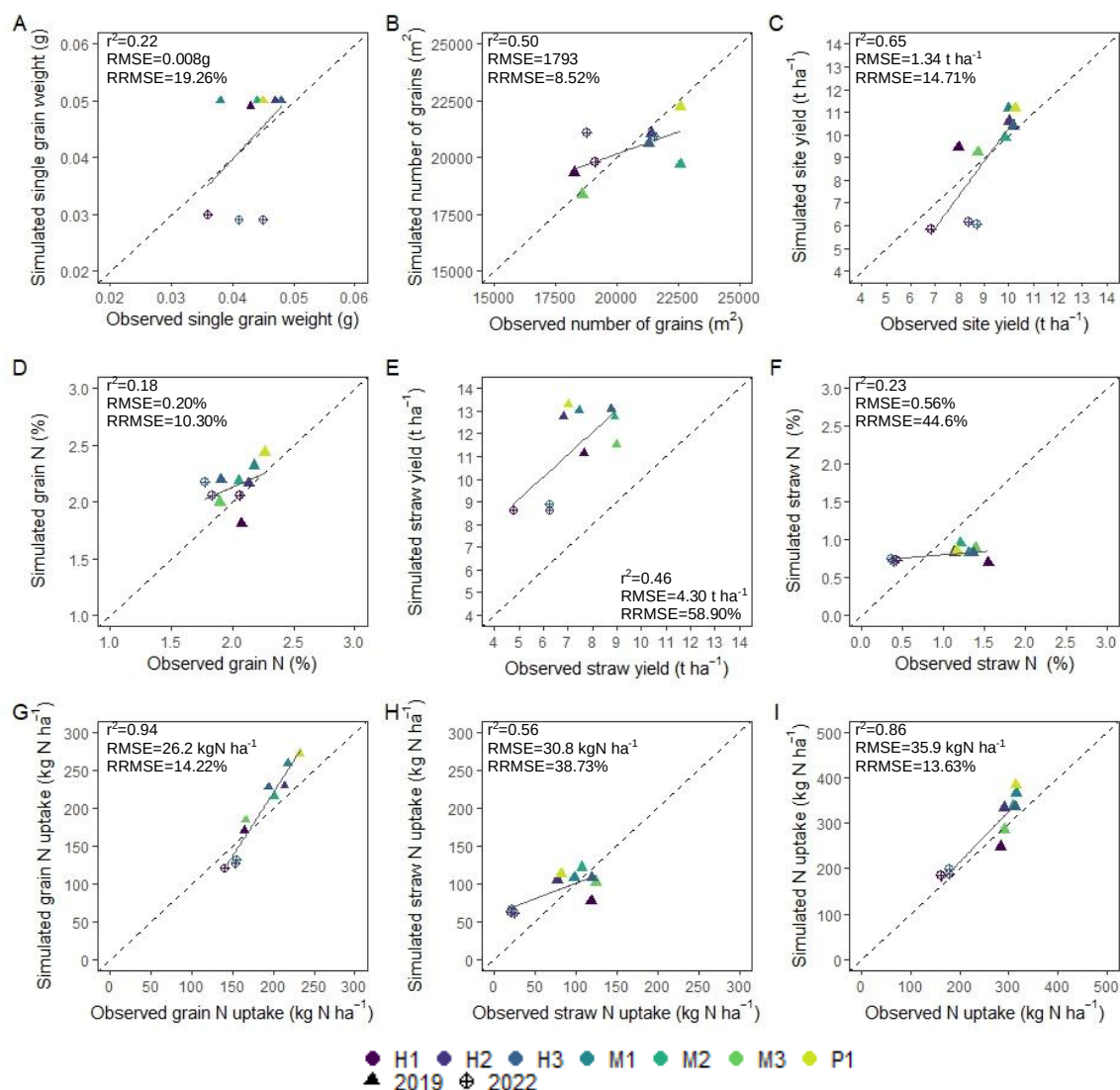


Figure 4-8 Observed and simulated crop properties for the seven SAMS sites (shapes) in 2019 and 2022 (colours) with parameterised plant populations and ear numbers; A: single grain weight, B: number of grains, C: site yield, D: grain N concentrations, E: straw (stem, leaf and chaff) yield, F: straw N concentrations, G: grain N uptake at harvest, H: straw N uptake at harvest, I: total N uptake at harvest.

largest simulated errors. Grain N concentration was simulated with a good level of overall accuracy (RRMSE = 10.3%), with a relatively small error of 0.2% RMSE. However, the spatial-temporal variability was poorly captured, as indicated by a low r^2 value of 0.18 (Figure 4-8D). Sirius simulated non-reproductive above

ground plant (straw) biomass and N concentrations poorly, with a RRMSE of 58.9% and 44.6% respectively (Figure 4-8E and Figure 4-8F). Sirius exhibited good performance in simulating grain N uptake, with an r^2 value of 0.94, indicating that the spatial-temporal variations were captured very well. The model's predictions closely aligned with observed values, as reflected by an RRMSE of 14.22% and an RMSE of 26.42 kg N ha⁻¹ (Figure 4-8G). While Sirius broadly captured the trends in spatial-temporal variation in straw nitrogen (N) uptake, with an r^2 value of 0.56, the high RRMSE of 37.37% and corresponding RMSE of 30.8 kg N ha⁻¹ indicate that the model generally performed poorly in simulating straw N uptake (Figure 4-8H). Overall, Sirius demonstrated a good level of accuracy of simulating total N uptake, with an r^2 value of 0.86 and a RMSE of 35.93 kg N ha⁻¹ (Figure 4-8I).

For comparison the evaluation was performed assuming plant populations and ear numbers were not known (Figure 4-9) i.e., not parameterising Sirius with observed agronomic data. Slightly improved grain weight predictions (RRMSE = 15.3%) however resulted in poorer grain number predictions (RRMSE=10.7%). Although overall grain yield predictions improved by RMSE of 0.53 t ha⁻¹. Errors for simulated grain N, straw yield, grain N uptake, straw N uptake and total N uptake all increased, however, small improvements in observed straw N content was recorded.

4.5.4 Sirius model application

Simulated NOpt varied across the different management zones, ranging from 163 kg N ha⁻¹ in M3 to 216 kg N ha⁻¹ in M1, with a mean value of 194 kg N ha⁻¹ across all zones (Figure 4-10, Table 4-2). Significant temporal variation in NOpt within zones was observed, though spatial influences also contributed to the variance. For example, M3 had the smallest interquartile range in NOpt, which was less than half the size of that in P1 and H1. A mean margin improvement of £5.1 per hectare was simulated compared to the farm standard of 218 kg N ha⁻¹, with improvements in margins ranging from £19.35 to £2.13 per hectare. However, when compared to the mean simulated NOpt of 194 kg N ha⁻¹ applied uniformly,

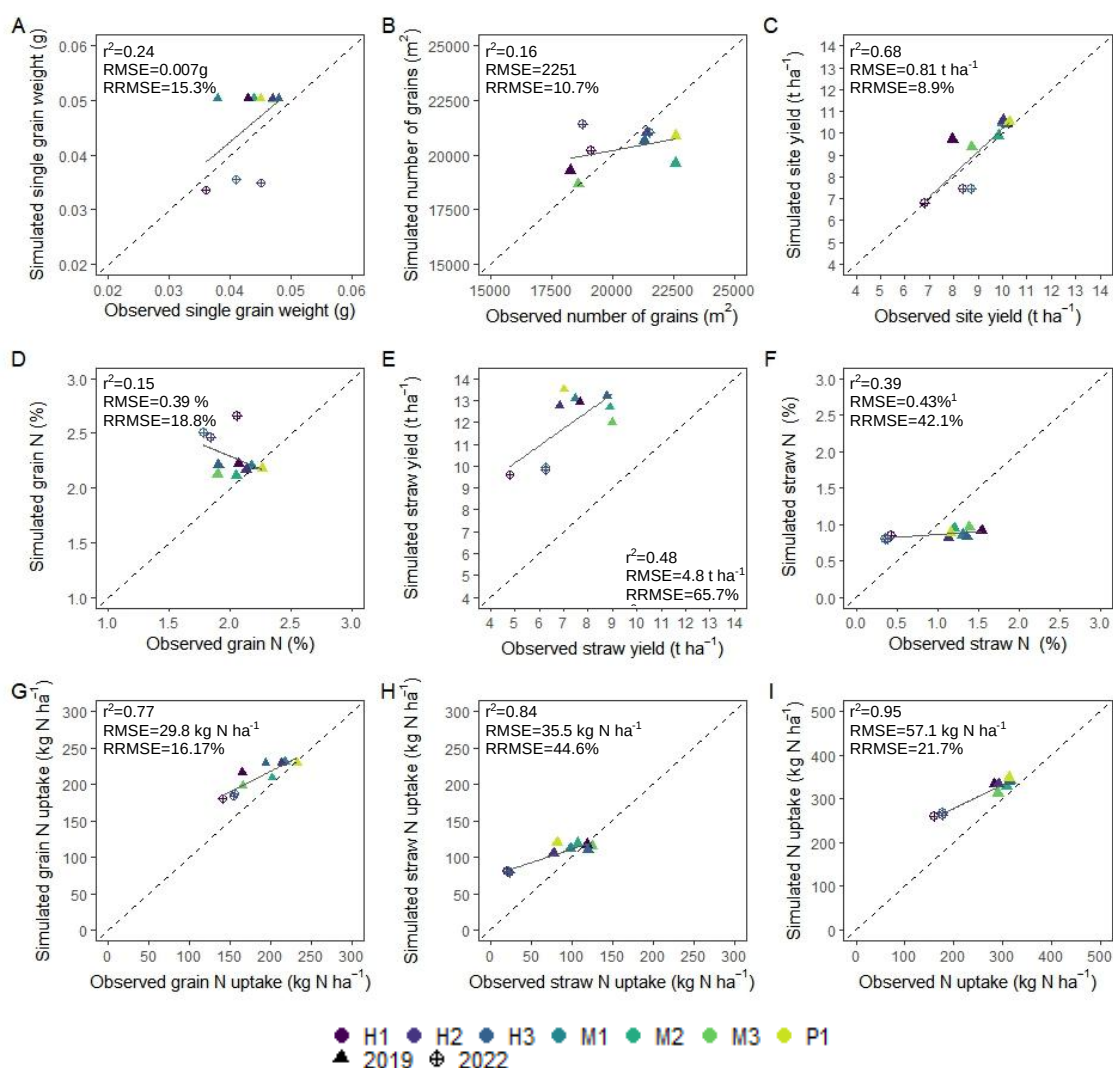


Figure 4-9 Observed and simulated crop properties for the seven SAMS sites (shapes) in 2019 and 2022 (colours) not parameterised with plant populations and ear numbers; A: single grain weight, B: number of grains, C: site yield, D: grain N concentrations, E: straw (stem, leaf and chaff) yield, F: straw N concentrations, G: grain N uptake at harvest, H: straw N uptake at harvest, I: total N uptake at harvest.

the simulated economic benefit was smaller, averaging £2.22 per hectare, and ranged from £6.96 to £0 per hectare.

REfertN increased by an average of 3.6% compared to the standard N rate of 218 $kg\ N\ ha^{-1}$, with improvements ranging from 0.3% to 11.1%. However, the REfertN gains were much smaller when compared to the uniformly applied

simulated N rate, with an average increase of just 0.4%, ranging from -1.9% to 5.9%.

Unutilised N at the simulated NOpt ranged from 43.1 to 69.9 kg N ha⁻¹. Compared to the standard 218 kg N ha⁻¹ rate, this represented a reduction of 10.6 kg N ha⁻¹ on average. The reduction was much smaller (0.8 kg N ha⁻¹) when compared to the uniform applied simulated mean NOpt. Applications of simulated NOpt across the 29 years for each management zone would have resulted in a reduction in CO2e emissions associated with the N fertiliser. Compared to the simulated blanket rate of 218 these savings were simulated to be on average 13.8 kg CO2e/t of grain.

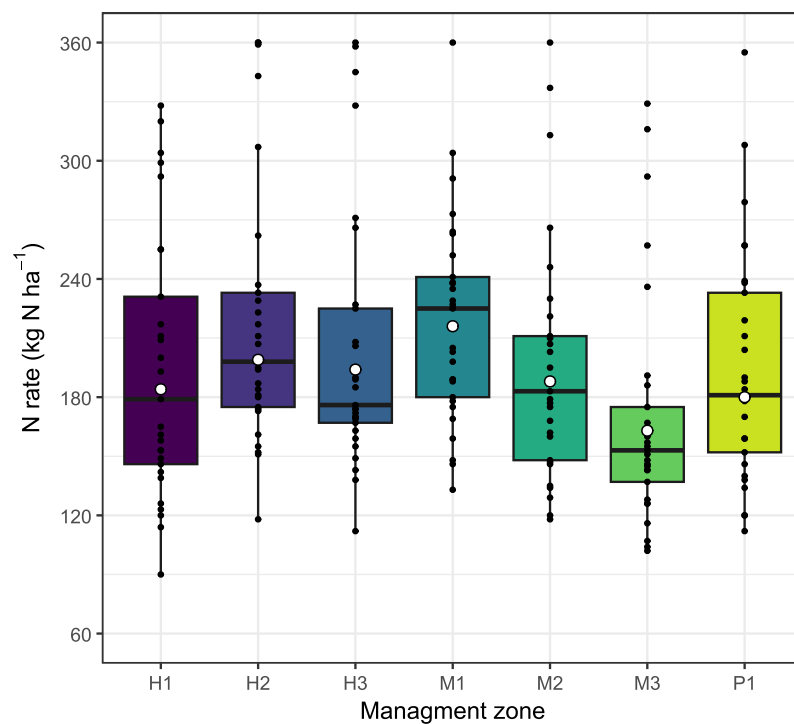


Figure 4-10 Nitrogen fertiliser rate with the largest economic return in each year (black dots) for each management zone/SAMS site. White circles represent the N rate with the largest mean margin across the 29 years simulated. The rectangular boxes represent the interquartile range, spanning from the 1st quartile to the 3rd quartile, with the horizontal line inside indicating the median. The whiskers extend to the minimum and maximum values within 1.5 times the interquartile range.

Table 4-2 Simulated NOpt (kg N ha⁻¹), Fertiliser-N recovery Efficiency (RE_{fertN}), Unutilised N (N_{UN}) and greenhouse gas emissions associated with N fertiliser applications per tonne of grain (GHG_N) for each zone. The difference between simulated NOpt, farm standard N rate of 218 kg N ha⁻¹ (Std N₂₁₈), and the mean simulated NOpt of 194 kg N ha⁻¹ (SStd N₁₉₄) for margin, RE_{fertN} and N_{un} across 29 years of observed weather. Means are weighted by management zone area so are representative of the entire 30 ha.

					Margin difference (£)		RE _{fertN} difference (%)		N _{un} (kgN ha ⁻¹)		GHG _N (CO ₂ e/t)	
Zone	NOpt (kg N ha ⁻¹)	Yield (t ha ⁻¹)	RE _{fertN} (%)	N _{un}	Std N ₂₁₈	SStd N ₁₉₄	Std N ₂₁₈	SStd N ₁₉₄	Std N ₂₁₈	SStd N ₁₉₄	Std N ₂₁₈	SStd N ₁₉₄
M1	216	11.6	87.8	60.2	2.28	3.54	0.3	-1.9	0.7	-6.3	-1.3	11.6
M2	188	10.8	87.0	60.5	2.13	1.40	4.5	0.8	13.6	2.2	-17.2	-3.5
M3	163	9.9	86.8	46.9	19.35	6.96	11.1	5.9	31.1	15.4	-35.1	-19.7
H1	184	10.3	87.1	44.5	8.70	1.53	6.6	1.8	18.7	4.8	-20.6	-6.1
H2	199	11.4	91.6	43.1	4.26	1.45	2.0	-0.5	5.8	-1.3	-10.5	2.6
H3	194	11.2	90.3	45.2	4.89	0.00	3.2	0.0	9.3	0.0	-13.4	0.0
P1	180	11.5	85.8	69.9	3.95	0.89	4.9	1.7	16.0	5.1	-20.6	-7.5
Mean	194	11.1	88.4	53.3	5.1	2.20	3.6	0.4	10.6	0.8	-13.8	-0.3

4.6 Discussion

4.6.1 Sirius as a spatial N management tool

This study evaluates the Sirius CSM as a spatial N management tool, demonstrating its potential to simulate within-field variation in wheat yield, nitrogen uptake, and crop performance across commercial fields. Using management zones derived from yield map data and soil electrical conductivity measurements, the model was parameterized to assess spatially targeted N applications.

4.6.1.1 Model evaluation for describing management zone performance

Overall, the use of soil parameters from a single site within a management zone to parameterise Sirius resulted in acceptable simulated yields compared to the mean management zone yield, although accuracy varied by year. Notably, Sirius overestimated yields at all sites in 2016. For Perowne's field (P1), which had the largest errors in 2016, which was its fourth successive winter wheat crop, increasing the risk of yield limiting diseases such as take-all decline.. Disease pressure (*Zymoseptoria tritici*) in 2016 was high. In experiments at Morley, a two-spray fungicide program, typical of that used on farm, recorded on average 9.7% leaf area infected (NIAB TAG, 2016). This level of disease has the potential for significant yield loss, , with yield loss estimated at 0.67% for every 1% of leaf area infected(Gosling and Roberts, 2017). This could explain the overestimation of yields at all sites in 2016. The overestimation of yield for H1 in 2019 is likely a result of large grass weed (*Lolium multiflorum* L) pressures recorded, through monitoring from the Morley SAMS project. Sirius does not account for yield losses resulting from disease or weed pressures therefore errors are more likely in simulation results when such agronomic pressures are present.

Measurement error can be a significant, unknown factor in evaluating crop models. Commercial yield map data has been shown to potentially contain significant systematic errors (Arslan and Colvin, 2002; Clarke et al., 2024a). Therefore, it is recommended that validation exercises using yield map data

should serve as a guide to the overall model performance by interpreting spatio-temporal yield trends rather than as an in-depth evaluation of the model structure.

When comparing the across-year mean yields for each site with those simulated by Sirius, the spatial trends in yield performance are well described. Historically, attempts to spatially parameterise crop models have relied on intensive grid-based sampling, even the least intensive often requiring approximately one sampling location per hectare (Chen et al., 2021; Johnen et al., 2014; Tewes et al., 2020a). While management zones have been proposed as a viable method for spatialisation, these approaches frequently involve multiple sampling points per zone (Albarenque et al., 2016; Cammarano et al., 2020; Tagarakis et al., 2019). This, however, increases the sampling intensity, making it less applicable due to the high labour and laboratory costs. Efforts to use single-zone sampling for parameterisation have been explored (Nijbroek et al., 2003; Wong and Asseng, 2006), but have been limited in the extent of model evaluation. Our study advances this body of work by demonstrating that a single sampling point within each management zone can be an effective method of crop model parameterisation. The model was evaluated across multiple years and found that, while some discrepancies emerged within individual years, the spatial variation in yield performance within management zones was well captured over time. While there is still significant expense in model set up, and obtaining zone specific soil parameters, many of these measures can be deemed temporally stable and, therefore, can be applied over many years, justifying this set-up expense (Sylvester-Bradley et al., 2005). The data can also be used for other targeted management decisions such as mapping spatial variation in soil carbon (Clarke et al., 2023) (see Appendix H). More temporally unstable parameters such as soil organic N can be sampled more frequently with costs offset against environmental schemes supporting farms in mapping topsoil properties by management zone (DEFRA, 2023c).

4.6.1.2 Model evaluation for site yield components and N uptake

To our knowledge cropping system models have not previously been assessed for describing spatial and temporal variation within fields for wheat in the UK.

While international evaluations have often focused solely on final grain yield, only a limited number of studies have assessed CSMs' ability to capture spatial variation in N uptake components, and those that do often concentrate on grain N uptake (Albarenque et al., 2016; Cammarano et al., 2020). This represents a significant gap, as many models simulate yield by accounting for the impacts of stresses and resources on specific yield components, which are influenced by different response variables. In the observed data, variation in grain number was the major contributor to differences in grain yield between sites (see appendix E.2), consistent with other studies analysing components of yield variation (Xie and Sparkes, 2021).

Sirius acceptable accuracy in simulating grain yield was largely due to its ability to simulate grain numbers well, rather than individual grain weight. In Sirius, the simulated grain number is a function of the dry mass accumulated in the ears prior to anthesis. Therefore, stresses reducing ear biomass before anthesis will lead to lower simulated grain numbers, along with heat stress response factors after anthesis (Stratonovitch and Semenov, 2015). Modellers directly influence grain numbers through two main parameters in Sirius: a parameter related to the ratio of ear weight at anthesis and grain numbers, and the number of ears specified in the simulation run. The former could not be addressed in this study as it would require detailed comparisons to assess the accuracy of the parameters for cv. Claire relative to the varieties grown in the study. Ear number is a key factor in determining final grain number (Darwinkel, 1978). Sirius does not simulate final ear numbers; instead, users can manually restrict this as a parameter. When the default 500 tillers per m² were inputted for all sites and years, Sirius' ability to simulate grain number was poorer. This is a noticeable limitation of Sirius for spatial applications. Ear numbers have been shown to be influenced by spatial variation in soil properties (see section 2.5.1.2). Therefore, to optimise Sirius' accuracy for spatial modelling, users would require prior knowledge of likely spatial variation in ear numbers - a crop parameter not easily measured. However, remote sensing techniques (Madec et al., 2019) or targeted counts in representative areas of management zones, as performed in this study, could improve the spatial applicability of Sirius.

Sirius demonstrated limited accuracy in simulating individual grain weight. Grain weight is calculated by assuming all new dry matter post-anthesis is allocated to grains, with up to 25% of the dry matter from vegetative organs at the end of the cell division stage available for transfer to the grain. Therefore, stresses before anthesis reduce this potential pool, while post-anthesis stresses reduce grain dry matter accumulation. In 2022, grain weight was significantly underestimated, leading to an underestimation of grain yield across all sites. Few studies have evaluated Sirius' ability to simulate individual grain weight, making it difficult to determine if this is a structural issue within the model or misparameterisation or simply a result of interactions within the dataset that were not accounted for. However, previous work using the closely related Sirius Quality CSM also reported lower accuracy in simulating single grain weight compared to grain number (Martre et al., 2006), suggesting that Sirius struggles more with grain weight variability. Grain number acts as a coarse-tuning mechanism, strongly influencing yield by responding to environmental conditions, whereas grain weight serves as a fine-tuning mechanism, predominantly affected by conditions post-flowering (Golba et al., 2013). One potential source of error could be discrepancies in the anthesis date; if phenological development is simulated incorrectly, stresses might impact crops at critical growth stages that were not observed in reality. While the parameters for cv. Claire have shown good accuracy in simulating harvest dates for UK wheat (see section 2.5.2.1), evaluating observed flowering and maturity dates in this dataset would have enhanced the assessment and allowed for a more detailed analysis of how specific stress events influenced simulated yield components. These measurements are now included in the SAMS monitoring programme to improve future modelling applications.

Grain N has a significant influence on total N offtake (Barraclough et al., 2010) and is a key component of NUE metrics (Congreves et al., 2021). Despite this, there have been few studies spatially validating CSM for simulating grain N concentrations (Albarenque et al., 2016; Cammarano et al., 2020; Moral et al., 2010). Sirius generally simulated grain N concentrations well, although with a slight overestimation, with the largest error at the H1 site in 2019, likely influenced

by grass weed pressures. The poorer model performance for grain N concentrations when plant and ear numbers are not parameterised can be explained by the mechanism through which N is partitioned within biomass in Sirius (Jamieson and Semenov, 2000). Grain N can increase when supply from the soil or the rest of the plant is high. Therefore, when tiller numbers are increased (as they were at all sites in 2022 by using default values), this logically increases the supply of N to the grain from stem and leaf biomass reserves, especially in years when grain yield is limited, as seen in comparison to yields of 2019. This loss of accuracy outweighs the improvement in overall yield simulation when calculating grain N offtake. This demonstrates the importance of evaluating a model's performance in simulating other crop components besides yield when used to inform N management.

Even accounting for small errors in the observed measurement data, such as biomass shedding during cutting or incomplete removal of straw down to the crown, straw biomass at harvest was poorly simulated. Previous studies have shown that Sirius can greatly overestimate biomass under optimal conditions (Sylvester-Bradley et al., 2005, Crout et al., 2014), and other structurally similar models have also been demonstrated to oversimulate leaf and aboveground biomass (Bannayan et al., 2003). The large discrepancies between simulated and observed straw nitrogen concentrations are likely due to Sirius' assumption that all dead tissue has a fixed nitrogen concentration of 1% (Jamieson and Semenov, 2000), whereas observed data from the SAMS sites show a range between 0.36% and 1.55%, with an average of 1%. These observations are consistent with other UK datasets, which report similar variability in straw nitrogen concentrations at harvest (DEFRA, 2019). While these errors did not compound, and the total simulated straw nitrogen uptake was more accurate than the individual components, overall simulations still performed poorly. Further work is needed to determine whether these discrepancies stem from limitations in the model structure or cultivar parameters that may not accurately represent modern wheat varieties with harvest indices above 50% (Shearman et al., 2005). Regardless, improvements in simulating straw biomass and nitrogen

concentrations should be targeted to enhance the overall accuracy of nitrogen uptake modelling.

For a model to be effective in a specific context, it must accurately represent the behaviour of the real-world system to an acceptable degree of precision. While the evaluation described above is inherently quantitative, sensibility tests are more subjective and based on the model's usefulness (Huth and Holzworth, 2005). This evaluation identified limitations in Sirius' ability to simulate specific yield components, biomass, and nitrogen partitions. However, it successfully modelled the spatial and temporal variation in grain N uptake, as well as total N uptake at harvest, particularly when considering the evaluation's constraints. Initial soil conditions for each season were unknown and had to be estimated, which likely increased modelling error, especially for initial nitrogen concentrations. The RMSE value of 35.9 kg N ha⁻¹ for total N uptake is likely to be sufficient to inform nitrogen management where variations in optimal N rates, such as those reported by Kindred et al. (2017), are large. However, it may be less reliable in situations with smaller responses, although the trends may still provide valuable information for deciding whether an area should receive more or less N based on a predetermined amount.

4.6.1.3 Management zone specific N rates

The management zone-specific soil parameters within Sirius were utilised to identify average optimal N rates for each each zone. Variability in simulated NOpt across different zones was recorded, particularly at Manns Field, where the variation was most pronounced. The M3 zone, which had the lowest PAWC, exhibited the lowest simulated NOpt. In contrast, M1 had the highest PAWC, simulated yield potential and NOpt. This suggests that when PAWC is the primary variable determining NOpt, areas with greater water-holding capacity can support higher N applications due to higher yield potentials. However, when large variation in soil organic N content is present this also influences NOpt.

The P1 zone, despite having the highest available water capacity and the second highest yield potential, had the second lowest NOpt of 180 kg N ha⁻¹. This can be attributed to the higher organic N reserves in the P1 zone, which contributed

to a larger pool of mineralised N, thereby reducing the need for additional N fertilisation. These findings contrast somewhat with current guidance, which suggests that in soils with organic matter content below 4%, influences on N rates are relatively small (AHDB, 2023a). However, the organic matter content in P1, at 3.8% (9.2 t ha⁻¹ of organic N), compared to 2.8% (7.2 t ha⁻¹ of organic N) in M1, appears to have a significant impact on the simulated NOpt, despite similar PAWC. These results suggest that even modest differences in soil organic matter can influence N fertiliser requirements for different zones. The limited variability in NOpt in Hackett's field can be accounted for by the smaller variations in PAWC across zones. Additionally, H1 zone with the lowest PAWC also had the lowest organic N stocks therefore despite lower yield potentials, it required additional fertiliser to offset smaller amounts of mineralised N.

The mean NOpt, weighted for zone size of 194 kg N ha⁻¹ is lower than the farms current farm standard of 218 kg N ha⁻¹. However, M1, with a mean ECa of 11.7 mS/m is representative of the broader farm (Figure 4-1A) and has a soil organic matter (used to estimate soil organic N) levels typical of the farm average (TMAF, 2023). In this zone the simulated NOpt of 216 kg N ha⁻¹ closely aligns with the current farm standard. Nevertheless, considering the possibility that the model may underestimate NOpt - potentially due to its inability to account for factors such as pest and disease pressures or waterlogging (Richter and Semenov, 2005) - the comparison between a uniform N application rate and zone-specific management was conducted at both the current farm standard (218 kg N ha⁻¹) and the modelled farm average (194 kg N ha⁻¹).

The simulated RE_{fertN} averaged 88% across all zones, which is higher than the multi-farm average of 73% reported by Baxter and Clarke (2023). However, a large range was presented in this study with 88% falling well within this. Additionally, in their study, in the absence of an untreated control, it was assumed that all soil nitrogen supply, as estimated using the RB209 assessment method, was fully taken up by the crop (AHDB, 2023a), potentially overestimating uptake from the soil N supply.

The implementation of modelled, management zone-specific N rates demonstrated moderate but valuable improvements in NUE with RE_{fertN} gains of 3.6%, reducing the N surplus (N_{un}) by over 10 kg N ha⁻¹ on average. In the M3 zone, which has a lower PAWC₁₅₀ with higher sand and stone content, these improvements were even more significant, with an 11.1% increase in RE_{fertN} and a reduction in N surplus by 31 kg N ha⁻¹. These results are particularly important because lower PAWC soils, higher in sand and stone content are known to be at higher environmental risk for N leaching (Gaines and Gaines, 1994; Sogbedji et al., 2000). Increased nitrogen surpluses are directly linked to higher nitrogen leaching rates (De Notaris et al., 2018). Therefore, positive changes to reduce N leaching risk on such soils can have the greatest impact (Li et al., 2023).

The moderate simulated improvement in economics from variable N applications is in line with previous studies reported benefits of spatially targeted N management. Colaço and Bramley (2018) found that studies using sensor-based technologies reported on average \$30 per ha improvement in profit with reported profits of \$0-10 per ha most common. This is in line with the potential savings of £5.1 per ha reported here compared to current farms standard N rates. These savings are small, on average, and unlikely to cover the costs of data procurement for model setup, even when accruing over several years. However, farmers can be paid £27 per ha annually through the government's sustainable farming incentive to apply variable rate N (DEFRA, 2024b), this incentive may potentially offset the parameterisation costs.

The comparison between farm standard and simulated uniform rates of 194 kg N ha⁻¹ is interesting within the context of government paying farmers to deliver actions designed to promote environmental good. Assuming that the simulated $NOpt$ is correct, and that 218 kg N ha⁻¹ is in most zones an over application of N, this highlights that if the farm standard N rate is optimised on farm, but applied uniformly, then the environmental and economic gains from spatial application of N are. That said, these results are specific to one farm, and outcomes will vary depending on the level of spatial heterogeneity. Nonetheless, the relationship

between soil ECa and standardised yield demonstrates what can be considered relatively high spatial variation in productivity.

While the simulated CO₂e savings of 13.8 kg CO₂e/t of grain are substantial, these should be considered in the context of broader farm-level mitigation strategies. Spatially optimised N management presents a viable yet complementary approach to reducing emissions while maintaining productivity. However, the modest savings of 0.3 kg CO₂e/t from a uniform model-recommended rate suggest that optimising farm-wide N rates alone may not be sufficient to achieve significant carbon reductions. While this study provides an in-depth evaluation of Sirius' ability to simulate observed spatial variability in nitrogen uptake across homogeneous management zones, it does not validate the model as a tool for determining optimal N management strategies. Pasquel et al (2022) argue that if a model is to be used for decision-making, its recommendations must be evaluated not only on its ability to simulate observed crop properties but also in terms of the practical outcomes of the recommended actions. Currently, the use of uniform management data from on-farm studies limits the ability to fully assess this. However, experimental or tramline trials with varying N rates, would allow for the comparison to model-derived NOpt and observed response. This approach represents the logical next step in the development of farm-level N management tools using crop simulation models. Additionally, here we made use of data collected through the Morley SAMS study to parametrise the model, therefore only management zones with a SAMS site could be evaluated. In further studies all identified zones within a field would be sampled and evaluated.

4.6.2 Spatial variation in soil plant available water and impact on yield

Sampling sites across varying ECa showed a significant relationship between ECa and soil clay and sand content, consistent with the understanding that ECa is influenced by soil texture, specifically clay content in low salinity soils (Domsch and Giebel, 2004; Mcbratney et al., 2005; Waive, 1999). This aligns with data from experimental trials at the same site (Clarke et al., 2024b). Higher clay

content soils are generally associated with higher water retention capacities. A moderate positive correlation between ECa and PAWC₁₅₀ suggests that ECa could be a useful proxy for estimating plant-available water capacity on these soils. However, variability in this relationship indicates that factors like soil compaction, soil organic matter and stone content which also influence PAWC₁₅₀ and soil ECa are potentially complicating the relationship (Daccache et al., 2015; Krajco, 2007; Lal, 2020). The use of intact soil cores for measuring water release characteristics also presents inherent limitations in measuring PAWC, with significant errors possible (Ritchie, 1981). The disturbance of the natural soil pore structure during sampling, caused by compaction and sample cutting can impact results. Large macropores caused by soil fauna or root mass can disproportionately impact single core water release characteristics. In soils with high stone content, such as those found at this site (Clarke et al., 2024b), the volume of small cores is insufficient to accurately capture the impact of coarser materials on the soil's water release characteristics. Therefore, they should only be used to represent the water holding characteristics of the fine earth fraction, once sieved and adjusted for any small stones present (Cresswell and Hamilton, 2002). This is a significant limitation on these soils, for which stone content has a large influence on PAWC₁₅₀. Even when these issues are mitigated, there are additional sources of error associated with pressure plate apparatus (Solone et al., 2012). Despite this, ECa effectively explains the spatial variation in PAWC₁₅₀ across the farm, and it is hypothesised that the relationship between ECa and PAWC₁₅₀ is stronger than the data suggests, because of the limitations discussed above. This is further supported by the observed relationship between yield, ECa, and weather conditions. Soils with higher ECa (between 9-15 ms/m), indicative of better water-holding capacity, often exhibit the highest within-field yields, suggesting that soil moisture availability is a critical determinant of crop productivity on the farm.

The relationship between SPEI for the months of April, May, June, and July on a one-, two-, three- and four-month lag respectively, and the variance explained in the relationship between soil ECa and yield, indicates that the yield response to soil properties associated with ECa is strongly influenced by seasonal variations

in weather conditions. In 2016 and 2018, the SPEI 1 (April) and SPEI 2 (May) were between 1 to 1.5, indicating “moderately wet” conditions compared to normal. The SPEI 4 (July) in 2018 identified the weather across the construction and production phases of wheat growth was “severely wet” (SPEI >1.5). This was influenced by an intense hyperlocal thunderstorm on June 2, 2018, which brought 70mm of rainfall. While nationally, the summer was categorised by drier than average conditions with impacts on crops (Holman et al., 2021), the weak relationship between ECa and within-field yield in these years suggests that soil moisture on the farm was likely sufficient for the yield potentials of that season across the variation in PAWC. However, in 2009, 2011, 2019, and 2022, ECa explained a much stronger degree of within-field spatial variation in yield. For SPEI 4 (July), all these years indicated drier than normal conditions over the key growth stages for wheat. The dry spring and summer of 2011 is a well-documented severe drought in England, with widespread impacts on crop growth and yields (Kendon et al., 2013). The impacts of this at Morley were most keenly felt on the low ECa soils, showing the second strongest correlation between ECa and within-field yields in the seven years.

In 2013, the relationship between SPEI and the variance explained by soil ECa on yield was the highest. This suggests that in 2013, soil ECa played a particularly significant role in influencing yield variation, even more so than in other years with overall drier conditions. While the available data sets do not allow for detailed interpretations, some plausible explanations can be provided. Firstly, drought severity indices calculated on monthly lags can hide small-scale short drought episodes that might still influence crop water availability. For example, in 2013, no precipitation was recorded in the first two weeks of June, typically coinciding with anthesis, a key period in wheat yield response to drought (Foulkes et al., 2002) . An additional 20-day period of no rainfall was observed at the beginning of July coinciding with grain filling. However, significant rainfall was recorded at the end of each month, resulting in near-normal SPEI values. Additionally, the summer and autumn of 2012 were among the wettest on record, resulting in poor establishment conditions for 2013 crops (Parry et al., 2013). It has been documented that high soil moisture content can limit root growth, which can

subsequently increase the impact of drier periods on crop productivity (Hodgkinson et al., 2017). Operations on wet soils in the autumn could have also increased compaction, potentially reducing root growth (Barraclough and Weir, 1988). Therefore, although rainfall was greater in 2013, poor and shallow rooting associated with autumn conditions may have reduced the crops' ability to utilise available soil water effectively.

This study demonstrates that using proximally scanned soil data in conjunction with spatially mapped yield data provides valuable insights into the drought risk associated with different soil types at the sub field scale. At Morley soils with lower ECa values often have yields limited by water availability, particularly during dry periods. In contrast, soils with higher ECa values (9-15 mS/m), which are indicative of better water-holding capacity, generally support higher yields. Identifying areas most susceptible to drought stress could allow for targeted management practices to mitigate this risk. Targeted application of plant growth regulators, which have been documented to provide some improvement in drought tolerance through several pathways, including maintaining plant photosynthetic efficiency (Zhang et al., 2022). While reducing the stem height, growth regulators do not appear to reduce root strength (Kubo et al., 2005) or limit root penetration (Hoad et al., 2001). Novel approaches such as the use of anti-transpirants where they are most likely to generate a response could be tested in field (Mphande et al., 2023, 2022). Additionally, soil management strategies can be optimised to generate the greatest benefits. By strategically applying the limited availability of organic amendments (Thomas et al., 2019), which can increase soil organic matter levels with regular applications, there is potential to enhance the soil water-holding capacity, with increases often greater in coarser-textured soils (Lal, 2020; Minasny and McBratney, 2018). Additionally, on farms where irrigation capacity allows, these areas are likely to see the greatest yield return from irrigation, which can be profitable in UK wheat (El Chami et al., 2015). For the focus of this study, we have demonstrated that water stress has spatial influences on crop growth and yield at the farm scale. This highlights the potential for co-limitation by other nutrients, particularly nitrogen (N), suggesting that N management strategies should address this co-limitation

while also accounting for other factors, such as the availability of mineralised organic N.

4.7 Conclusion

This study highlights that the spatial variability of PAWC, inferred through ECa, can be linked to within-field yield performance and weather patterns. Such analysis allows for targeted drought risk management and the potential to manage the co-limitation of other nutrients, particularly nitrogen. On-farm yield map datasets were used to identify spatially coherent management zones, while the mean ECa of each zone indicated likely variation in PAWC. By targeting single sampling sites within each zone, the spatialisation of the Sirius cropping system model was evaluated. This demonstrated Sirius's ability to capture spatial variability in N uptake across zones. However, improvements in simulating straw biomass and nitrogen partitioning would enhance the accuracy of total N uptake modelling. Future work should focus on developing better cultivar parameters to reflect these improvements. It was demonstrated how a spatially parameterised CSM can be used to inform N management in UK wheat. Future studies should validate such model-derived recommendations to achieve both economic and environmental benefits, as well as compare how different models with varying structures simulate N responses across zones.

4.8 References

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5 Integrated discussion and conclusion

The purpose of this integrated discussion is to synthesise the findings from the individual manuscripts (forming Chapters 2–4) and demonstrate how they collectively contribute to the development of cropping system modelling as a potential tool for nitrogen management in UK wheat crops. By integrating the results from each study, this discussion highlights the connections between the manuscripts and examines the broader significance of the research. It also demonstrates the contribution of this work to advancing both the theoretical understanding and practical application of cropping system models for on-farm decision-making. Additionally, this section reflects on the methodological innovations introduced, critically assesses the limitations, formally documents other research consideration undertaken and outlines future research directions.

5.1 The Sirius CSM to support on farm N management

The aim of this research was to evaluate the potential of cropping system models to inform economically and environmentally appropriate nitrogen (N) management, accounting for within-field spatial-temporal variations in soil properties for UK wheat crops. The studies presented across individual chapters have collectively addressed this goal.

The use of crop models as tools for managing spatial variation on farms is not a new concept. Early attempts were identified through the systematic review (Basso et al., 2001; Paz et al., 1999; Sadler et al., 2000). However, over the last 25 years, progress has been slow. Recent studies continue to describe the limited application of crop models for managing spatial variation (Cammarano et al., 2020; Pasquel et al., 2023), and research remains geographically concentrated, primarily in the USA and Italy. These studies often use the same fields repeatedly (Basso et al., 2016a, 2012, 2011c, 2007). In contrast, studies based in the UK are scarce, with only a single investigation using the DSSAT model for spring barley (Cammarano et al., 2020).

Currently, there are no commercial, industry, or levy board-supported crop modeling tools available to growers in the UK. The concept is criticised as being

too inaccurate for practical farm applications (Sylvester-Bradley et al., 2017). However, there are limited studies to support or refute this notion, and Cammarano et al (2020) report generally good model performance in their work on spring barley. To address this gap, the primary objective of this research was to test the widely validated and applied Sirius CSM for simulating within-field spatial variation in yield and nitrogen uptake.

5.1.1 The Sirius CSM

The Sirius CSM was selected for this research for several key reasons. Primarily, it is one of the most validated and widely used crop simulation models in the UK, with proven accuracy in simulating crop responses to nitrogen and weather over time (Harkness et al., 2020; Jamieson and Semenov, 2000; Semenov et al., 2007). Additionally, prior experience with Sirius (Clarke et al., 2020), facilitated appropriate model setup and application, which is crucial for accurate simulations (Confalonieri et al., 2016).

Sirius includes cultivar-specific parameters for a relatively modern UK wheat variety, cv. Claire (Wolf, 1989), which was widely grown in the UK from the late 1990s until around 2015 (Figure Apex B 14). While this model setup is beneficial, using cultivar-specific parameters introduces potential modeling errors, as genetic variation across cultivars is well-documented (Senapati et al., 2019a; Senapati and Semenov, 2020). Therefore, while the parameters for Claire are adequate for simulating yield and nitrogen uptake, future work should aim to generate parameters for more modern varieties (see 5.3.1).

Despite the advantages of Sirius, it does possess some limitations. One key challenge is its limited integration with other data handling and analysis software. Other CSMs have successfully been linked to programming languages and software environments (Alderman, 2020; Miguez, 2024). For this research, custom scripts were developed to generate Sirius input files and process the results using R, although model runs still had to be manually initiated. Future work should focus on improving Sirius's integration with spatial and computational tools to enhance its scalability for broader farm applications.

5.1.2 Sirius's ability to simulate spatial variation in N uptake efficiency

This research has conducted one of the most in-depth evaluations of the Sirius model to date. By using a long-term experimental dataset, the evaluation minimised the risk of errors often present in farm-scale yield map data. Long-term experiments provide a more controlled environment for model validation, as protocols are more robust, and measurement apparatus are verified. Moreover, these experiments include detailed grain N/protein data, crucial for evaluating N uptake but often missing in farm datasets.

Sirius was evaluated across different soil types and under contrasting seasonal conditions, including drought (2010) and wet years (2012) (Parry et al., 2013). While Chapter 4 extended the evaluation across a much larger area, the limited temporal resolution of the SAMS dataset (covering only two years) restricted the analysis. Nevertheless, this framework set out a method for spatialising CSMs across farms, highlighting the importance of validating data accuracy before applying CSMs to precision agriculture techniques.

While the errors in grain N concentrations were not large in both studies, the spatial-temporal variation in grain N concentrations was not simulated with the same degree of success as grain yield, consistent with other spatial applications of CSMs (Albarenque et al., 2016; Cammarano et al., 2020). Evaluation not only quantifies the errors associated with model use but is also crucial for improving performance by identifying areas where the model's structure requires refinement (Johnston and Poulton, 2018; Wallach et al., 2006). In this case, a key limitation in Sirius was identified in its ability to simulate lower-than-expected grain nitrogen concentrations. For example, grain protein concentrations recorded as low as 6.3% (equivalent to 1.1% grain N) were observed in the NFS-RE dataset. However, based on older datasets (Spiertz and Ellen, 1978), the structural nitrogen limit in the model was fixed at a minimum of 1.5%, preventing the simulation of lower observed concentrations.

Before contacting the developers of Sirius, a comparison of the NFS-RE data with the WGIN dataset, which features low fertiliser rates (0 and 100 kg N ha⁻¹) across

modern wheat varieties (DEFRA, 2019), confirmed that grain N concentrations below 1.5% were not uncommon, especially at N rates below 100 kg N ha⁻¹. Based on these findings, we presented the data to the principal developer of Sirius, Dr. Mikhail Semenov (personal communication, 2023). Following discussions, it was agreed that while there wasn't sufficient evidence to make the minimum grain N a cultivar-specific parameter, the structural limit in Sirius should be lowered. As a result, the latest version of Sirius now incorporates a structural nitrogen limit reduced to 1%, based on our findings. This adjustment is expected to improve Sirius's ability to model spatial variation in nitrogen uptake more accurately under low-N conditions.

Sirius simulated spatial-temporal variation in grain N uptake with a reasonable degree of accuracy (RMSE = 21.3 kg N ha⁻¹ in Chapter 3; RMSE = 26.4 kg N ha⁻¹ in Chapter 4). These errors are not insignificant, but they were likely influenced by the absence of initial soil N conditions and the use of non-cultivar-specific parameters. Additionally, the model does not account for disease pressures, which can significantly affect nitrogen use efficiency. Therefore, any model-derived recommendations should be interpreted as best-case scenarios.

Additionally, for Sirius to derive spatial N_{Opt} recommendations, it must be simulated with a range of N rates. Therefore, the model should accurately simulate crop response across the variation in management zones if accurate management decisions are to be obtained (Sadler et al., 2000). The evaluation in Chapter 2 across the NFS-RE and Straw Incorporation Experiment datasets increases our confidence in this aspect. Sirius successfully simulated yield and grain N uptake across a range of N rates, meaning our confidence in simulating response to nitrogen is greater than if only a single N rate had been evaluated. On-farm datasets could further improve this by incorporating tramline N rate trials and untreated blocks, which would allow for more robust testing of the model's performance across varying nitrogen management scenarios.

5.1.3 The application of soil ECa in deriving water holding characteristics for crop models

Accurate parameterisation of soil properties is critical for the effective spatialisation of CSMs in precision agriculture. While direct measurements of soil hydraulic properties, such as water release characteristics, provide the most reliable data, they are often time-consuming and expensive, particularly when applied to large-scale commercial farms. In Chapter 4, soil parameters were obtained using measured water release characteristics via pressure plate apparatus, as collected through the Morley SAMS study. However, such measured data were not available for the NFS-CE/NFS-RE dataset in Chapter 2, necessitating the use of pedotransfer functions to estimate soil hydraulic properties based on more readily available data such as texture and organic matter.

Pedotransfer functions offer a practical solution in cases where direct measurement is infeasible, providing an indirect method to estimate critical soil properties such as soil water retention and hydraulic conductivity (Patil and Singh, 2016). This method was applied in Chapter 2 to derive soil parameters across the spatial variation in ECa, allowing the Sirius model to run simulations even in the absence of detailed measured data. However, while PTFs provide utility, they are associated with inherent uncertainty. These uncertainties arise because PTFs rely on empirical relationships and can vary significantly depending on the dataset used to derive them. As a result, model outputs—such as crop growth simulations—may be sensitive to the specific PTF applied, which in turn can affect the accuracy of predicted water availability and crop yield (Gagkas et al., 2018).

Given the importance of soil water availability in determining crop response to N as demonstrated in chapter 4, future research should not only focus on selecting the most appropriate PTFs but also on validating them against direct measurements where possible. A useful approach would be to compare the predictions of PTF-derived parameters with direct measurements of soil hydraulic properties, such as those from the Morley SAMS dataset. Such a comparison

would help determine the reliability of PTFs across varying soil types and conditions, thus improving model robustness and accuracy.

While pedotransfer functions allow for the estimation of soil parameters in the absence of direct measurements, proximal soil electrical conductivity (ECa) scans present an additional tool that can enhance the spatialisation of CSMs by capturing spatial variation in soil plant available water (Domsch and Giebel, 2004; Mcbratney et al., 2005; Waite, 1999). In both Chapter 2 and Chapter 4, ECa scans were used to map variation across the fields, and this information was essential in explaining yield variability. The ability of ECa to capture within-field variability in soil properties provides valuable insights for parameterising CSMs like Sirius, especially when combined with targeted soil sampling.

However, as demonstrated in both chapters, the relationship between ECa and certain soil properties such as Plant Available Water Capacity (PAWC) is not always straightforward. At Morley, as with other soils across eastern England, varying gravel and stone content complicates the relationship between ECa and PAWC (Cooper et al., 2020). This complexity posed a challenge in generating accurate PAWC maps from ECa data using linear methods (Daccache et al., 2015; Wong and Asseng, 2006), particularly due to insufficient data points related to stone volume. In both Chapter 2 and Chapter 4, spatial variation in ECa was successfully used to explain yield variability, justifying the application of CSM. In Chapter 4, the variation in management zone ECa values provided confidence that these zones were driven by spatial variations in soil properties, which the Sirius model could interpret.

Moving forward, the integration of ECa data and pedotransfer functions holds promise for improving the spatialisation of CSMs across large farms. Although no studies from the systematic review employed this specific approach, the use of intact, undisturbed soil core samplers could help bridge the gap between ECa scans and accurate soil parameter estimation. Modern sampling rigs can now rapidly collect 113 mm diameter cores down to 1 m depth, capturing both fine and coarse soil particles, which could be used to generate PAWC maps derived from ECa data. They are large enough that stone content can be determined as well

as soil bulk density. A sieved sample of fine earth can then be sent for particle size analysis. These corers have been used to sample root biomass (Figure 5 1).

To explore this further, grant funding has been secured to sample up to 30 management zones across a commercial farm in eastern England. These samples will be used to spatialise CSMs for managing N demand, while also generating farm-wide CSM parameters for water release characteristics. However, it is important to recognise that due to the heterogeneity of topsoil organic matter, each management zone will likely require separate topsoil sampling to accurately assess soil organic nitrogen content. By combining these methods—pedotransfer functions, ECa scans, and direct sampling—future research can develop more reliable, spatially explicit models that better inform precision N management.



Figure 5-1 Clarke operating a smaller diameter version of the soil corer rig in 2017 on a plot experiment in Cambridge

5.2 On farm yield map data sets to support precision agriculture

While the methodologies developed and presented in Chapter 3 do not contain any crop simulation modelling, they defined how Sirius was applied and evaluated

in Chapter 4 as well as supporting wider application of precision agriculture and spatial on-farm management decisions. The quantification of large potential errors in on-farm yield map data sets demonstrated the caution required when using these data sets for CSM evaluation and other on farm decisions. This shaped how evaluations in Chapters 2 and 4 were carried out, focusing on quality of data sets with a long-term experiment and the Morley SAMS project rather than attempting a wide scale multi farm parameterisation. Additionally, the delineation of homogeneous yield performing management zones can support wider on farm applications including measuring soil carbon or yield based N management.

5.2.1 Yield based N management

Farmers in the UK can increase or decrease N rates by 10 kg N ha⁻¹, from the soil N index recommended rate for every additional 0.5 t ha⁻¹ of yield above or below 8 t ha⁻¹(AHDB, 2023a). However, this requires accurate quantification of yield spatially. The validated and corrected yields allowed for greater confidence when making spatial N application maps based of the above guidance (Figure 5-2 N recommendations based on management zone mean corrected winter wheat yield (2011-2020).). Variation in yield-based N recommendations varied by as much as 83 kg N ha⁻¹. However, the relationship between NOpt and yield is inconsistent and often weak (Kindred et al., 2018a). This was evidenced in chapter 4, the simulated NOpt for P1 was the lowest, because of higher soil organic N stocks, despite it having the highest mean yield in 2019. Having validated and corrected yields for management zones will also improve with other nutrient offtake calculations and improve targeted applications of P, K and Mg (AHDB, 2023b; Watson et al., 2002; Willoughby et al., 2022).

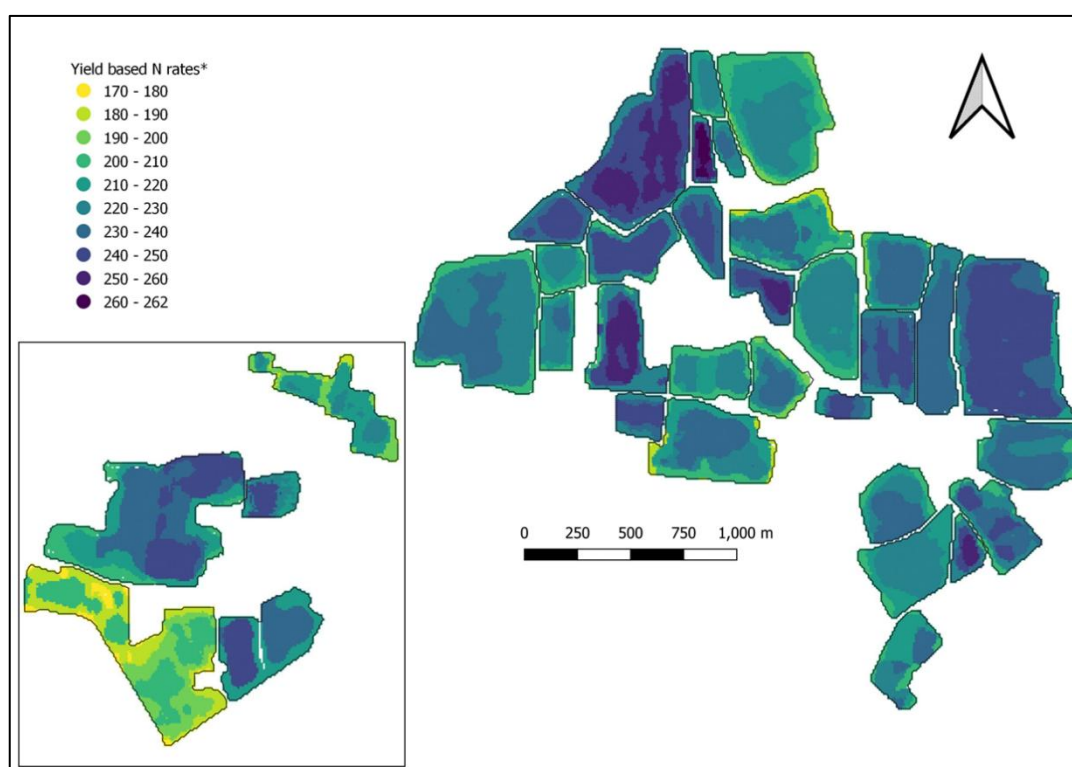


Figure 5-2 N recommendations based on management zone mean corrected winter wheat yield (2011-2020).

5.2.2 Capturing spatial variation for soil carbon monitoring through management zone sampling

The slow rate of change and large heterogeneity make identifying management induced changes in soil organic carbon at the field and farm level difficult, more so than at regional levels (Oldfield et al., 2022). Measuring soil carbon stocks accurately is also challenging; soil carbon stocks can be equal or greater in the subsoil (Gregory et al., 2016), and other soil properties such as stone content and bulk density are required for accurate measurements (Rytter, 2012). Farmers are encouraged to measure soil carbon stocks and implement practices that stabilise and where possible increase soil organic matter contents to improve productivity and compensate global emissions (Deb et al., 2015; Minasny et al., 2017; Poulton et al., 2018).

As part of a NIAB commercially and charity-supported project, we investigated the potential to use homogeneous management zones, identified through the

methods outlined in Chapter 4, using the fuzzy c-means clustering algorithm (Hassall et al., 2019) to quantify spatial variation in soil carbon within and across fields. In one part of the assessment, soil carbon stocks were evaluated using a horizon-based sampling strategy (De Feudis et al., 2022; Grüneberg et al., 2010) across three management zones in each of six fields in southern England. These were then compared to the management zone-standardised yield. The same comparison was performed on SAMS sites at Morley where fields had more than one site per field. The results were presented in an academic poster presented at the Wageningen Soil Conference, 2023 (see Appendix H)

In summary, both data sets recorded significant correlations between standardised yields and management zone carbon stocks. This is likely explained by the symbiotic relationship between soil properties that generally support higher soil carbon stocks (i.e., water-holding capacity, clay content, lower stone content) and promote higher yields in rainfed agricultural systems. Additionally, higher soil organic carbon stocks can directly enhance productivity. The higher residue returns from high-yield management zones are also likely to increase soil carbon inputs in these zones. This work demonstrated that, in the absence of other spatial variation in soil properties within fields, yield-based management zones can be used to quantify the spatial variation of soil carbon stocks on farms and support the cost-effective monitoring of management impacts on these stocks.

While this PhD has focused on modelling spatial variation in crop nitrogen uptake and water dynamics, this extension project demonstrated how other agroecosystem models, such as the Roth-C carbon model (Coleman and Jenkinson, 1996), could be parameterised spatially and used to inform the management. Such models could be parameterised with current management strategies in mind and used to simulate long-term trends in soil carbon across management zones, as well as to predict the likely response to changes in management strategies (Coleman et al., 1997; Liu et al., 2011).

5.3 Future research directions

5.3.1 The calibration of other CSM to support multi model ensemble

A key limitation of this research is that only a single CSM, Sirius, has been spatially parameterised and evaluated. While the systematic review identified few studies that compare multiple models, differences in performance and simulated outcomes suggest that a multi-model ensemble approach could be beneficial (Wallor et al., 2018). Although other models have been used in the UK, they remain limited, and representative cultivar parameters for modern UK wheat varieties are largely unavailable.

The Sirius model primarily focuses on wheat but has been applied to other cereals (Fletcher et al., 2009). However, its use for N management in non-wheat crops is limited, complicating rotational modeling and surplus N fate assessments. Recognising this, efforts have started to generate cultivar parameters for modern UK wheat varieties for other CSMs. For example, using data sets from NIAB at Morley and Rothamsted, parameters for the widely grown UK winter wheat variety cv. Skyfall (Figure Apex B 14) are being calibrated, initially with the DSSAT model, with plans to extend calibration to other models. Initial calibrations can be seen in appendix F.4)

5.3.2 Validating model derived management strategies

It is recognised that the most complete validations of a CSM include an evaluation of the model's intended use. Specifically, if the model is used to estimate a variable, it is that variable which must be evaluated. Conversely, if the model is used to inform decision-making, then the decision itself should also be validated (Pasquel et al., 2022a). The model must not only be sensitive to the mean observed yield but also to the derivative of the yield in response to inputs such as nitrogen (Sadler et al., 2007).

For instance, the concept of precision N management has been suggested to be validated against the null hypothesis: "Given the large temporal variation evident in crop yield relative to the scale of a single field, the optimal risk-aversion strategy is uniform management" (Diacono et al., 2012).

The alternative hypothesis to explore to validate the approach would be:

“Cropping system model-derived nitrogen management recommendations improve economic and NUE outcomes in UK wheat crops.”

The research presented in this thesis has advanced us to the point where this hypothesis can now be tested. We have demonstrated how the Sirius CSM can be parameterised across fields using spatially coherent management zones, and how these models can be evaluated using on-farm data sets, such as yield maps, or through targeted zonal crop sampling for more thorough evaluations. Once evaluated, the model can then be used to derive management zone-specific nitrogen rates. The next step is to determine whether model-derived management recommendations lead to the simulated economic and NUE gains. Using the example described in Chapter 4, does an N rate of 163 kg N ha⁻¹, instead of current rate of 218 kg N ha⁻¹ for the M3 Management zone on Manns field at Morley, deliver an average margin improvement of £19.35 and a fertiliser N recovery improvement of 11.1%?

While this work was beyond the scope of this research, as it requires extensive small-plot field trials and several years of observations, grant funding was sought to undertake this next stage of model evaluation. This work has begun as part of the AHDB Strategic Cereal Farm East Programme in 2024 and is set to continue in 2025 on Manns field, a site where model-derived N rates were determined in Chapter 4. Model-derived recommendations will be compared with observed NOpt through replicated N response experiments carried out within management zones, following a similar approach to those identified in the systematic review (Albarenque et al., 2016). These N response experiments will allow for the determination of actual management zone-specific NOpt (Kindred et al., 2018a). Observed NOpt can be compared to both long-term simulated and season-specific model-derived NOpt, thereby evaluating the effectiveness of model-derived recommendations.

Additionally, the farm installed a Yara ALS 1 N sensor™ for the 2024 season allowing for management zone sensor-based prescription maps be compared to observed NOpt and simulated NOpt.

Future work could explore how integrating long-range weather forecasts within each season could potentially improve climate-based simulated NOpt in response to expected seasonal conditions (Boas et al., 2023; Calanca et al., 2011). Additionally, the integration of satellite and N sensor data could enhance season-specific simulated NOpt. However, these aspects can be investigated post hoc, once several years' worth of data from a range of management zones has been collected. Furthermore, the impacts of climate change on agriculture have been shown to vary considerably at fine spatial scales due to differences in soil and climate conditions. Climate change impact assessments have often focused on regional climate variability (Harkness et al., 2020). However, at Morley, we observed that plant-available water capacity can vary between 131 mm and 86 mm within the same field. Fine-scale climate change impact assessments could be conducted using local future climate scenarios generated from the observed long term-weather data set for the site to investigate whether sub-field spatial variation is likely to change over time and to quantify the overall farm-level impact on productivity.

5.4 Conclusion

This study successfully demonstrated parameterisation and application of the Sirius CSM to manage spatial variation in nitrogen requirements for UK wheat, addressing a key research gap in sub-field scale CSM applications. The evaluation of Sirius showed that CSMs can effectively capture the co-limitations of nitrogen and water availability, particularly when variation in plant-available water and organic N are the primary drivers of yield variability. Model-derived N recommendations were used to inform site-specific nitrogen management, providing a structured approach for precision fertiliser application. The integration of long-term on-farm datasets—such as yield maps and soil electrical conductivity data—to delineate homogeneous yield performance zones for CSM spatialisation was demonstrated. Additionally, a framework for data cleaning, validation, and parameterisation was developed, improving the reliability of farm-scale CSM applications and ensuring robust model outputs for decision-making. The findings reinforce the practical value of CSMs for precision nitrogen

management, offering economic and environmental benefits by optimising fertiliser applications at a fine spatial scale. While some model limitations remain, particularly in biomass and nitrogen partitioning, this study establishes a strong foundation for further refinement of CSMs and their role in on-farm nitrogen decision support. Future work should focus on multi-model comparisons to assess uncertainties and field validations of model-derived recommendations to fully realise the benefits of this approach. Additionally, while this study simulated economic and environmental benefits from site-specific N recommendations, further work is needed to validate these impacts. The systematic review highlighted a critical gap in field-level validation of CSM-derived N recommendations, reinforcing the need for future studies to compare model outputs with real-world nitrogen responses.

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Appendix A Ethical approval letter



17 December 2020

Dear Mr Clarke ,

Reference: CURES/12467/2020

Title: Site-Season Effects On Crop Productivity To Support Sustainable Intensification

Thank you for your application to the Cranfield University Research Ethics System (CURES).

We are pleased to inform you your CURES application, reference CURES/12467/2020 has been reviewed. You may now proceed with the research activities you have sought approval for.

If you have any queries, please contact CURES Support.

We wish you every success with your project.

Regards,

CURES Team

Appendix B Crops simulation models supporting precision agriculture – a Systematic review

B.1 Research context

A critical step in a systematic review is defining the review, recognising the likely gaps and uncertainties and how the questions are conceptualised within the literature (Armstrong et al., 2011). In the context of UK wheat cultivation, cropping system models (CSM) have been utilised for various purposes, such as yield forecasting (Bannayan et al., 2003), assessing the impacts of extreme weather and climate change (Clarke et al., 2020; Harkness et al., 2020), optimising management strategies like seed rates and sowing dates (Ghaffari et al., 2001), and identifying traits for future breeding programs (Semenov and Shewry, 2011; Semenov and Stratonovitch, 2015). Despite their use as research tools, reviews exploring the evolution of CSM have pointed out the unrealised potential of modelling techniques to inform practical applications (Jones et al., 2016). With a limited number of studies applying CSM within precision agriculture contexts (Keating and Thorburn, 2018b) and recent UK-based studies recognising limited applications of CSM for managing spatial variation (Camarano et al., 2020). It was therefore expected that by focusing on studies within the UK or similar agroecological systems, the scope of this systematic review might be somewhat constrained. While the primary aim of this research is to develop modelling-based approaches for nitrogen management in UK wheat crops, its recognised that calibration, parameterisation, and evaluation methods utilised outside these systems may offer valuable insights. Therefore, the review maintained a broad approach, encompassing temporal, geographical, and agricultural system variations.

The primary focus of this review is examining the methodologies employed in spatialising (Pasquel et al., 2022) CSM at the sub field scale, documenting the datasets used for this purpose, and how CSM are evaluated and implemented to manage spatial variation.

B.2 Introduction

Soil properties within a field can vary as much as that across a region (De Wit and Van Keulen 1987). This can be variation in inherent soil physical properties such as soil texture and depth (Lammoglia et al., 2019; Usowicz and Lipiec, 2017) or a result of external influences, such as compaction caused by agricultural machinery (Pentoś et al., 2021). Soil chemical and biological properties can also vary due to interactions with physical variation and/or independently (Gülser et al., 2016; Kassim et al., 2021; Usowicz and Lipiec, 2017). This variation in soil properties often interacts with crops causing large spatial variation to crop nutrient requirements (Kindred et al., 2015; Mittermayer et al., 2021) and/or water demand (Abioye et al., 2020) and subsequently in yield (Kindred et al. 2017; Maestrini and Basso 2021; Clarke et al., 2023). Therefore, uniform management, with whole-field approaches is likely to lead to the inefficient use of nutrients and resources, with the potential for losses to the environment through runoff, leaching and gaseous emissions. Sub field variation in soil properties have also been demonstrated to require different seeding rate and depth (Munnaf et al., 2020), cultivations (Heege, 2013) and levels of pesticide (Forbes, 2019; Metcalfe et al., 2016). Spatially accurate nutrient applications and other management decisions can therefore greatly reduce environmental losses and improve economic outcomes and form the foundation of precision agriculture (PA) (Nawar et al., 2017). Following the definition of in-field variations in soil characteristics, the challenge for farmers, advisors, and researchers, is in identifying how best to manage this variation considering the economics of the production system, with the need to minimise any negative externalities to the environment (Miao et al., 2018). This is made more complex as the impact of spatial variation is not always temporally stable, with weather and crop type potentially changing how crops respond to spatial variation (Basso et al., 2007; Martinez-Feria and Basso, 2020).

It is not possible through conventional field experiments to evaluate all the possible soil, crop, and management interactions across many seasons and across areas of defined spatial variability to ascertain the most suitable management strategy for a given area (Albarenque et al., 2016). Those methods

that do try to develop site specific management decisions are currently mainly driven by economic considerations focused on yield and economic return, with little emphasis on the externality to the environment (Banger et al., 2017). For example, canopy N sensors fail to consider the underlying factors influencing observed variation and how applying less, or more importantly more, nutrients to an area might interact with soil properties and the wider environment (Colaço and Bramley, 2018). CSMs have the potential to overcome these limitations. Bringing together soil and plant process models, describing changes in system states in response 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, 2018a).

Using multi-objective optimisation CSM can be used to evaluate the trade-off between maximising yield and economics while identifying optimal management strategy for the environment, e.g., reducing potential N losses through leaching (Finley et al., 2011, Udvardi et al., 2021, Maestrini and Basso, 2018). Spatially explicit soil parameters, weather data and crop specific coefficients can be inputted into a CSM along with historic management practices including fertiliser applications and drilling dates. CSM models can then be run, based on the observations at a spatial scale smaller than field level and compared to recorded data such as yield maps, or satellite data to ensure the model outputs are correctly replicating observed responses to spatial variation in soil properties. Models for decision support systems are seen as critical in improving nutrient use efficiency (Udvardi et al., 2021). Despite this, although CSMs have been used in a variety of cropping systems and environmental conditions, their application in scenarios exploring and managing spatial and temporal yield variability is perceived to be limited (Cammarano et al., 2020; Ma et al., 2016) and globally there is yet to be a wide adoption of management inferred from CSM on farm. For example, the USDA irrigation and management survey shows that fewer than 1% of growers in the USA use CSM for irrigation management (Kim and Kisekka, 2021). Therefore, this systematic review aims to provide a synthesis of current CSM methods for managing spatial variability.

The specific review objectives are to:

1. Provide a contextual overview of which CSM have been used in quantifying spatial variation and in what context, such as country and cropping systems.
2. Identify and describe the methods used in CSM parameterisation, calibrations and evaluation procedures at the sub field scale.
3. Describe model calibration and validation procedures and reported successes of these methods.
4. Assess how modeling outputs are being used to identify spatially explicit management options considering economic and environmental considerations.

B.3 Method

In the following section the process of the review is set out in detail using a PRISMA statement (Preferred Reporting for Systematic Reviews and Meta Analysis) (Moher et al., 2009). Studies that used CSM to support PA were retrieved from the online database Scopus, in December 2022. Only studies published in English between 1998 and 2022 were included. Book chapters and reviews were excluded. The search terms used were: ‘crop model’ ‘crop simulation model’ ‘crop modelling’, ‘soil model’, ‘precision agriculture’ ‘spatial variability’ and ‘management zones’. Terms in the same group were grouped with logical “OR” and combined with a different group with “AND”. The final search string was thus: ("crop model" OR "crop simulation model" OR "soil model" OR "crop modelling" OR "cropping system model" AND "precision agriculture" OR "spatial variability" OR "management zones"). For search terms where variation in spelling could arise the search was performed with all spellings, i.e., modeling and modelling. These search terms were chosen based on the aim of the review as well as reviewing the keywords of relevant studies over the last decade (Basso et al., 2016a, 2011b; Cammarano et al., 2020; Wallor et al., 2018).

To be included in the review, the literature selected were studies that: i) were empirical studies applying CSM to manage or explain spatial variability; ii) CSM applied at a sub field scale, i.e., more than one simulation point per field; and iii) Simulations performed on an arable crop. Since this review specifically aimed to identify calibration, parameterisation, and evaluation methods, as well as assess the suitability of CSMs for spatial management decisions, theoretical, review, or discussion papers without data collection or analysis were excluded, theoretical, review or discussion papers without data collection or analysis were discarded. Only studies that simulated above-ground (plant) and below-ground (soil) processes were included, thus crop models without a soil component such as SAFY (Gasó et al., 2019) were excluded. Studies that used or repeated the same data and study site as a previous study, without novel applications or change, were also excluded. The initial publication describing the model application was retained for inclusion.

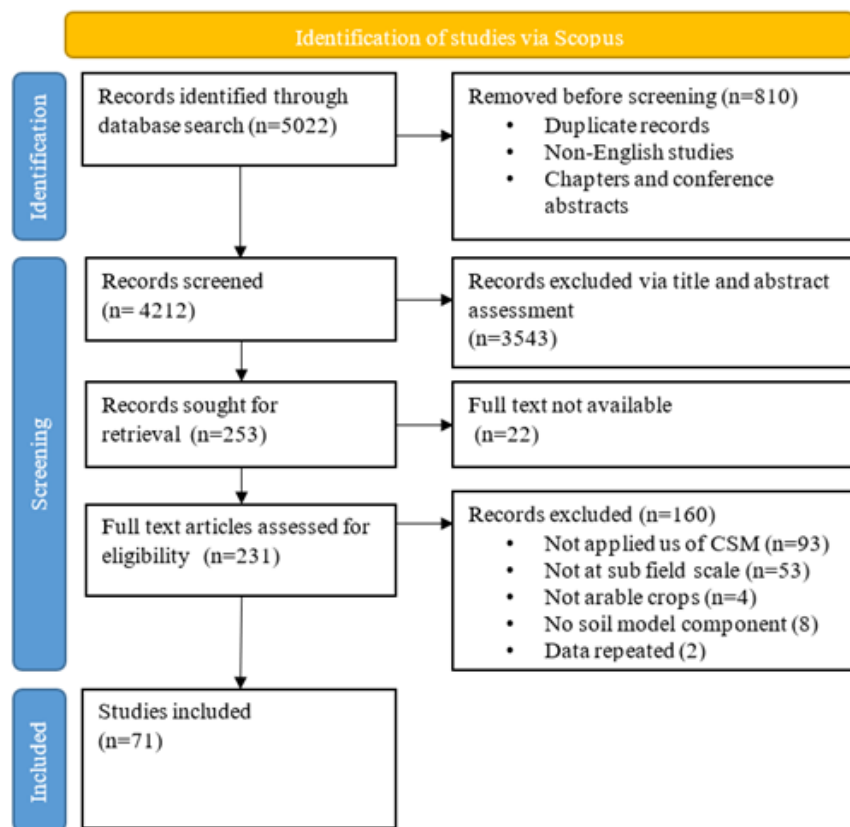


Figure Apex B-1 PRISMA flow diagram

The identification and screening procedure is described through a PRISMA flow diagram (Figure Apex B-1). After removing book chapters, non-English and duplicate records, some 4,212 articles titles and abstracts were reviewed to identify potential studies for inclusion. Some 253 studies were sought for full text review. Full text articles were not available for 22 studies. Based on the criteria described above; 93 articles were excluded for not featuring the applied use of CSM, 53 studies were excluded as they did not apply CSM at a sub field scale, 4 studies did not feature an arable crop, 8 studies didn't include a soil modelling component, and 2 studies used data already reported in another study included in the review. A total of 71 studies were thus identified for review for the current use and applications of CSM to support PA.

B.4 Studies context

B.4.1 Publications

The year with the most publications (9 studies) was 2021 (Figure Apex B-2), demonstrating the concept is still of relevance in the PA research community. However, research using CSM to support PA has not seen consistent accelerated growth in publications over the last two decades unlike those documented in reviews for other PA technologies (e.g. Ahmadi et al., 2021) or other applications of CSMs (Wang et al., 2022). A similar trend was reported by Keating and

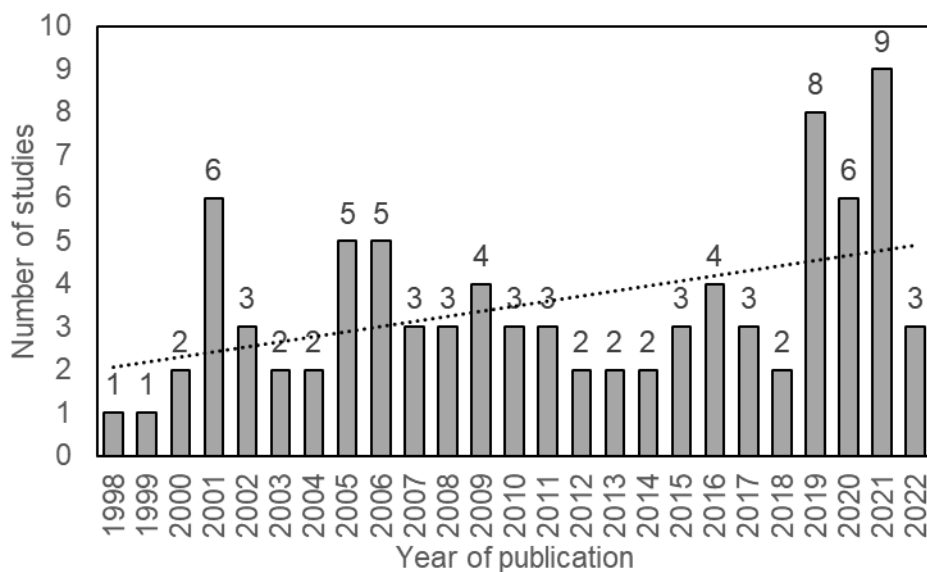


Figure Apex B-2: Number of studies by year of publication

Thorburn, (2018b), who showed the proportion of papers on Web of Science using the DSSAT or APSIM CSMs in the field of precision agriculture was no more than 2 in 2005 and 2015, compared to for example the field of climate change which had 5 studies in 2005 and over 45 in 2015. Despite the opportunities CSM could provide for managing spatial variability, research development appears to being limited by some key research and adoption barriers, this review will explore some of these barriers providing research development framework for CSM techniques to manage spatial variation.

B.4.2 Locations

The majority (87%) of reported studies were in USA (31 studies) or Europe (31 studies) (Figure Apex B-3). The uptake of PA is comparatively high in these regions compared to other regions. Therefore, the adoption of new PA technologies, such as prescriptions from CSM, is likely to be encounter fewer barriers. Variable Rate Technology (VRT) is already used on 29% of US maize area and 31% of UK wheat area (Lowenberg-deboer and Erickson, 2019), therefore recommendations from CSM for site-specific management could be implemented without additional technology investment. Additionally, key data sources for CSM calibration and validation for on-farm use such as yield mapping and soil survey data are already widely available in these regions, 68% of maize area is yield monitored and 22% soil mapped in the US (Lowenberg-deboer and Erickson, 2019). Only 2 studies have used CSM to identify and manage spatial variability within fields in the UK, with no evidence of CSM being applied for wheat at the sub field scale. The validation of a model in one locality or cropping system doesn't mean it is applicable in another (Sargent, 2000). Before it is used to inform decisions, models must be validated or evaluated in the context of that production system across the range of plausible conditions (Bellocchi et al., 2010).

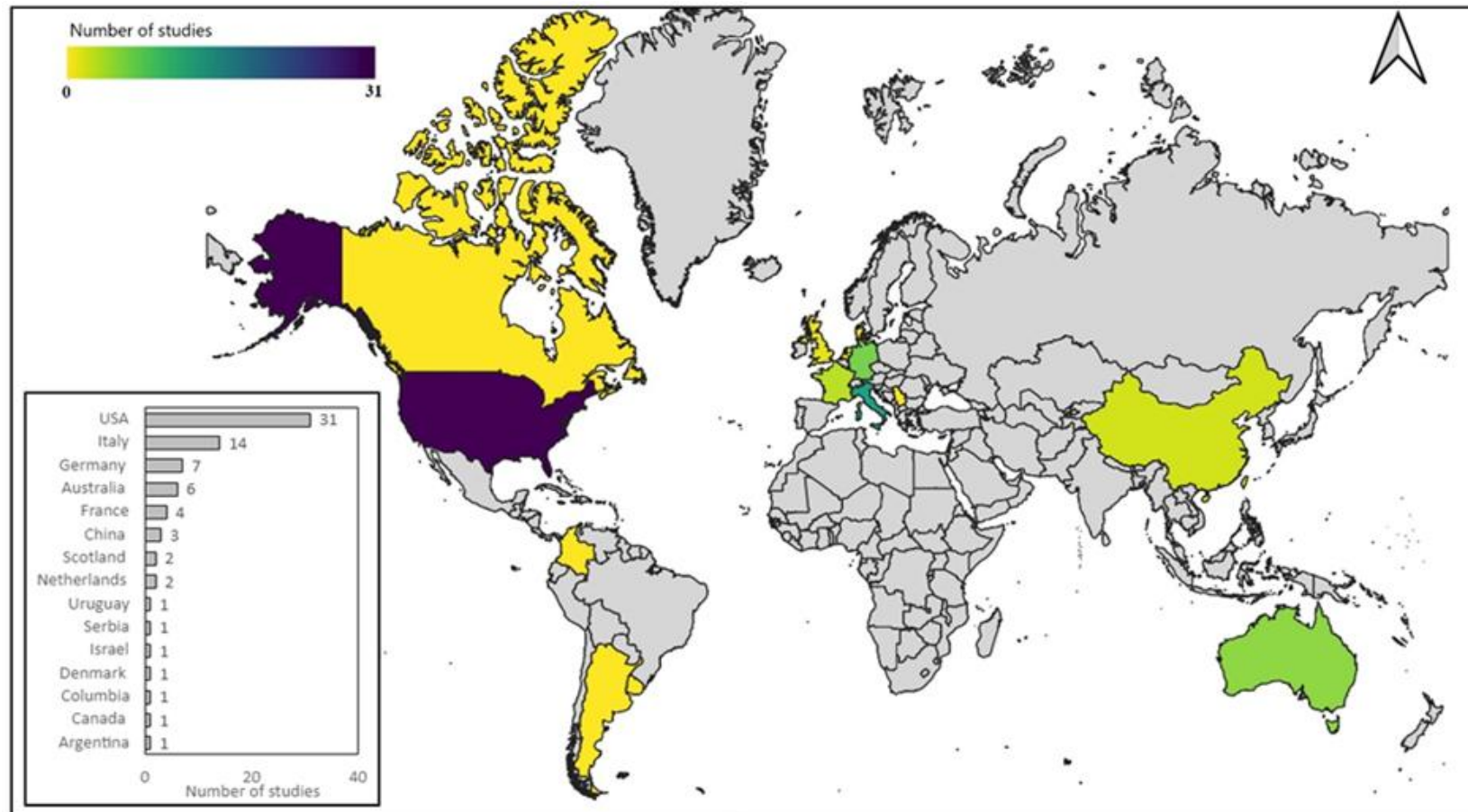


Figure Apex B-3: Number of studies by country

Greater importance is placed on model reliability when users are making real-time, real-world decisions based on modelling scenarios (Huth and Holzworth, 2005). Therefore, before models are used to inform nitrogen management on farms in the UK, they need to be evaluated for their ability to accurately describe and reproduce observed fine-scale spatial and temporal variations in crop growth and nitrogen use within its agroecological context.

B.4.3 Crops and rotational modelling

The majority (86%) of studies consulted included the modelling of maize or wheat crops, with 33 and 28 studies respectively (Figure Apex B-4). Maize and wheat are the most widely grown crops globally, accounting for around 30% of global agricultural area (FAO, 2022). They are also the two crops with largest amount of fertiliser (N+P₂O₅+K₂O) use globally (IFA, 2022), therefore the economic and environmental benefits of site-specific management through PA is potentially the largest for these two crops. Only 6 studies (8%) model the spatial variability across multiple crops. Spatial variation in crop growth is not always consistent, with crops with different development stages (i.e. winter or spring drilled crops in

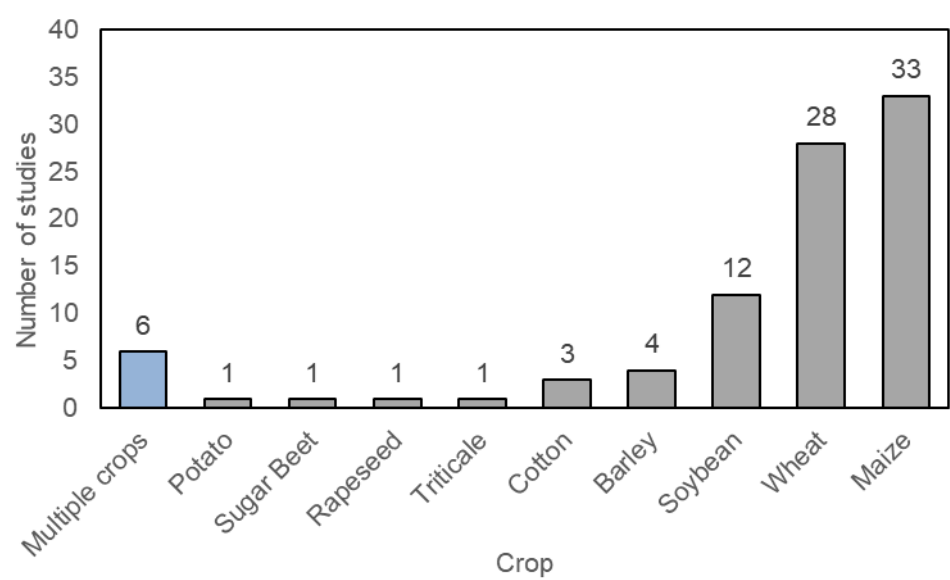


Figure Apex B-4: Number of studies by crop. If more than one crop is modelled the study is counted both the individual crops column and multiple crop column

Europe) interacting with soil characteristics and weather differently (Brogi et al., 2020). Therefore, a complete assessment of yield variability should consider several years of data covering the full crop rotation, including, when grown, different crops (Joernsgaard and Halmoe, 2003). The spatial variation in yield and nutrient use efficiency from one season/crop can also potentially have influences on soil properties for the next through the inter-annual transfer of water and nutrients (Wallor et al., 2018). Anwar et al. (2009) modelled the spatial response to different N rates in wheat and barley over two growing seasons, reporting that the low yielding zones had higher levels of nitrate N before sowing, potentially a result of the proceeding low yielding crop (*cf.* to high yielding zone) utilising less nutrients. Other rotational influences might impact crop responses, improved NUE is often reported in crops grown after an unrelated crop or following the use of cover crops (Angus et al., 2015; Constantin et al., 2011; Storr et al., 2021). Therefore, many studies using CSM for managing spatial variation are limited in their application as they reinitialise the CSM at the start of each season and then fail to track model state variables over multiple years (Thorp et al., 2007). This is also a common limitation in other modelling applications including climate change impact assessments (Wallor et al., 2018). Modelling approaches that provide a continuous simulation are intrinsically more complex and more difficult (McNunn et al., 2019). Additional information on the management of the previous crops is required, as well as suitable model inputs such as cultivar parameters that represent that crop well. Across-season modelling can also cause modelling errors to accumulate, reducing the overall performance of the model as compared to model runs of single seasons (McNunn et al., 2019).

B.4.4 Crop models

Across the studies considered, 28 CSM have been used (Figure Apex B-5). Decision Support System for Agrotechnology Transfer (DSSAT) (Jones et al., 2003) was the most widely used model (23 studies). Agricultural Production Systems Simulator (APSIM) (Keating et al., 2003) was used in 11 studies and SALUS in 9 studies. As no spatial crop simulation model has been developed specifically for the use in PA (Pasquel et al., 2022) it is perhaps unsurprising that

researchers have often used models, such as DSSAT and APSIM (40% of the studies included in this review) most widely used in other modelling scenarios (Asseng et al., 2014). It is beyond the scope of this review to identify a CSM most suitable to support PA. Appropriate model selection depends on a variety of influences including crop type, the sub-processes to be modelled, user experience and the data available for calibration (Adam et al., 2012). Of the 71 studies only 3 studies validate and compare the results from multiple models (Chen et al., 2021; Thorp and Bronson, 2013; Wallor et al., 2018). There is a need for more studies comparing the spatial-temporal performance of different models to provide users with a better understanding of modelling uncertainty in management recommendations. This concept is discussed further in B.7.

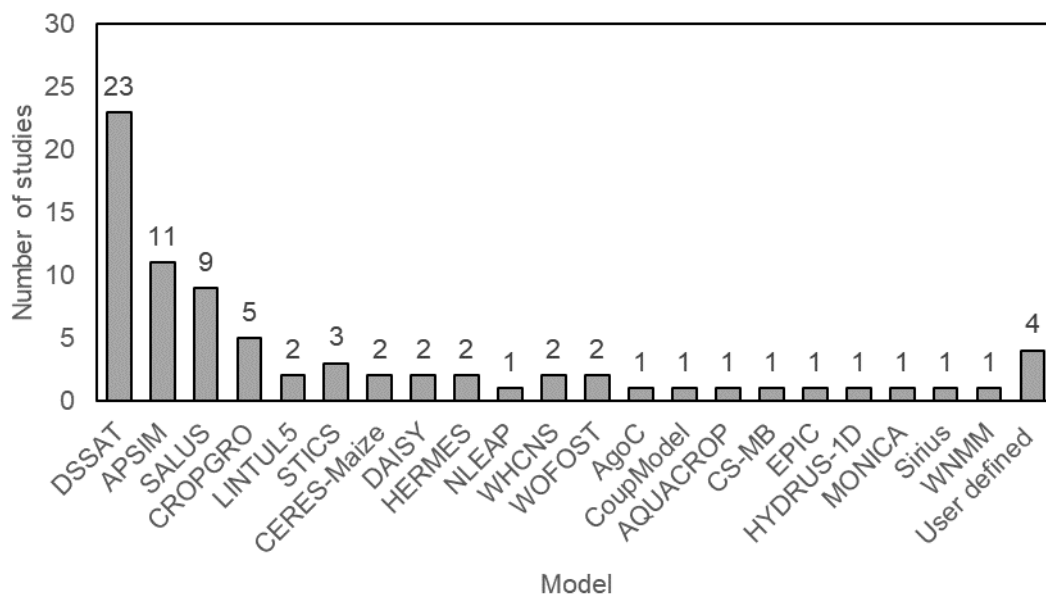


Figure Apex B-5 Number of studies by crop simulation model

B.5 Model parameterisation and calibration

Most CSM are “point-based”, parametrised for a homogenous area, usually representative of an agricultural experiment or a single field or representative soil profile (Heuvelink et al., 2010; Van Ittersum and Donatelli, 2003). Spatialising CSM is defined as applying models over an area larger or smaller than that for which it was originally developed (Faivre et al., 2004). In the context of this review, we are interested in studies that apply CSM at the sub field scale (i.e.

more than one modelling point per field). Typically, model inputs are provided at the same spatial scale as required for the model outputs (Pasquel et al., 2022). Model parameters and outputs have varying levels of spatial and temporal variability that are accounted for when spatialising a crop model (Figure Apex B-6).

Weather - Studies in this review assume weather is likely to have little impactful variation within a field (e.g. Wallor et al., 2018). However, weather does have high temporal variability, changing across minutes/seconds for precipitation for example. The majority of the CSM operate at a daily time step, requiring daily temperature, solar radiation, and precipitation data as a minimum (Jones et al., 2003; Keating et al., 2003). On-farm-operated weather stations (Carroll et al., 2011; Jenkins Yateley, 2014), national station networks (Cooper et al., 2021), or gridded weather data, demonstrated to be suitable for CSMs (Van Wart et al., 2015) mean that representative daily weather data sets are likely available for most fields. Therefore, the model parametrisation for weather variables is not examined in this review. Accurate weather data, however, is critical for spatially accurate model simulations (Heinemann et al., 2002; Nonhebel and Nonhehe, 1994; Watson and Challinor, 2013). A high level of data validation and assurance must be taken when generating a weather data sets for a field/farm.

Management - Model evaluation involves parametrising of CSMs with recorded historic management information such as sowing date, fertiliser rates/timings and observed weather and comparing simulated model outputs such as yield with those historically spatially observed. Management options can vary across both time and space with seasonal variations in operation date and application rate of seed, fertiliser inputs and pesticide applications. Management decisions are likely to vary spatially between fields and within fields if PA technology is already being implemented on farm. In technologically advanced agricultural systems, farms record this information in farm management systems to comply with agricultural standards, product quality and safety and to support management decisions (Fountas et al., 2015). It is therefore assumed that historic management data/information required for CSM calibration and validation, will in most cases

be easily available for most farms, therefore this review does not provide comment on sources of agricultural management information used in model validation.

Cultivar parameters - Farms commonly change varieties (cultivars) to address challenges such as disease and pest control as well as preferred phenological traits (Fischer and Edmeades, 2010). While cultivars typically remain consistent within individual fields, it is not uncommon to grow multiple cultivars across a farm. This practice can be driven by the need to meet different end market requirements or mitigating risks by spreading workloads and exploiting the contrasting traits of various cultivars (e.g., early, or late maturity). Inadequate cultivar parameters that are not representative of the system being modelled will lead to large sources of uncertainty in the crop model projections (Manschadi et al., 2021). This review therefore collated the methods used to obtain cultivar parameters that capture this temporal and spatial variability in varieties grown.

Soil physical properties - Soil hydraulic properties are often driven by stable soil properties such as soil texture, organic C and stone content and soil depth which are unlikely to vary considerably over short to medium timeframes (Pasquel et al., 2022). One exception to this would be when deformation occurs through compaction which can affect soil water release characteristics over shorter time frames through changes in bulk density; although most modelling studies assume temporal stability in bulk density (Gregory et al., 2010; Matthews et al., 2010). These properties can however exhibit a high degree of spatial variability within fields (Lammoglia et al., 2019) and are often expensive, time consuming and often associated with inaccuracies in measurements (Schindler, 2015). Soil organic matter comprises organic N components, which are gradually mineralised into ammonium by soil microorganisms during the decomposition of organic matter. Mineralisation provides nitrogen in plant available form (Stockdale & Gaunt, 1997). Therefore, the quantities of inorganic N and parameters influencing its mineralisation are key model parameters (Jamieson et al., 1998). A primary focus of the studies included in this review was how spatial variation in soil physical parameters, including organic carbon (C) and nitrogen

(N), is parameterized using measurements, pedo-transfer functions, and/or calibration..

Soil chemical properties and soil water content - Some soil nutrients (e.g. nitrogen), and soil water content can vary over both short temporal periods, particularly when fertiliser is applied or after leaching events (Anas et al., 2020) and fine spatial resolutions at the sub field level (Kindred et al., 2015; Marchant et al., 2012). Soil properties also vary with depth and for models to accurately describe soil-water-nutrient-plant interactions the vertical (variation in horizon properties) and horizontal (how these horizons vary across space) needs to be captured. As well as important for model parametrisation/initialisation parameters these represent key model state variables simulated across the modelling time frame, therefore represent modelling outputs as well as inputs.

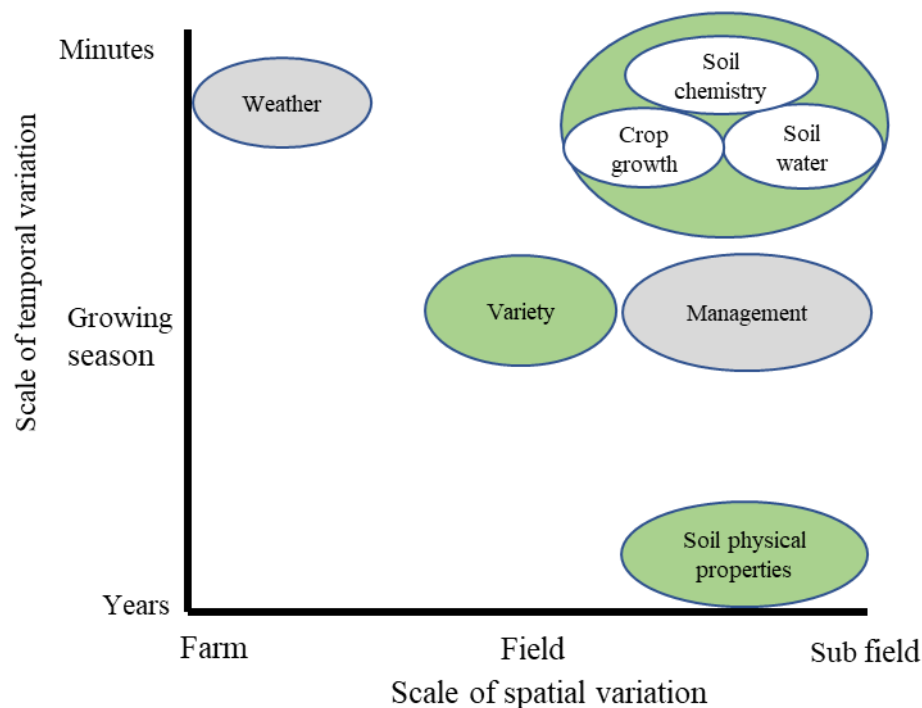


Figure Apex B-6: Conceptual diagram of spatial temporal interaction for crop model parameters, green represent those addressed in this review, white are often both input and output (simulated) parameters of CSM

Crop growth – Crop growth will change daily, based on the interactions of weather, nutrient availability, pest and disease pressure and other limiting factors. It is the primary aim of a CSM to recreate observed or simulate predicted crop growth given the inputted parameters. However, within season spatial monitoring of crop growth through remote sensing applications has allowed for models to be updated within season, based on observed leaf area index (LAI). Therefore, studies within the review which assimilate remote sensing data into model applications will also be reviewed.

B.5.1 Soil parametrisation

Point-based models can be applied spatially across an area by a process termed spatialisation (Pasquel et al., 2022). By which a model is no longer applied across field average properties assuming a homogenous field area, as originally designed (You et al., 2022) for the context of PA this is at a within field scale (Pasquel et al., 2023). Most studies in this review focus on modelling responses to within field spatial variation in soil properties and therefore require multiple parametrisations or calibrations to capture this variation in soil properties. The subsequent sections will assess the four primary methodologies employed by the studies within this review to spatialise CSM to account for variations in soil properties at a sub-field scale. These include grid sampling, zonal sampling, the use of soil survey data and parameter calibration (Figure Apex B-7).

Grid and zonal sampling rely on some form of soil sampling to parameterise the spatial variation in soil properties within a field. What properties are measured also varies between studies (Figure Apex B-8). A large proportion of studies (46 studies) measure soil texture (particle size) either through sedimentation (Wallor et al., 2018), laser diffraction, or hand/visual methods (Johnen et al., 2014). Soil texture describes the proportions of clay, silt, and sand content of soil. Soil texture is temporally stable, and has a large influence on soil fertility, porosity and water holding characteristics. It is the primary input into many Pedotransfer Functions (PTF) that allow water release characteristics to be estimated. PTF are the primary way the water holding characteristics are determined using measured

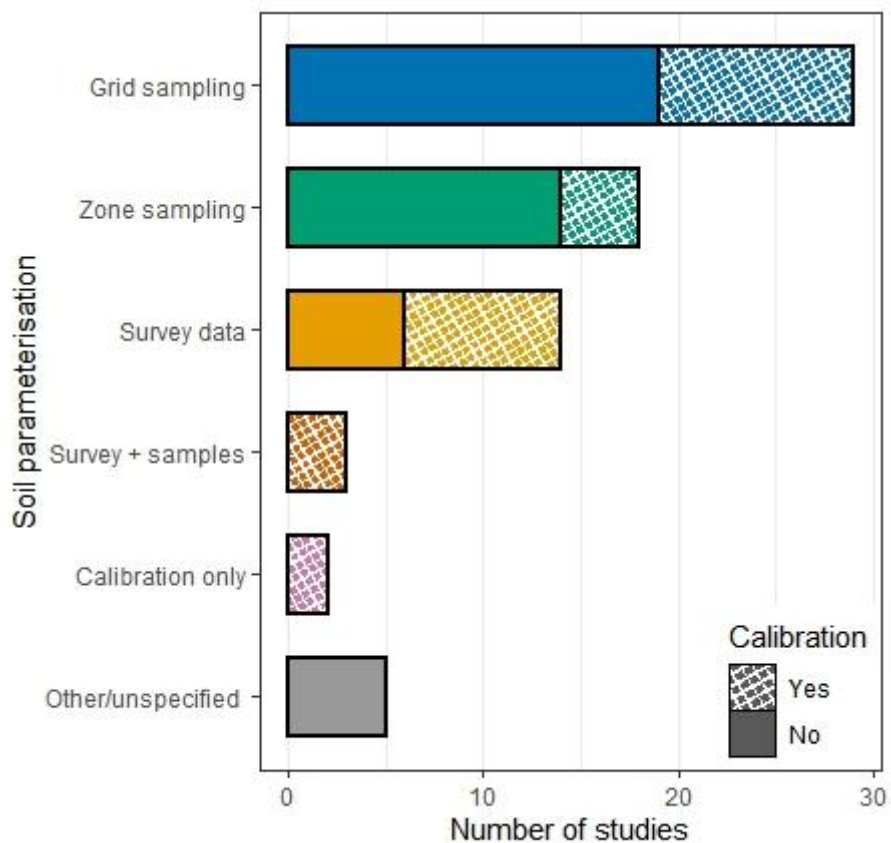


Figure Apex B-7 Number of studies by soil parameterisation method. Studies with no calibration (solid colours) used recorded soil properties only, calibration used calibration methods to obtain some soil parameters that were not measured (hashed colours).

data (Figure Apex B-9). Soil organic carbon (SOC) or soil organic matter (SOM) (often measured as a proxy for SOC) was also measured in a large proportion (27) of studies. Like texture SOC is a key predictor variable in many PTF estimating soil water holding characteristics (Patil and Singh, 2016a). It can also allow for the estimation of soil organic N content (Shepherd et al., 1996), which a proportion is mineralised to provide soil N supply to crops, a process simulated in many CSM (Jamieson et al., 1998; Jones et al., 2003). The estimation of soil organic N from SOM/C has inherent limitations, not accounting for local soil organic matter dynamics and composition (Shepherd et al., 1996). Likely in recognition of this, a proportion of studies (8) measure soil organic N directly.

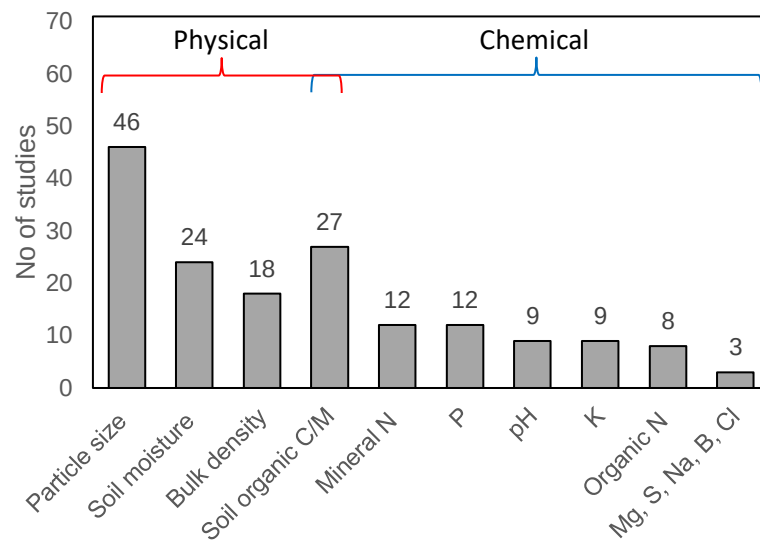


Figure Apex B-8 Soil properties measured spatially by number of studies

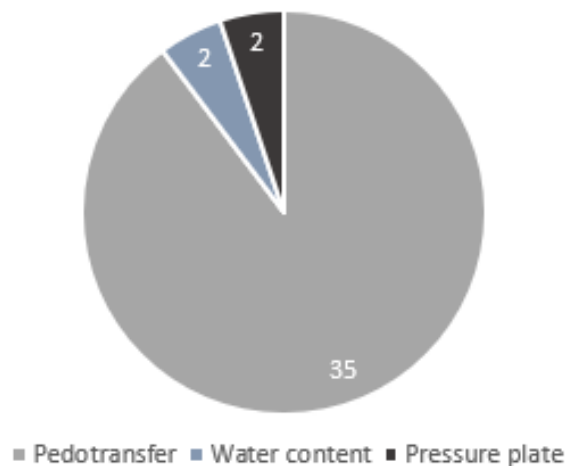


Figure Apex B-9 Methods used by studies using measured properties to generate spatially specific water holding characteristics.

The measurement of soil moisture in 24 studies has study specific purposes. In climates where overwinter or in season rainfall is often not sufficient to fully recharge soil moisture (field capacity) initial soil moisture parameters can be influential in model simulation results. Therefore, in model evaluation exercises this can be measured at sowing to ensure accurate model initiation (e.g. Anwar

et al., 2009; Basso et al., 2011b; Delgado et al., 2005). Where initial properties are not measured simulations can be run prior to sowing, based on observed weather patterns to obtain a simulated starting soil moisture (Anwar et al., 2009). Although rare, a sensitivity analyse to initial starting conditions, would confirm the importance of these measurement in a system prior to modelling applications. Another primary purpose of soil moisture is for model evaluation purposes. Many studies use CSM to inform on the spatial response within field to plant available water, requiring the accurate simulation of spatial temporal variability in soil water contents (e.g. Albarenque et al., 2016; Batchelor et al., 2002; Cammarano et al., 2020). The measurement of soil moisture when the soil is believed to be at field capacity (i.e. overwinter or after irrigation) and when close to permanent wilting point (can be directly entered as these respective CSMs parameters (e.g. Braga and Jones, 2000; Fraisse et al., 2001). Although less common than using pedotransfer functions, 2 studies use this method for parametrisation (Figure Apex B 7) (Ma et al., 2016; Wong and Asseng, 2006).

Soil mineral nitrogen (N) is measured in a limited number of studies for the purposes of either model initiation or validation of soil N supply (Cammarano et al., 2020; Chen et al., 2020a). Other soil nutrients and properties, such as phosphorus (P), potassium (K), magnesium (Mg), and pH, are often assessed to eliminate other potential nutrient limitations that are not often accounted for within CSMs.

Grid sampling

Grid sampling techniques are the most popular method of obtaining spatially relevant soil properties for model parametrisation, used as the only source of soil information in 19 studies (27%). Grids can either be regular, distributing sampling nodes equally across the study area (e.g. Basso et al., 2001; Chen et al., 2020; Ma et al., 2016) (Figure Apex B-10) or irregular, distributing sampling points unequally, but stratified to cover all possible variability (e.g. Basso et al., 2011b; Tewes et al., 2020). While the latter is not a grid, by definition, its intention is to cover the spatial area of the field without any predetermined knowledge of the

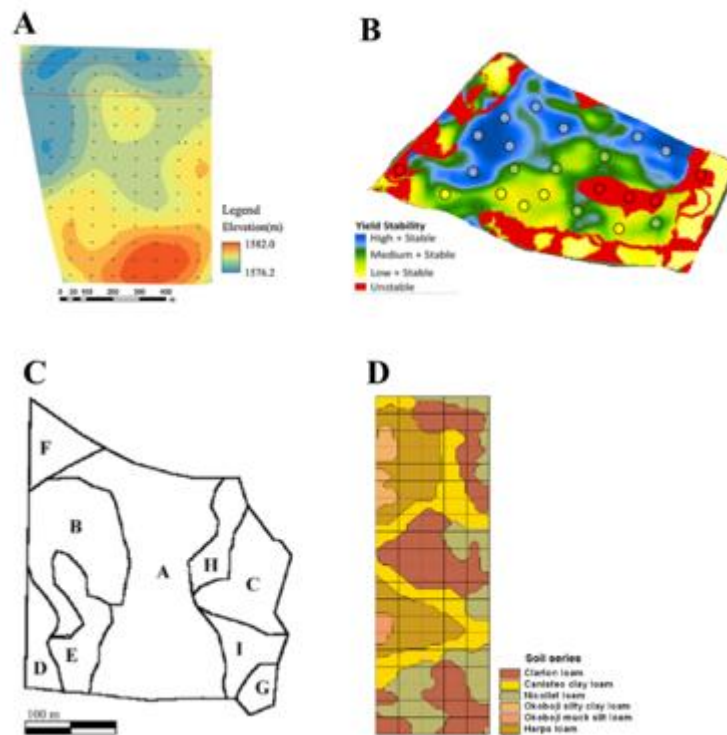


Figure Apex B-10 examples of parameterisation by A; grid sampling (Chen et al., 2020) , B; multiple points per management zone (Cammarano et al., 2021), C; Single sampling points per management zones (Nijbroek et al., 2003), and D: soil survey data (Thorp et al., 2008)

spatial variation within the field, therefore we classify it as grid sampling in this review. In its simplest form soil samples can be taken in a structured grid and all CSM parameters can be either measured or calculated (e.g., using PTFs) and the spatialised model can be run at the same footprint of each of the grid cells/points of measured parameters (Chen et al., 2020a). Model outputs can either be reported at the sampling scale or interpolated over the entire area using geostatistical techniques such as kriging (Chen et al., 2021; Pasquel et al., 2022).

For fundamental research using CSM to manage spatial variation, grid sampling likely ensures spatial variation in soil properties and its influence on crop growth is most accurately attained (Muhammed et al., 2017). The finer the grid resolution the better the spatial variation in soil properties is captured (Gotway et al., 1996;

Rafael Nanni et al., 2011) although every field is likely to have a different optimal sampling resolution, based on the scale of the variation and the potential economic benefit of spatially explicit management (Rafael Nanni et al., 2011). Soil mapping using gridsampling strategies is a popular application of precision agriculutre, with an estimated 38% of cereal farms in the UK soil mapping (Lowenberg-deboer and Erickson, 2019). However, this is typically for topsoil nutrient content and pH only, relatively inexpensive measurements. Crop simulation models require detailed description of soil characteristics for the complete rooting zone. It is therefore recognised that spatially parametrising a model through grid sampling alone is not financially feasible across large areas, or even relatively small areas outside of experimental studies (Basso et al., 2007; Mittermayer et al., 2022). Figure Apex B-11 shows the studies in this review for which total study area (hectares) and number of sampling points could both be accurately ascertained or estimated (53 studies, 75%). For studies less than 10 ha in size, grid sampling is the most common method of parametrising soil properties (9/12 studies, 75%), with an average sampling resolution of 16

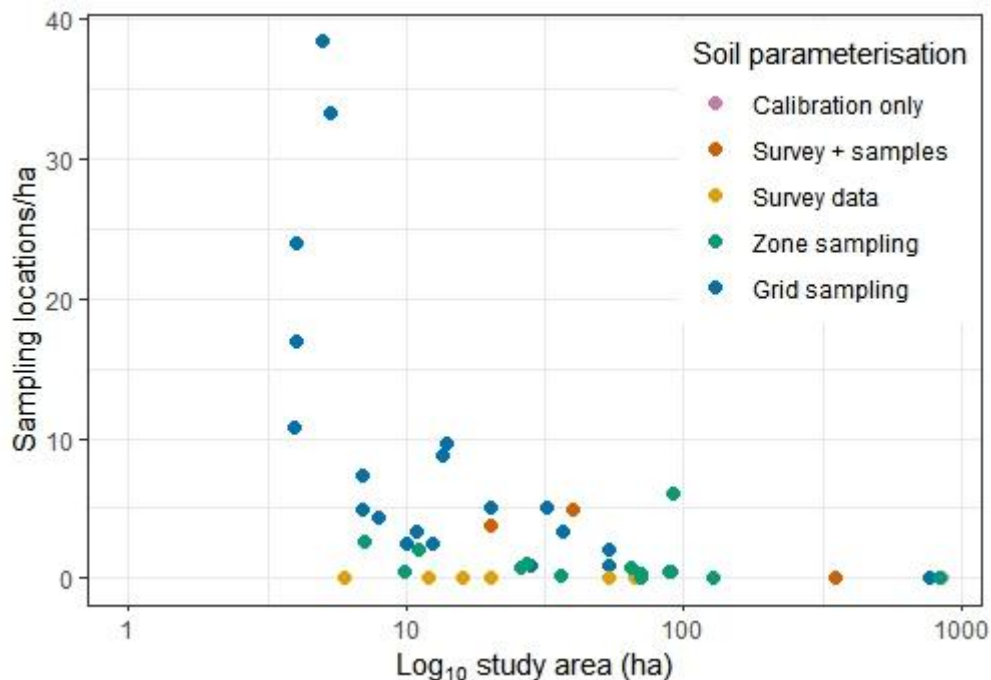


Figure Apex B-11: Study area Log₁₀ transformed in relation to number of sampling points used for obtaining soil parameters

sampling locations per ha. For studies over 10ha grid sampling is used in just

35% of studies (14/43 studies) with an average grid sampling resolution falling to 4 sampling locations per ha. When the average sampling density (number of sample locations per hectare) of studies utilising some form of soil sampling for model parametrisation is plotted against study area, both log₁₀ transformed, it becomes evident that there is a need to reduce sampling intensity as scales increase (Figure Apex B-12). As studies move away from a single experimental field and to scales more representative of that required for CSMs to inform decision making on farm, researchers generally employ strategies that reduce the number of sampling points, for determining soil parameters such as zonal sampling strategies (Mittermayer et al., 2021).

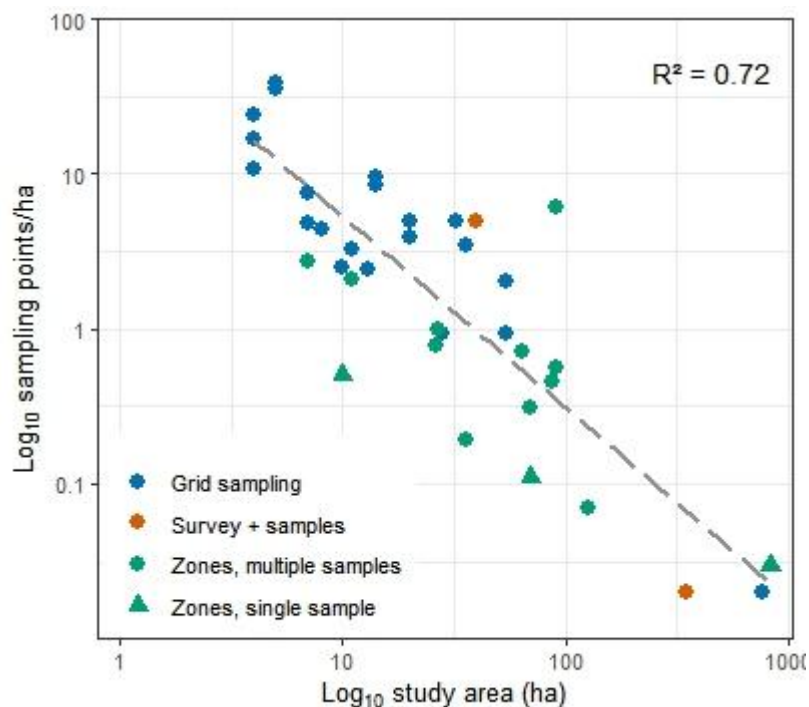


Figure Apex B-12: Study area (Log₁₀ transformed, ha) in relation to the number of sampling points (Log₁₀ transformed, points per ha). The R² value represents the strength of the relationship on a log-log scale.

Management zone sampling

The delineation of management zones aims to balance the need for measured soil properties for model parametrisation, whilst reducing the amount of soil sampling locations required to capture spatial variation in soil properties (Basso

et al., 2001). Management zones are defined as a sub-region of a field that expresses relatively homogenous yield limiting factors for which a single management strategy can be applied (Doerge, 1990). Sampling can then be targeted within these zones to determine soil properties assumed to be representative of the zone as a whole (Frogbrook and Oliver, 2007). Of the studies in this review 20% (14 studies) use predefined management zones to target soil sampling and provide spatial units for modelling results. There is an entire scientific discipline on methods to delineate management zones through grouping spatial units, often grided variables of soil or plant measurements, resembling each other more strongly than those within other zones (Lark, 1998), however there is no single widely adopted method (Guastaferro et al., 2010a). Within this review, studies investigated use a variety of methods including: clustering algorithms (Albarenque et al., 2016; Pedersen et al., 2021; Tagarakis et al., 2019); the use of multi-year means of standardised measures and stability measures (Anwar et al., 2009; Cammarano et al., 2020; Dixit and Chen, 2010); and the use of primary outputs from geophysical or topographic surveys (Brogi et al., 2020; Fry et al., 2017; Hoffmann et al., 2017). Management zones have been identified from single layers or combination of data layers (Nawar et al., 2017). Within the studies in this review data layers used included: yield maps or remotely sensed canopy reflectance images (Anwar et al., 2009; Cammarano et al., 2020; Oliver and Robertson, 2009; Wong and Asseng, 2006); soil apparent electrical conductivity or topographic (elevation) properties (Albarenque et al., 2016; Brogi et al., 2020; Fry et al., 2017; Hoffmann et al., 2017; Tagarakis et al., 2019); or a combination of yield or remote sensing plant indices and soil or topographic properties (Fraisse et al., 2001; Nijbroek et al., 2003). Yield data is among the commonest agronomic measure used for delineating management zones, although using this alone can be inefficient at determining zones (Nawar et al., 2017). Management zones based solely on yield performance can be poorly correlated to variation in soil properties that may not limit yield but might deliver economic or environmental benefit from alternative management practices i.e., excessively high soil nutrient concentrations (Muhammed et al., 2017). However,

Oliver and Robertson, (2009) showed that the misclassification of management zones and yield limiting factor often only has small impacts on profitability.

Once management zones have been identified, soil properties representative of the management zones as a whole need to be obtained. Several methods are used to obtain representative soil parameters. The most intensive method is to sample at multiple specific locations within each zone providing a context of the variation of soil properties within zones (Figure Apex B-10B). Brogi et al., (2020) sampled horizon type and thickness at 100 locations and grain size distribution at 552 sites over 18 zones across 552 ha. Cammarano et al., (2020) sampled on average at 8 locations within 3 yield performance zones across an 11ha field. Despite employing intensive strategies like these, the typical sampling density in studies using multiple point zonal sampling approaches averages 1.2 sample locations per hectare. This figure is notably lower than the 9.0 sample locations per hectare for grid sampling methods. While zonal sampling does decrease the sampling intensity, it may still be too demanding to maintain economic viability as a sampling technique for model parametrisation. Moreover, it remains at a finer resolution than commercial soil nutrient sampling strategies, typically sampling at a 1 ha resolution (Marchant et al., 2012). With a UK average field size of around 12 ha (Vickery et al., 2002) the soil properties required for measurement at more than 12 locations a field will likely prove to intensive for an economically viable parametrisation strategy.

The least intensive sampling method is to sample a single representative location within each zone assuming uniform soil properties within the zone (Nijbroek et al., 2003; Oliver et al., 2010) (Figure Apex B-10C). This does not provide any information of within zone variation in soil properties and sampling/measurement errors are likely to be more influential than if part of a mean made up of multiple locations within a zone. Hence, greater caution is necessary when delineating management zones, ensuring that homogeneous performance within zones arises from homogeneous soil properties within that zone. While not extensively used in the literature proximally sensed soil scans could serve as a tool in establishing a relationship between zone yield performance and underlying soil

properties before sampling. This would allow for targeted soil measurements to be conducted, facilitating the creation of location-specific relationships between measured soil properties and spatial soil scans. Brogi et al., (2020) used apparent Electrical Conductivity (ECa) survey at 6 depths across 90 ha in Germany to derive 18 zones with similar ECa and through 100 profile investigations were able to generate model parameters from the 18 soil layer descriptions. Wong and Asseng, (2006) determined Plant Available Water Capacity (PAWC) from 8 locations across the variation in yield in a five-year combined yield map for a 10ha field in western Australia. They found that soil ECa mapped across the area strongly correlated to PAWC ($r^2 = 0.78$) and therefore was able to transform a kriged ECa map into PAWC and using model response to the range of PAWC was able to extrapolate model responses across the field area. Hoffmann et al., (2017) also demonstrated how using ECa maps and how low spatial resolution targeted sampling (9 samples across 127 ha in one field) can be used to parametrise CSM (APSIM) where there is a strong influence from soil texture and/or soil depth. The application of management zone delineation to decrease soil sampling is likely a pivotal tool in spatialisation of CSM. However there remains limited evidence of its effectiveness across extensive areas beyond a few fields. Further efforts are needed to integrate spatial datasets such as yield maps and proximally sensed soil scans to enhance sampling efficiency.

Soil survey data sets

The use of soil survey data to obtain spatially explicit soil parameters drastically reduces the cost of parametrisation, as it can mean no soil sampling is required (e.g. Shuai and Basso, 2022) (Figure Apex B 10D). Soil survey data is used in 23% of studies (16 studies). At the highest resolution, studies use detailed first order (Franzen et al., 2002) soil surveys available for the study location (Irmak et al., 2006, 2002; Paz et al., 1999). Such data sets are likely limited in the availability and not likely to be a widely applicable method of parametrisation. Even at scales less than 1:1,000,000, survey data only covers about one third of the total global terrestrial area (Hartemink et al., 2013; Ranst, 2003). A common approach is extracting soil information from digitised county and national soil

survey data, including SSURGO in the USA (e.g. Jin et al., 2017; McNunn et al., 2019; Shuai and Basso, 2022) and CanSIS in Canada (Jégo et al., 2012). Even where relatively high-resolution soil survey data is available the ability to describe sub field variation in crop performance from them, and subsequently as tool for PA has been criticised (Bobryk et al., 2016; Jin et al., 2019). There are limitations on what parameters survey data can provide. It is primarily only used to supply relatively steady state variables such as texture, bulk density, and water release characteristics. Soil organic carbon and nitrogen, nutrients and moisture contents that are temporally less stable either need to be estimated (e.g. Thorp et al 2005) or measured (e.g. Paz et al., 2003). One approach to overcome the insufficient spatial scale of survey data to describe within field variation is to assign properties of known soil series based on other geospatial attributes. Jin et al (2019) assigned the least, medium and most productive attribute tables to the least the medium and most productive areas of a field respectively. This approach appears to be the most plausible method for leveraging survey data to spatialise CSM when the resolution is insufficient to explain the observed spatial variation. A lookup table containing plausible soil physical properties derived from local survey data could be employed to calibrate the model, aligning it with observed spatial variations such as crop yield. Using the profiles for zones that provide the best model fit. However, it is likely that, at the very least, sampling of topsoil nutrient and organic nitrogen content will be necessary, as these factors can be influenced by broader land management practices rather than just soil geomorphology. The comparison of survey obtained parameters compared to measured parameters is limited. Tewes et al (2020b) compared pedotransfer derived plant available water from measured and data extracted from SoilGrids™, a global map of soil profile information generated from profile samples and environmental map layers. They demonstrated no strong relationship between the measured and the SoilGrids plant available water across 14 fields in Europe. While the LINTUL5 model accuracy was not significantly better than the soil grids data in modelling within field heterogeneity, this was largely down to poor model performance at modelling water stress.

It's unlikely that soil survey data is currently sufficient resolution spatial for accurate determination of crop model input for describing within field spatial variability in soil properties for modelling purposes.

Calibration of soil parameters

Soil properties needed for CSM parameterisation can be expensive and labour intensive to obtain across large areas. Therefore, soil parameters are often estimated by calibration (inverse modeling). Calibration involves fitting the model to observed data through parameter adjustment or using a parameter search technique (Sanft and Walter, 2020). Among the reported studies in this review, 27 (38% of studies) undertake some form of soil parameter calibration, with two studies relying entirely on calibration for obtaining soil parameters (Figure Apex B-7).

There is no consensus on the best method for calibrating crop models, even within the same model structure or data sets (Wallach et al., 2021). Most models don't offer an automated calibration procedure, requiring external coupling of model software with a chosen calibration program or algorithm. The computationally simplest way to obtain soil parameters is through trial and error. Fry et al (2017) used measured data for soil texture and bulk density to obtain soil water physical characteristics but manually adjusted the runoff curve number fitted with a single year of soybean yields at 19 sites across two fields. Jones and Barnes (2000) adjusted soil water holding capacity until model predictions of LAI were consistent with remotely sensed estimates. Manual adjustment methods can allow for greater supervision over the calibration procedure (Wallach et al., 2021). However, adjusting parameters by trial and error to optimise calibration would become cumbersome for multiple location with spatially variable parameters (Zanella et al., 2015). Therefore, more efficient automated methods are required for spatialising CSM to support PA. Automatised optimisation algorithms also ensure user bias doesn't impact calibration results (Ma et al., 2016).

There are various parameter search techniques in the literature, with different computational complexity, but generally these search through feasible values

within a multidimensional space with the goal of minimising an objective function (Braga and Jones, 2000). Within the studies in this review methods include simulated annealing (Braga and Jones, 2000; Miao et al., 2006; Paz et al., 1999; Thorp et al., 2015), Generalised likelihood uncertainty estimation (Lammoglia et al., 2019), Bayesian melding (Finley et al., 2011), genetic algorithms (Timlin et al., 2001) among others. More important than the method is the choice of parameters to calibrate, and the data sets used to fit the modeling parameters (Braga and Jones, 2000). Which and how many parameters to calibrate also requires careful consideration. If too many parameters are calibrated, parameters might fit a calibration data set well but be poor predictors of future drivers of spatial variation (Wallach et al., 2006). The most calibrated soil parameters are soil water retention characteristics (field capacity and permanent wilting point), soil hydraulic conductivity, maximum rooting depth, and drainage and runoff characteristics (Batchelor et al., 2002; Fry et al., 2017; Jin et al., 2019). These are crucial for model performance in rain fed systems but are expensive and difficult to measure (Braga and Jones, 2000).

The simplest calibrations calibrate a single parameter not available through measured data or could be calculated through PTF. Fry et al (2017) and Irmak et al (2006) adjusted the soil water flow parameter “runoff curve number” in DSSAT for subfield locations to obtain the best fit between simulated and observed yield. Cheng et al (2019) estimated soil mineral nitrogen supply through differences in remotely sensed LAI. Johnen et al (2014) used a mixed approach first calculating water release characteristics for each spatial unit from soil texture classes, then in locations where measured soil moisture in June/July (assumed to represent permanent wilting point (1500 kPa) differed from simulated values the texture class was changed. Then the saturation water content was adjusted at location where simulated soil moisture values differed greatly from measured soil moistures in early spring. Jin et al (2019) adjusted maximum rooting depth in the APSIM model to reflect spatial variability in water table depth. While the above studies use this calibration as a way of obtaining parameters that are not measured, they still often rely on primarily measured data for model parameterisation.

Yield data is the predominant data set used to spatially calibrate soil parameters (e.g. Finley et al., 2011; Fry et al., 2017; Zanella et al., 2015). Yield data are widely collected through combine yield maps (Lowenberg-deboer and Erickson, 2019), often available over multiple years (Blackmore et al., 2003; Muhammed et al., 2016) and yield is generally the primary response variable of interest (i.e. economic output). However, it is necessary that the parameters being estimated are identifiable within the data sets used to calibrate them. i.e. they have a direct and quantifiable influence on the data being used for calibration (Wallach et al., 2014); a concept termed parameter identifiability (Luo et al., 2009).

Several studies in this review highlighted parameter identifiability as a significant limitation in the calibration of spatially relevant soil parameters. Lammoglia et al (2019) demonstrated using a sensitivity analysis how multiple parameters can influence the spatial variation in yield for a single year, and the influence of these parameters is not temporally stable, for example in wet years plant available water capacity has little impact on yield and therefore calibration would be poor if a wide range of seasons are not included in the calibration. This has been evidenced by Thorp et al (2007), in their study validation errors of the DSSAT model decreased by 32% when 5 years of maize yield data, compared to 2 was used in model calibration. This reliance on sufficient temporal spatial data sets poses a significant challenge for model soil parameterisation via calibration; for instance, in the UK, the range of simulated yield losses due to drought averages over 3 t ha⁻¹ when 20-years of yield loss data is included in the calculations (Figure Apex B-13). However, this range decreases by 43% (to 1.8 t ha⁻¹) when calculated with 5 years of data on average (Clarke et al., 2020). As of 2019, more than a quarter of farms using combine yield maps in England have adopted the technology since 2012 (DEFRA, 2020, 2012). With a single crop unlikely to feature more than in 50% of cropping years, it is unlikely that many farms currently have sufficient yield map data to adequately capture the extremes of temporal variability in weather and the spatial response to this. Any calibrations would also

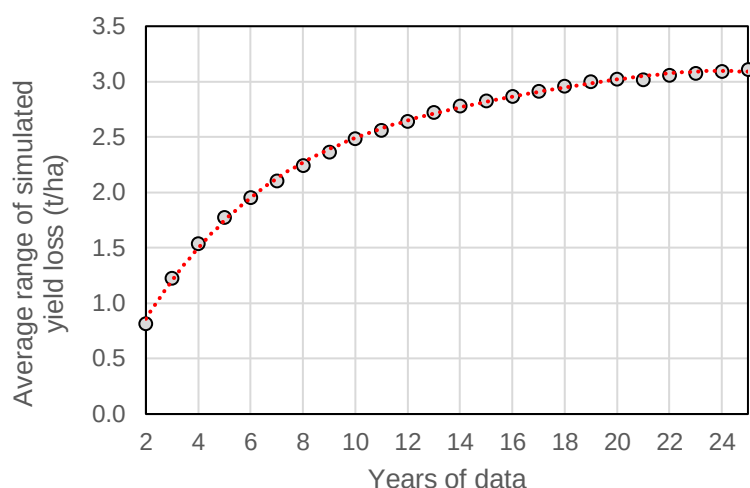


Figure Apex B-13 Average simulated range (maximum simulated loss – minimum simulated loss) of yield loss due to water limitations for rainfed wheat in Cambridge UK depending on how many years of data included in calculations. Yield loss data extracted from 106 years of simulated wheat yields from observed weather data (Clarke et al., 2020).

warrant a large proportion if not all the data set to be used in calibration leading to suboptimal validation data sets (described further in B.6.1), however techniques such as leave-one-out cross validation can help overcome this (Thorp et al., 2007, 2005). Calibration data itself often contains inherent variability and errors (He et al., 2017a). This is likely to be large for on-farm combine harvester yield map data sets, which are well documented to have potential sources of significant error (Blackmore and Marshall, 1996; Morgan, 2020). Consequently, temporal and spatial inaccuracies in these data could lead to poor estimates of soil parameters.

Using crop data in the objective function can result in inaccurate parameters, as crop growth can also be influenced by external factors not represented in the model, such as disease, weed, pest pressures, and nutrient deficiencies outside those accounted for in the model. This can lead to attempts to adjust soil parameters to account for yield and growth responses that are unrelated to the parameters being calibrated. It is therefore recommended that calibration data

sets should be directly related to the parameter being estimated, such as soil moisture to calibrate soil hydraulic properties (Fraisie et al., 2001). Braga and Jones, (2000) reported that using yield data for parameter estimation led to acceptable errors in modelled yields but large errors in modelled soil moisture contents, while using soil moisture as the metric for optimisation lead to acceptable errors in both simulated yield and soil moisture. However, the measurement of such parameters spatially is unlikely to be viable across commercial farms.

In summary, while calibration methods can be useful for estimating soil parameters, they often fall short in providing reliable and accurate parametrisation across diverse conditions. The necessity for extensive and temporally variable data sets poses a significant challenge for on-farm applicability (Pasquel et al., 2023), particularly when relying on yield data that may not adequately capture the influence of specific soil parameters. Given these limitations, calibration may not always be the optimal approach for CSM soil parametrisation. Instead, integrating measured data wherever possible and combining it with calibration for the parameters that are most challenging to measure might offer a more balanced and effective strategy. Furthermore, the use of CSM on farms requires the trust and understanding of the end user. Therefore, spatial variation quantified through tangible measured parameters might be seen by the end user as a more trustworthy source.

B.5.2 Crop cultivar coefficients

Most CSM require cultivar-specific parameters describing the growth and development of the species and allow for the description of traits between cultivars within these species. The complexity of these parameters varies between models but commonly consists of 10-40 species/ecotype parameters and a further 5-15 cultivar (within species) parameters (Wallach et al., 2014). The miscalculation of cultivar specific parameters describing phenological development and crop growth is a major source of crop modelling errors and uncertainties (Manschadi et al., 2021) and is attributed to poor model performance within this review (e.g. Batchelor et al., 2002; Joshi et al., 2019;

Shuai and Basso, 2022). For reliable modelling outputs cultivar parameters require careful calibration using high quality measured data along with robust validation procedure (Coudron et al., 2021; He et al., 2017b). The calibration of cultivar parameters often relies on experimental data from research stations, with the selection of calibration data often driven by data availability rather than specific considerations for the applicability for model use (Xiong et al., 2008). For studies attempting to model a general agroecological system validation data sets for a previously calibrated cultivar can be sought (e.g. Clarke et al., 2020), or a previously calibrated and validated cultivar can be applied directly (Cho et al., 2012; Senapati and Semenov, 2020). While models being applied to directly inform on farm management decisions will require cultivar specific parameters representative of those of the application context and on-farm data sets being used for model evaluation and application.

There is large diversity in genetic material grown across farms. For example, the most popular variety grown in the UK occupied only 14% of the total wheat area in 2022 (AHDB, 2022). New cultivars are released frequently, resulting in high turnover of varieties across years (Figure Apex B-14). Varieties within a specific agroecological system (i.e. country or region) can display large variance in phenological and crop growth characteristics. The flowering date of modern Northern European wheat varieties can vary by up to 14 days, meaning conditions at key growth stages might be different between cultivars (Sheehan and Bentley, 2021). Nutrient use efficiency has also been shown to vary in UK elite wheat varieties (Barraclough et al., 2010a). Therefore, the calibrated parameters of a variety will potentially become obsolete if farms switch to varieties with considerably different growth characteristics (Joshi et al., 2019). The studies in this review employ various methods of obtaining cultivar parameters that reflect those of their studies (Figure Apex B 15). The following section will review these methods and discuss their applicability for on farm applications of CSM.

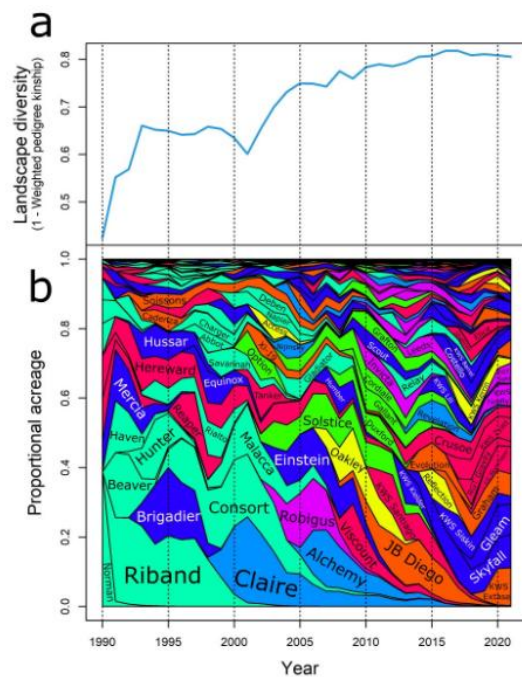


Figure Apex B-14 A: diversity of wheat grown in England since 1990. B: proportion of area of wheat varieties from NIAB Seed Stats service (graph produced by Nick Fragley)

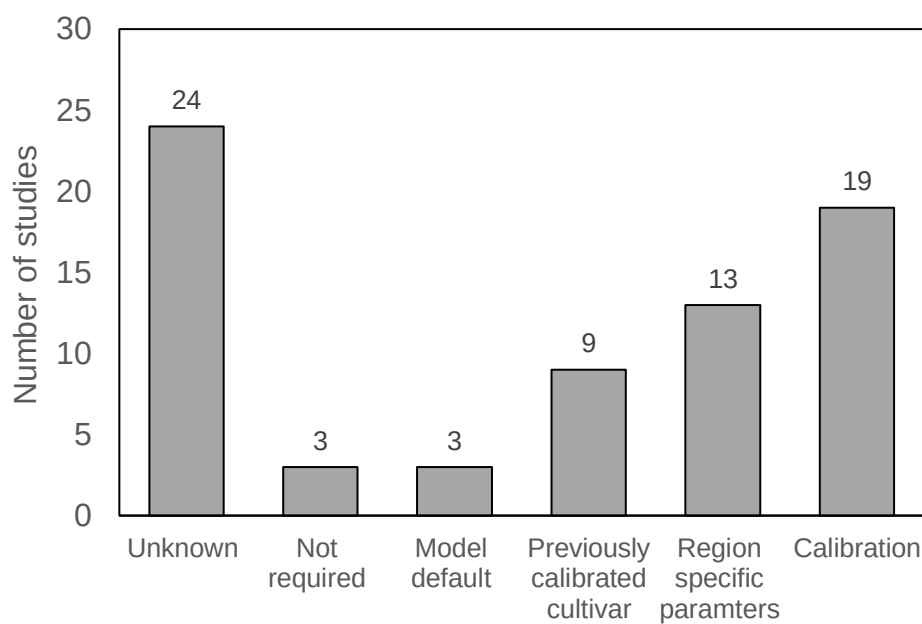


Figure Apex B-15 Methods used for obtaining cultivar parameters

Unspecified, default parameters or parameters not required

One third of studies (24, 33%) failed to describe cultivar parameterisation methods (e.g. B. Basso et al., 2009; McNunn et al., 2019; Thorp et al., 2008). The absence of detailed information on calibration methods employed by modelers and the lack of model calibration guidelines are acknowledged as challenges in crop modelling literature (Seidel et al 2018). This review highlights the necessity for modelling research to enhance transparency regarding the procurement of cultivar parameters and to define any associated limitations in these methodologies.

A small proportion (3) of studies used default parameters provided within their chosen model. It must be assumed these were demonstrated outside of the published information to represent that of the cultivar(s) grown within the study (Fry et al., 2017). Default model parameters are unlikely to be representative of cultivars grown in a large proportion of systems (Dente et al., 2008) and therefore this approach is not seen as a suitable method for the wide scale application of CSM to manage spatial variation on farms. A further 3 studies used models either designed within the study or do not have capability for cultivar specific parameters.

Calibration within the study

When suitable cultivar parameters are not available for the system being studied calibration of cultivar parameters is required to improve simulated responses to climatic, soil and management factors (Rosenzweig et al., 2013). From the studies identified in this review 19 (27%) undertake some form of cultivar parameter calibration. Differences between models, data sets required, model structure and modelers preference mean there is no standard approach to crop model calibration (Seidel et al., 2018). However, its generally agreed that there are optimal data sets and strategies for obtaining accurate cultivar specific parameters (He et al., 2017a; Hunt and Boote, 1998; Rosenzweig et al., 2013; Seidel et al., 2018). In summary:

- Data should include contrasting conditions and environments, with sufficient years in relation to the number of parameters being fitted to avoid overfitting.
- Data sets should contain at least the date of main phenological stages, yield components, and biomass at harvest .
- It generally preferred to calibrate in stages, first fitting the model to phenology data, then to other crop variables such as yield components.
- While calibration by trial and error does allow greater supervision over the calibration procedure it is computationally time consuming and can lead to bias. Therefore, automated methods such as a simplex algorithm searching for optimal parameter values (e.g.Nelder and Mead, 1965) is recommended (Wallach et al., 2023).

The high quality, high temporal resolution data sets required limit the applicability of calibrating cultivar parameters from on-farm agronomic data sets, often just comprising of combine yield data(Jin et al., 2017). Zanella et al (2015) calibrated crop parameters based on two years of combine harvester yield data for maize. Approaches which only use final grain yield is like to lead to a poor estimate of parameters (Boote et al., 2016). Other studies recognise the limitations of farm data sets for model calibration therefore set up more experimental research designs within fields to calibrate crop coefficients. These generally involve monitoring phenology and LAI or biomass through the season and final grain yield across multiple sites within the study field(Chen et al., 2021; Johnen et al., 2014; Ma et al., 2016). However, due to the extensive field work required such methods are often limited to a single year of data (Dixit and Chen, 2010; Fraisse et al., 2001; Ward et al., 2018). Joshi et al (2019)collected biomass samples across two years alongside farm collected yield map data, however such methods are likely to labour intensive for wide scale modelling applications. Where large scale research grade field studies were not possible number of other methods of calibration were performed including:

- Satellite data – While the assimilation of remote sensing data has the potential to improve parameter estimation (Jin et al., 2018). Jin et al (2017)found the availability of images through the growing season

restricted the applicability. While they found that update parameters performed better than the model default parameters, they were not compared to more conventional calibration techniques for that variety.

- Independent data set – recognising on farm data sets suitable for model evaluation but not calibration Morari et al (2018) calibrated the Italian wheat variety cv Biensur using an independent experimental data set.
- Provided by the seed company/breeders – (Basso et al., 2011b) used coefficient reported directly from the seed company. While information on some parameters are likely to be recorded it's unlikely wide scale recording on all crop model parameters is performed by breeders, and there is no guarantee these will be shared.

Previously calibrated parameters

A method that does not depend on site- or variety-specific calibration but aims to consider local cultivar-specific traits is the use of calibrated parameters from a previous study. The cultivar featured in 9 studies (13%) had previously been calibrated for the model being applied (e.g. Cammarano et al., 2021; Cheng et al., 2019; Finley et al., 2011). In these situations, it's likely the researchers had some control over the variety grown or identified a study site that featured a previously calibrated cultivar. Only a very small proportion of cultivars within a region are currently calibrated for modelling purposes (Fukui et al., 2015). Consequently, finding appropriate parameters for a specific variety in the existing literature for a given model is unlikely. A logical next best approach is therefore utilising parameters previously calibrated for a cultivar representative of those cultivated in the study application, which share similar phenological development and growth characteristics. Within this review 13 studies (16%) use previously calibrated parameters said to be similar to that of that grown in the on-farm application (e.g. Jin et al., 2019; Shuai and Basso, 2022; Thorp et al., 2007). The modelling process involves a set of mathematical equations that “represent” the system, while the simulation process produces numerical results (e.g., yield) that “represent” the system's behaviour. Cultivar parameters that accurately represent the breadth of cultivars within the system could be calibrated using high quality

experimental data sets and protocols. These parameter datasets would allow off the shelf parametrisation reducing the complexity of applying CSMs on farms.

It's important to recognise that current nitrogen management strategies, such as estimated soil N supply-based methods (AHDB, 2023a) and national appraisals of optimal N management (Kindred et al., 2018), do not account for variety-specific responses beyond classification into broad end-market groups. Therefore, care should be taken in advocating for excessively detailed calibration procedures using suboptimal data sets if they constrain the ability of CSMs to potentially inform on-farm management decisions. Likewise, it is also important that any on-farm applications demonstrate the suitability of any previously calibrated parameters, through appropriate model evaluation.

It is recognised that there is a lack of access to available data sets suitable for multi-cultivar calibration exercises that would allow the generation of a library of cultivar specific parameters (He et al., 2017a; Peng et al., 2020). Studies have shown how high-quality field trial data with sufficient in-season and end of-season measurements can be used to parameterise multiple cultivars within an agroecological system (Fukui et al., 2015; Mongiano et al., 2019; Perondi et al., 2022). Such databases would allow modelers to select the variety, or one representative of the field/farm for which they are looking to develop modelling applications or generate them, based on the model(s) they are using. Such databases have wider applications, there is the potential for varieties best suited to the agroecological conditions within and across fields to be identified through modelling exercises. Variable cultivar selection has also been identified by farmers as a potential practice that could provide improved net returns (Batchelor et al., 2002). This has been confirmed using the calibrated parameters of 70 soyabean variety's that optimal cultivar choice could vary spatially across field (Paz et al., 2003). While few other modelling studies exist, modern wheat varieties have also shown specific adaptation to soil type (Smutná and Tokatlidis, 2020).

Access to genetic coefficients covering the varieties grown in a validation data set and those in which management decisions are to be derived is key for

application of CSM to manage spatial-temporal variation on farm. On farm data sets are sub-optimal for the calibration of site-specific parameters, it seems more suitable to pursue the generation, collection, and identification of exiting independent data sets that are suitable for calibrating cultivar specific parameters representing the genetic diversity within an agroecological system.

B.6 Model evaluation

There are multiple definitions for model evaluation (Bellocchi et al., 2010). Simply, model evaluation attempts to quantify how well model simulations and predictions are represented by real observations (Pasquel et al., 2022; Wallach et al., 2006). This is usually achieved by comparing the modelled output, such as crop yield against a measured data set (Matthews et al., 2008). Measured data should be independent, and not have been used in model calibration (Bellocchi et al., 2010). Model performance is commonly evaluated using a metric or indicator measuring the residuals between observed and simulated data, the Root Mean Square Error (RMSE) is a popular metric:

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2} \quad \text{(Appendix B-5-1)}$$

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

Pasquel et al (2022) maintain that the method of evaluation should be relevant to how the model is being used. For example, if a model is used to estimate a variable such as yield then this is the variable that needs to be evaluated, however if a model is the be used for decision making, such as how best to manage a within field management zone for N fertiliser, then this decision/recommended course of action should be evaluated. It could be argued that both these could be true for studies in this review. The first aim would be to

evaluate how well a model describes the observed spatial variation within a field, the second to validate the management decisions derived from multi objective optimisation, i.e. delivering economic or environmental benefits, thus turning a crop model into a decision model (Jones and Barnes, 2000).

Of the 71 studies featured in this review 64 performed some form of model evaluation for simulated crop responses (Figure Apex B-16). It was less common for models to evaluate the success of CSM for modeling spatial variation in soil processes and state variables. Of the studies reviewed 15 studies evaluated soil moisture spatially and 5 studies evaluated soil mineral N content.

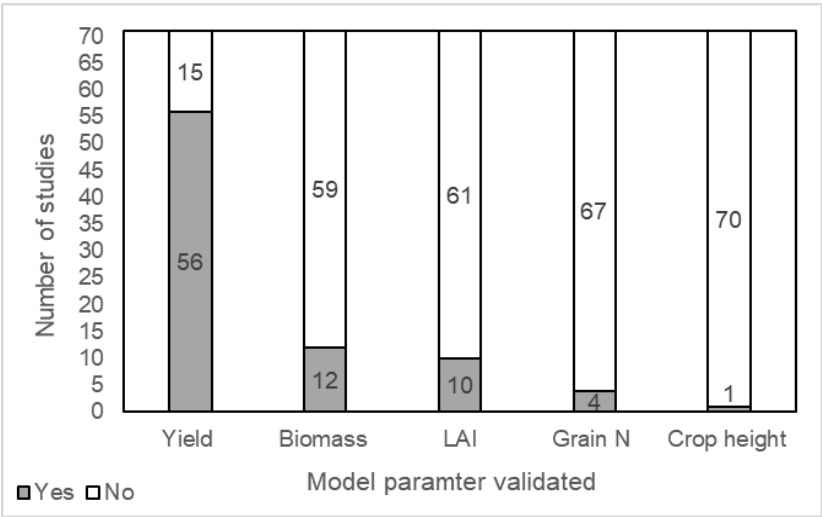


Figure Apex B-16: Agronomic model outputs validated by number of studies

B.6.1 Yield

Yield is often the greatest economic driver in arable cropping and perhaps the most complex (Thorp et al., 2015). Spatial variability in grain yield is the consequence of dynamic interaction between genetics, environment, and management (Shuai and Basso, 2022). Therefore, the most common approach to model evaluation is to quantify how spatially variable input model parameters such as soil plant available water can recreate observed spatial variation in yield. The widespread adoption of combine yield mapping has facilitated the recording of spatial and temporal variations in yield (Lowenberg-deboer and Erickson,

2019; Muhammed et al., 2016). Therefore, researchers looking to spatially validate or calibrate a model using yield data can use data sets collected on farm. Yield is validated in 56 of the 71 studies identified in this review (78%). The RMSE and/or rRMSE are the most common metrics used for model evaluation and were extracted from the relevant papers. Of the 56 studies evaluating yield 37 studies allowed for a RMSE and 31 studies allowed for a rRMSE to be extracted or calculated. When more than one model parameterisation method where used the best performing method was selected (Basso et al., 2001; Dixit and Chen, 2010; Wallor et al., 2018b). For wheat the mean RMSE reported was 0.57 t ha⁻¹, 0.80 t ha⁻¹ for soybean and 1.22 t ha⁻¹ for maize (Figure Apex B -17A). The mean rRMSE was 17.5% for wheat, 16.0% for soybean and 12.1% for maize (Figure Apex B-17B). It can therefore broadly be concluded that CSM appear to be capable of describing spatial temporal variation in crop yield within fields to a good level of accuracy, although site, model and crop variation does exist.

The following sections summarise the key consideration when evaluating a CSM for managing spatial temporal variation in yield.

Dataset suitability: Model evaluation is considered essential in any application, as it compels users to define the objectives of the modelling exercises, allows them to interpret the model's suitability, and is crucial for model improvements (Wallach et al., 2014). Despite this, some studies do not perform direct model evaluations, instead referencing independent evaluations of their chosen models (Oliver et al., 2010; Pedersen et al., 2021). Every effort should be made to conduct some level of evaluation prior to application. Particularly demonstrating the benefit of modelling-based recommendation to a farm specific scenario.

Any data used for model evaluation should be independent of any calibration procedures (Thorp et al., 2005). However, the lack of available data often mean evaluation and calibration data sets are amalgamated (e.g. Anwar et al., 2009; Fraisse et al., 2001). This makes validating the model difficult and can lead to a statistically bias estimate of model performance (Tewes et al., 2020b).

It is recognised that ‘measured’ data from agricultural field experiments have a level of uncertainty/error in them that should be accounted for in model calibration and validation (He et al., 2017a). For experimental data, errors and variance is reported to be around 13.5%, and this should be considered when interpreting modelling accuracy (Asseng, 2013; Taylor et al., 1999). For data sets collected on farm errors can be greater. Yield maps in controlled tests have been shown to have mean errors between 1-10% (Reyns et al., 2002). The limitations of such data sets have been highlighted in several studies. Jégo et al (2012) noted that calibration using yield map data may have caused the underestimation of yield when validated against hand-harvested samples. Kersebaum et al (2005) demonstrated very good simulations of yield with the Hermes model when using hand-harvested yields, but poor performance when using yield map data, which differed by as much as 28% from hand-harvested yields. Studies have

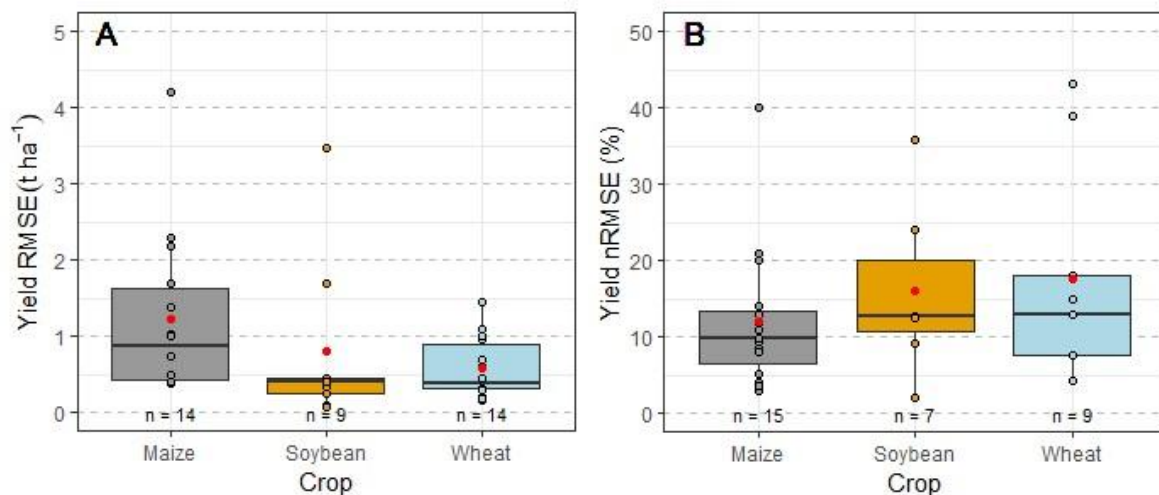


Figure Apex B-17 Evaluation of CSM for simulating spatial variation in yield A: RMSE B: RRMSE for those studies that report these metrics

demonstrated inaccuracies in yield map data ranging from 5%-10% (Grisso et al., 2002; McNaul and Darr, 2020; Morgan, 2020). However, these studies were relatively small experimental validations under optimal combine operation conditions. Studies testing the accuracy of combine yield maps acquired over commercial farms across rotations are lacking. For models to be appropriately validated on-farm, the accuracy of any spatial yield data must either be ensured, or possible inaccuracies be acknowledged and dealt with in the model application.

Temporally sensitive evaluation: The studies in this review use CSM to describe and manage spatial temporal variation within fields. Therefore, like calibration data sets, evaluation data sets should capture the temporal influences of spatial variation. For example, while in dry year's spatial variation is likely to be strongly driven by spatial dependencies in soil available water, these soil properties might have smaller or no effect in years with adequate rainfall, a CSM should be tested across these scenarios. Limited availability of appropriate spatial yield data resulted in 22 studies performing evaluations on just a single year of data (e.g. B. Basso et al., 2009; Cammarano et al., 2020). When temporally rich yield map data sets are available, evaluations can be performed over greater periods of time, the stronger evaluation exercises use between 5 – 7 seasons (Basso et al., 2011b; Sadler et al., 2000; Thorp et al., 2005). With the availability of spatial yield map data sets such evaluations should be the target for demonstrating CSM for managing spatial variation in yield.

Spatially sensitive evaluation:

The use of aspatial statistics such as RMSE, when used inappropriately can be misleading when evaluating a spatialised CSM. Any evaluation should consider the spatial scales that the evaluation is performed on (Pasquel et al., 2022). Albarenque et al (2016) evaluated the SALUS CSM across homogeneous zones within two fields. Despite sampling multiple points per zone, the reported RMSE and regression analysis were not stratified by management zone. Consequently, it was not possible to determine if the CSM's performance varied across different zones or fields. Although net revenue simulations under varying N rates were conducted for each zone, the lack of zone-specific evaluation prevents the uncertainty in the recommendations within each zone to be considered. The importance of such methods has been demonstrated in several studies reporting spatial patterns in model performance (Thorp et al., 2007). Paz et al (1999) identified that low-lying areas of the field demonstrated poorer model performance, potentially due to the model's inability to account for surface and subsurface water exchange between grids. Subsequently, any model-derived management techniques will have greater uncertainty in these areas.

Response sensitive evaluation:

When using a CSM to optimise a management option, the CSM should be evaluated not only against observed variations in soil and weather but also across all combinations of possible management strategies, such as different N rates (Sadler et al., 2000). In this review, 24 studies simulate the spatial response to N management; however, only a third of these validate the CSM for simulating yield responses to varying N rates. While evaluating responses to spatial and temporal variation can be performed using standard on-farm data sets, such as yield maps from standard farm management, assessing the response to a management strategy requires multiple management approaches across observed spatial variations over several years. One method to acquire such response information is to set up experimental response trials across the observed spatial variation (Albarenque et al., 2016; Anwar et al., 2009; Delgado et al., 2005; Kersebaum et al., 2005). However, this is very research intensive and not possible on all fields/farms to which CSM might be applied. One method that has not been extensively employed in the literature is the use of farmer applied strips with different treatments covering the extent of the spatial variation. Such methods have been used to quantify spatial response to different management strategies, such as N rates (Sidhu et al., 2021; Stamatiadis et al., 2020) and have been used to validate other PA technologies such as canopy sensors (Li et al., 2022; Montgomery et al., 2020; Walsh, 2015). Such strips could be used to evaluate CSM performance at simulating the response of observed spatial variation to varying inputs, providing confidence in a model's ability to derive accurate responses.

A third way to test a CSM's accuracy in simulating a response variable spatially is to use pre-determined CSM-based recommendations. This approach, by definition, becomes a model validation exercise, as it demonstrates whether CSM-based recommendations achieve their objectives, such as improved margins or environmental outcomes. This has traditionally been done by splitting a field into grids/zones and applying a farm standard and model recommended

and comparing simulated and observed yield response (Basso et al., 2016b; Kersebaum et al., 2005).

B.6.2 Biomass, leaf area index and grain nitrogen

All CSM operate with a plant subsystem characterised by above ground biomass and Leaf Area Index (LAI). LAI acts as an intermediate state variable, that is influenced by individual and a combination of simulated processes (Wallach et al., 2014). In the Sirius crop model for example, the soil profile represents a reservoir for water and N, as these are utilised, the effects of deficits are calculated through their influences on LAI (Jamieson and Semenov, 2000). Therefore, the accurate simulation of LAI is vital for accurate modelling of environmental influences on harvested organs (i.e. yield).

Above ground biomass is evaluated in 12 studies. This is almost exclusively done by collecting hand grab samples from gridded or zoned sampling sites. The least intense and most common method is to collect biomass sample at harvest from selected points within a field (Albarenque et al., 2016; Dixit and Chen, 2010; Wallor et al., 2018). Some studies measure biomass at several points through the growing seasons (Cammarano et al., 2020), however, this is not feasible outside of experimental studies.

The measurement of LAI through handheld devices is quicker than collecting and processing biomass samples and is used in several studies (e.g. Chen et al., 2021, 2020a; Jones and Barnes, 2000). The use of non-destructive handheld devices to determine spatially optimal N rates, such as the Yara N-Tester is already practised on some farms (Ortuzar-Iragorri et al., 2005). Therefore, there is the potential that handheld LAI measurements targeted within management zones, to reduce sampling requirement, could be used on farm for evaluating CSM, accounting for spatial variation in LAI.

With the rapid growth of remote sensing technologies, it has become easier to monitor the spatial temporal variation in crop growth within and across fields and regions (Weiss et al., 2020). Using the unique spectral response of leaves, LAI estimates can be retrieved directly from satellite (Amin et al., 2021; Delegido et

al., 2011; Kamenova and Dimitrov, 2021; Pasqualotto et al., 2019) and unmanned aerial vehicles (UAV) data sets (Kanning et al., 2018; Zhu et al., 2019). There have been numerous reviews and syntheses of methods documenting how remotely sensed data can support the spatial applications of CSM through assimilation (Jin et al., 2018a; Kasampalis et al., 2018; Weiss et al., 2020). Broadly these methods can be categorised as model calibration, by which parameters are adjusted to obtain the best fit between simulated and observed state variables, such as LAI, the example of Jin et al (2017) has been described in section 0. Forcing methods replace simulated state variables with those observed through remote sensing applications to improve the accuracy of other simulated variables such as yield. Updating/re-initiation adjusts simulated variables to those on which days of observed values are available, with the assumption the model will then provide more accurate simulations of succeeding days. Tewes et al., (2020b) used LAI derived from Sentinel-2 imagery to re-initiate the LINTUL5 CSM, employing an ensemble of simulations based on varying parameters. In season measurements from remote sensing sources can also be used for improved model evaluation. Jones and Barnes (2000) used handheld LAI measurements to generate a linear model of satellite derived LAI and demonstrated agreement between observed and simulated LAI for two management zones in a cotton field in USA. Despite these examples demonstrating value, the use of remotely sensed data for CSM at within fields scale evaluation and applications remains limited.

Grain N has a large influence on total N offtake (Barraclough et al., 2010a) and is a key parameter in NUE calculations (Congreves et al., 2021). It is also a key quality indicator for grain markets (Edney et al., 2012; Godfrey et al., 2010). Despite its importance, especially in studies utilising crop CSM for managing spatial variation in N demand, only four studies validate grain N (or protein) concentrations spatially. Albarenque et al (2016) found that the SALUS crop model simulated maize grain N poorest among all evaluated parameters, with a mean error of 36% across 21 sites within seven management zones in two fields in Argentina. Cammarano et al (2021) also reported that grain N had the lowest D-Index (indicating poorer model performance) compared to other evaluated

variables in a spring barley field in Scotland, though this was from a smaller sample size, and the RMSE appeared small (0.06%). Morari et al (2021) demonstrated poorer model performance in simulating management zone grain protein compared to yield (nRMSE = 16.4% compared to 4.3%), with errors as large as 3.5% protein content. It's recognised that although most CSMs do simulate grain N content, CSM development and evaluation has been yield and biomass focused. There is a need for broader evaluation and further development of models at simulating grain N concentrations under varying environmental and management scenarios (Nuttall et al., 2017; Yin et al., 2017). This review highlights this should include the evaluation of CSM to simulate the dynamics of within field spatial variability in grain N concentrations.

All studies evaluating grain N in this review collected grain samples manually. Like many other agronomic measures, this reliance on manual spatial sampling and processing limits wider spatial validations. Despite this, sampling grain for nutrient content spatially within management zones is of agronomic interest for nutrient offtake and budgeting, and is being encouraged on farms (FAS, 2023). Therefore, every effort should be made to validate models at the sub-field scale for grain N concentrations, particularly if better spatial N management is the CSM end use. Emerging technologies such as combine harvesters fitted with near infrared spectroscopy for spatially determining grain N content are at the commercial stage of development and, will in the future make such spatial evaluations easier.

B.6.3 Soil water contents and mineral Nitrogen

The evolution, development and application of crop models has primarily focused on modelling crop growth in relation to water and soil nitrogen supply (Keating and Thorburn, 2018a). These are the most modelled system responses to spatial variation in the studies reviewed. Model equifinality is the concept that multiple combinations of model parameters can perform similarly when evaluated against a limited data set, such as yield (He et al., 2017a). For example, a deep sandy soil with many stones might have the same plant-available water as a high clay content soil with a shallow impermeable layer. Therefore, yields in response to

water and nitrogen may be similar, while the below-ground nitrogen and water dynamics would differ. The former is more prone to leaching, whereas the latter might experience surface runoff. It is therefore important, particularly when using CSM to infer environmental risk (i.e. leaching potential) to evaluate the accuracy of the modelled process as well as final grain yield. The previously mentioned study by Braga and Jones (2000) demonstrated this with a range of hydraulic parameters able to simulate yield well but those only close to real values were able to simulate soil water contents correctly.

In data driven experimental studies within field sites are frequented multiple times during the growing season and soil moisture is measured through oven-dried soil samples or soil moisture probes. Albarenque et al (2016) and Cammarano et al (2020) demonstrated that the SALUS and DSSAT models simulated whole profile soil moisture with an RMSE of 26 mm and volumetric water contents from 0-60 cm with an RMSE of 3%, respectively, across multiple sites in management zones over a growing season. These good agreements between measured and simulated soil moisture contents are essential for using simulation models to determine optimal management in crops and soils sensitive to soil water limitations (Albarenque et al., 2016). A more practical approach for on farm validations would be to install in situ soil moisture sensors that log soil moisture across the whole growing season. Such technology is already employed in irrigation scheduling (El-Naggar et al., 2020). Although not feasible across all management zones, a selection of zones covering the contrasting spatial variation in soil properties identified through geophysical surveying (Brogi et al., 2020) is a plausible approach that requires further demonstration.

Soil mineral nitrogen content is temporally variable, with significant fluctuations possible over short periods due to leaching, crop uptake, and fertiliser applications. Technology for measuring soil nitrogen in real time within field, is under development not yet at a widely adoptable stage (Capstaff et al., 2021). Therefore, studies must manually sample soil and determine soil mineral N in the laboratory to quantify concentrations, while costly, extensive sampling and evaluations can be performed across spatial variation within a field (Cammarano

et al., 2021, 2020). A less intensive but valuable approach is to measure and evaluate simulated soil mineral N post-harvest. This residual N will provide an indication of crop fertiliser use efficiency, assuming the mineralised component can be accounted for /estimated as well as representing N with the potential to overwinter leaching in certain agroecological systems (Chen et al., 2020a; Kersebaum et al., 2005).

B.7 Addressing modelling uncertainty

Crop modelling has inherent uncertainties, which were recently decoupled in a review paper (Chapagain et al., 2022). Modelling uncertainty arises because, models are simplification of cropping systems and therefore will always fail to achieve complete determinism (Walker et al., 2003). Model uncertainty can be categorised into three sources: observation/measurement uncertainty, model uncertainty, and prediction uncertainty (Chapagain et al., 2022).

Observation uncertainty relates to the potential intrinsic errors within the data used to calibrate and parametrise CSMs. Such uncertainty can arise from random measurement variation in the experimental data used for calibration. For agricultural field trials random errors and variance are approximately 13.5% (Asseng, 2013; Taylor et al., 1999). The use of on-farm data for model evaluation, such as combine yield map data, planting information and lack of additional observational data, frequently collected in agricultural field experiments such as weed, and disease incidence is likely to increase observation uncertainty in such data sets. Most studies in this review using yield map data assume it is a true spatial-temporal record of crop yield, very few studies, demonstrate these data sets are of sufficient accuracy for modelling applications, despite evidence they likely contain systematic errors. A wider scale assessment of the systematic uncertainties of on-farm yield data sets would provide modelers with a better understanding of the uncertainty associated with such data sets and allow for more appropriate application within a modeling context.

A large proportion of studies quantify soil hydraulic parameters using pedotransfer functions, with their own individual levels of uncertainty in their predictive capabilities (Hollis et al., 2012a; Van Looy et al., 2017). Another source

of observation uncertainty particularly important for spatialisation of crop simulation models is the spatial-temporal resolution of observations. In the studies reviewed, the finest grid sampling resolution is approximately 10 samples per hectare (Figure Apex B-9). Even at this high spatial resolution, soils within a 1,000 m² area are typically spatially aggregated into a classification of single soil profile, often based on soil samples taken at a single point in time and assumed to represent the average conditions for the area. However, soils, establishment, and crop growth are likely to exhibit heterogeneity within and across seasons that are not accounted for in this approach. When soils are categorized by larger areas, such as management zones, this uncertainty increases. It is therefore important to contextualise such uncertainties within the modelling results, assessing how well the model outputs align with the zone mean and the variance within the zone mean.

Model uncertainty encompasses the distribution of simulated results due to uncertainties in model inputs, model structure and parameter uncertainty.

There are many CSMs available to users, over 40 for wheat alone (White et al., 2011). Each using differing combinations of equations for simulating processes such as LAI and light interception, yield formation, phenological development, water dynamics and evapotranspiration (Wallor et al., 2018). How these models differ in their outputs within the same agroecological systems (model inputs) indicates model structure uncertainty (Chapagain et al., 2022). Over the last decade modelers are increasingly accounting for model structure and model prediction uncertainty using multimodal ensembles (MMEs) (Wallach et al., 2018; Wallach and Thorburn, 2017). The mean or median of the output/prediction of the MMEs can be used to represent the system as a whole (Asseng et al., 2015). While the variation between these outputs represents the uncertainty arising from model structure.

The use of MMEs as a tool for quantifying modelling uncertainty in managing within field spatial variation is limited. In this review only three studies compared the results of multiple model predictions. Chen et al (2021) evaluated the APSIM and WHCNS models, with contrasting mechanisms for simulating water balances and

soil water movement, for maize in a 54 ha. field in China, both models performed well (nRMSE <13%) although the WHCNS model generally had better prediction accuracy. Thorp and Bronson (2013) compared the DSSAT and AQUACROP models across a 14 ha of a cotton field in Texas, USA. They found when using soil hydrological properties estimated from PTF that AQUACROP had the largest errors in predicted yield, primarily due to large underestimates of yield in a dry season. And only through individual calibration of the drained upper limit parameter did models perform to similar levels of accuracy.

Wallor et al (2018) conducted the most comprehensive comparison of CSMs to assess within-field variability, evaluating an ensemble of 11 CSMs across two European fields. In the first field, nearly all models demonstrated acceptable accuracy in simulating soil water content, though soil nitrogen dynamics exhibited a wide range of accuracy. Notably, accurate soil moisture simulations did not consistently translate to accurate yield development predictions. In the second field, the evaluation focused solely on crop yield, biomass, and LAI. While almost all models successfully simulated LAI variation, significant discrepancies were observed in crop development simulations. The multi-model mean failed to capture both inter-annual and within-season variability in crop yield and biomass. Input uncertainty was identified as a likely cause of significant model errors. In the first field, the models' inability to directly account for stone content was cited as a probable cause of poor performance. In the second field, the absence of subsoil hydrological parameters and issues with data collection and aggregation were likely factors impacting the modeling results. Despite these challenges, it was concluded that within-field spatial variation of yield driven by variations in soil texture was reflected by only a few models. Additionally, it was acknowledged that user experience could have influenced some modeling outcomes, a common limitation of MMEs (Chapagain et al., 2022).

These limited studies underscore the necessity for broader multi-model comparisons, incorporating more comprehensive soil data for spatial parameterisation to account for differences in model input parameters. Additionally, these evaluations were confined to observed seasons, and models

were not extrapolated beyond these periods to generate management recommendations. Model outcome uncertainty, defined as the cumulative uncertainty from all sources (Walker et al., 2003), is a primary concern for decision makers. This is a crucial next step, as systems such as the spatially economic optimum management N rate or seed rate are intrinsically uncertain (McNunn et al., 2019). Consequently, model uncertainty can exacerbate this intrinsic system uncertainty. The uncertainty in prescribed precision agriculture (PA) management practices from multi-model ensembles (MME) remains unassessed and should be prioritised in future research. Studies using single model outputs do go on to use the CSM to infer spatially appropriate management decisions, what decisions and how these are derived are reviewed in the following section.

B.8 Determining spatially appropriate management from CSM outputs

Of the studies in this review, 30 evaluated a CSM at a sub-field spatial scale but did not apply the CSM to explore sub-field responses to different management strategies to guide PA techniques (Figure Apex B-18). Model evaluation exercises are crucial for demonstrating that a model's structure and parameters are suitable for a particular application, considering the different contexts of the application. Optimal calibration and modeling approaches might not be the same for all sites. Wide-scale, repeated validation studies provide end users with confidence in using the models within the validation context (Bellocchi et al., 2010). Among the studies reviewed, DSSAT has been validated for maize at the sub-field scale across the USA and Europe in 12 studies. The average RMSE was 0.93 t/ha (n=6), and the rRMSE was 11.47% (n=4) for grain yield, demonstrating that the model structure generally provides a good level of accuracy in simulating sub-field variation in yield. Users can, therefore, reasonably expect that with appropriate parameterisation, the model can perform well within this context. However, demonstrating a CSM's capability at predicting site-specific yield responses is only part of the prerequisite for supporting PA

management decisions. Determining the most effective way to apply CSMs to provide land managers with actionable information and appropriate management recommendations presents a more complex task (McNunn et al., 2019).

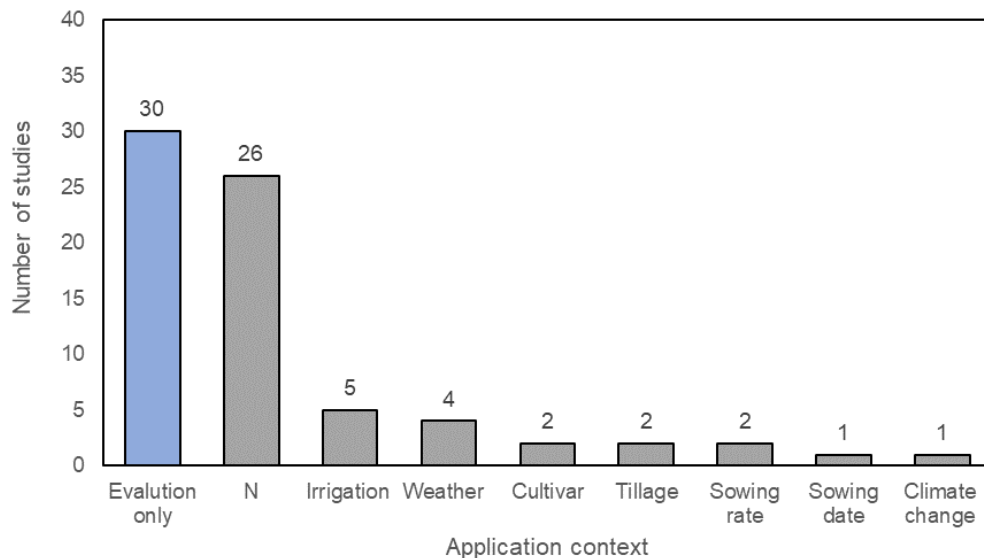


Figure Apex B-18 number of studies by application context for deriving within field spatially appropriate management decisions, evaluation only means models were not applied to generate management decisions just evaluated at describing observed spatial variation.

For management decisions with little impact on other model response except crop growth and yield a simple cost-benefit analysis can be performed on varying model inputs (e.g. seed costs) and subsequent model outputs (modelled grain yield). For example, Jin et al (2017) used a sensitivity analysis to demonstrate that plant density had little simulated impact on simulated N leaching or N mineralisation therefore just economics need be considered. Other management decisions can also be made, based on simply what model input returns the highest grain yield on average across multiple simulated seasons including choice of cultivar. Batchelor et al (2002) used marginal net return comparing the predicted yield for cultivar parameters for 70 soybean varieties for 100 grid squares of a 20-ha field. This is like the approaches adopted by Miao et al (2006) and Paz et al. (2003) for identifying site specific cultivar choice and Anwar et al. (2009) for optimal sowing date.

The most common spatially specific management decision informed by CSMs is the determination of nitrogen fertiliser application rates (26 studies). Understanding site-specific optimal N fertilisation efficiency requires long-term studies, as field experiments limited to a few years are unlikely to reflect the average crop response to seasonal weather variations (Basso et al., 2009). Kindred and Sylvester-Bradley (2014) argue that the only feasible way to determine spatially appropriate N requirement recommendations is by conducting multiple N experiments across every field in every season. This is, of course, infeasible, while more farmer-friendly methods, such as tramline trials, have shown limited applicability (Kindred et al., 2018). CSMs allow us to conduct these experiments in a simulated environment, replacing the need for actual experiments. Therefore, a large proportion of studies determine site-specific management decisions by simulating N response experiments across observed spatial variation within fields, using historical weather data to identify a climate, soil, and management-specific modelled average economic optimal N rate (e.g. Pedersen et al., 2021; Ward et al., 2018; Wong and Asseng, 2006). Albarenque et al. (2016) to simulate maize yield response over 41 years of weather data to four N rates within seven management zones across two fields in Argentina. When applying CSM outputs solely for the calculation of the economic optimum N rate to inform management decisions, it can be argued that we are not harnessing the full potential of CSMs to support on-farm management decisions, as this approach neglects the interplay of crop, soil, and system losses. Economic N_{Opt} can still result in significant within-season losses and leave quantities of mineral nitrogen in the soil post-harvest, leading to potentially negative environmental consequences where leaching risk is high (Thorp et al., 2006).

Multi-objective optimization allows for both economic and environmental optimum nitrogen to be accounted for in management decision-making. A common approach is to compare the cumulative probability function of economic N_{Opt} with that of a modelled environmental consequence, such as N leaching (Basso et al., 2007; Bruno Basso et al., 2009; Thorp et al., 2006). This method quantifies the probability of exceeding a certain environmental risk threshold. Thorp et al., (2006) and Basso et al., (2007) both use an example policy where growers should

not apply N rates that are modelled to exceed nitrogen losses of a certain level (40 and 30 kg N/ha in their respective studies) in 80% of seasons. A simpler approach is to simply select the N rate that increase yield without increasing N leaching (Basso et al., 2016b).

Another approach is to estimate the direct economic cost of a certain environmental outcome. Jin et al. (2019) calculated the associated societal costs from N leaching and N₂O emissions within the US Corn Belt, estimating the cumulative costs associated with negative impacts on human health and the environment. They used a median cost of \$18.54 and \$16.18 per kg N for N leaching and N₂O emissions, respectively, to demonstrate the potential economic value of adopting variable rate applications, based on the simulated economic N_{Opt} and modelled leaching and N₂O emissions.

Such approaches can currently demonstrate that spatially appropriate N management can deliver environmental benefits (Jin et al., 2019) or estimate an appropriate level of environmental risk (Basso et al., 2007). However, currently the economic costs of N losses are associated external to the farm (Sobota et al., 2015). Therefore any guidelines associated with an optimal simulated environmental risk probability or outcome will either need to be enforced by regulation, market forces or through environmental incentives.

While a large proportion of studies use CSM to determine site-specific management practices, few validate the recommendations to demonstrate improvements in economic and environmental performance at the field level. Basso et al. (2016b) conducted what they describe as a unique study where they assessed N rates derived from the SALUS CSM over two years of wheat cropping in an Italian field. They found that in areas with lower yields due to non-N limiting factors, the lower N rate did improve economic outcomes. No further evidence was found of studies validating economic or environmental benefits from CSM derived applications, or comparing their relative performance compared to more conventional VRT such as canopy sensors or a soil sampling-based approach.

B.9 Framework for applications of CSM for managing spatial variation

This review explored the current state of the application of CSM for managing within-field spatial variation in soil properties and crop performance. A key knowledge gap, relevant to the specific aims of this thesis, was identified due to the lack of studies on winter wheat in the UK, this thesis aims to address this gap extensively. Additionally, several broader knowledge gaps were identified regarding the widespread application of CSM as on-farm management tools.

1. Lack of Studies on Winter Wheat in the UK

- **Gap:** There is a significant lack of studies applying CSM to winter wheat in the UK, leaving a key knowledge gap for precision agriculture practices in this region.
- **Requirement:** Conduct extensive research focusing on the application of CSM at fine spatial resolutions for wheat in the UK, incorporating detailed calibration and validation specific to the UK's agroecological conditions.

2. Calibration and Parametrisation for Soil Properties

- **Gap:** Spatial parametrisation for soil properties at a sub-field scale is resource-intensive, limiting the practical application of CSM. Currently, few studies cover scales larger than 100 ha, constrained by the requirement for detailed soil characterisation.
- **Requirement:** Develop cost-effective methods for soil parametrisation. Integrating management zone sampling with proximal sensing technologies potentially could help reduce sampling requirements and requires further investigation.

3. Calibration of Cultivar-Specific Parameters

- **Gap:** Lack of access to multi-cultivar calibration data sets limits the ability to accurately parametrise cultivar-specific traits within CSMs.
- **Requirement:** Create and maintain databases of cultivar-specific parameters using high-quality field trial data, including phenological stages, biomass, and yield components, to support accurate CSM calibration for diverse agroecological systems.

4. Development of Rotational Modelling Studies

- **Gap:** Few studies model across crop rotations with multiple crops, potentially limiting the accuracy of CSM by not tracking state variables over multiple years, thus reducing their applicability.
- **Requirement:** Develop rotational modelling approaches that track state variables such as nitrogen mineralisation and leaching across multiple years and validate these models to account for the risk of accumulating errors.

5. Comparison and Assessment of Modelling Uncertainty Using Multiple Models

- **Gap:** Limited comparative studies exist that evaluate the spatial-temporal performance of different CSMs. Additionally, few studies incorporate multi-model ensembles to account for modelling structure uncertainty.
- **Requirement:** Conduct comparative studies using multiple CSMs to assess and quantify modelling uncertainty. Increase the use of multi-model ensembles to manage uncertainties and provide robust CSM-derived management recommendations for precision agriculture.

6. Use of Remote Sensing for Model Calibration and Validation

- **Gap:** Limited use of remote sensing data (e.g., satellite or UAV-derived LAI) for within-field CSM calibration and validation.
- **Requirement:** Expand the integration of remote sensing technologies to monitor spatial-temporal variation in crop growth, using these data to calibrate and validate CSMs at the sub-field scale for improved accuracy. Additionally, explore the potential for CSM to complement or integrate conventional VRT methods, such as canopy sensors.

7. Temporal and Spatial Data for Model Evaluation

- **Gap:** Insufficient long-term and high-resolution spatial data sets limit the effectiveness of model calibration and evaluation, often limited to yield and final biomass. Additionally, on-farm data sets, such as yield maps, often contain systematic errors that impact their suitability for application in CSM exercises, although the scale of such errors is poorly quantified and rarely recognised.

- **Requirement:** Gather long-term, high-resolution spatial and temporal data sets, including multi-year yield maps data sets, to enhance model calibration and validation. Ensure the accuracy of on-farm data sets by assessing and mitigating systematic errors to improve the reliability of model simulations of crop responses to varying conditions.

8. Validation of Economic, Environmental, and Practical Performance of CSM-derived Recommendations

- **Gap:** Few studies validate the economic and environmental benefits of CSM-derived recommendations, such as nitrogen management strategies, at the field level. Additionally, there is a lack of practical performance evaluation of CSM-derived management recommendations.
- **Requirement:** Perform field-level validations of CSM-derived recommendations to demonstrate their effectiveness in improving economic outcomes and reducing environmental impacts, such as nitrogen leaching and greenhouse gas emissions. Implement studies that compare these recommendations against conventional VRT methods, such as canopy sensors, assessing their economic and environmental benefits, and validating their practical performance in real-world scenarios.

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Appendix C Industry Events and Media

C.1 Webinars

This research has been prominently featured in various webinars and online training sessions, primarily hosted by the Agricultural and Horticultural Development Board (AHDB). These events include:

1. How do different fields perform in different years; can we predict profitability? 30th November 2020, AHDB ([Hyperlink](#)).
2. Yield map data sets – To support on farm decision making, 15 November 2023, AHDB ([Hyperlink](#)).
3. The good, the bad and the ugly - identifying your marginal land “how to” workshop – Foundation, 6th July 2021, AHDB ([Hyperlink](#)).
4. The good, the bad and the ugly - identifying your marginal land “how to” workshop – Advanced, 6th July 2021, AHDB ([Hyperlink](#)).
5. Identifying marginal land, 30th November 2021, AHDB ([Hyperlink](#)).
6. Can “marginal” land be managed differently to improve margins and deliver on Environmental Land Management, 1st December 2022, AHDB ([Hyperlink](#)).

C.2 Industry talks

1. NIAB Professional development group East – Monitoring spatial variation for targeted soil and crop management – NIAB Cambridge, 10th January 2022.
2. Soil Benchmark agronomy conference – Making use of farm spatial data sets, NIAB Cambridge, 7th December 2022.
3. NIAB Professional development group East – Measuring and managing spatial temporal variation across farm, NIAB Cambridge, 11th January 2024.
4. TAG Consulting Regional Agronomist Conference – Monitoring spatial variation for targeted soil and crop management, [online], 11th January 2022.

5. The Morley Agricultural Foundation Winter Talks and AGM – Capture, cleanse, and correlate yield data to guide best field management. Morley, 3rd February 2022.
6. REAP conference – Making sense of Agriculture with Emerging Agri-Tech: Crop models the new sabermetrics? Cambridge, 8th November 2022.
7. NFU East Anglia Development Board – Long term research at Morley, Morley 13th December 2022.
8. Indigro crop. Soil and environmental consultants – long term research at Morley, Morley 23rd February 2022.
9. AHDB Strategic Farm East Open day – Identifying and managing “marginal” land, 21st June 2022.
10. AHDB Monitor Wisbech Talk – Identifying and managing “marginal” land, Wisbech, 23rd February 2023.
11. Engagement day with G's Group, Crop Science Centre, University of Cambridge and NIAB – Quantifying, measuring, and modelling spatial temporal variation on farm and long-term experiments, Crop Science Centre, Cambridge 11th October 2023.
12. The Gatsby Charitable Foundation and Sainsbury Family Charitable Trusts visit to Cambridge Crop Science Centre and NIAB – NIAB Long Term Farming Systems Experiments – supporting extension research, Cambridge Crop Science Centre, Cambridge, 11th December 2023.
13. CUPGRA Annual Conference- Combining satellites and in-field monitoring to guide crop management 15th December 2021, Robinsons College, Cambridge
14. NIAB Professional development group South - Measuring and managing spatial variation – crop models as a on farm management tool [online], 16th November 2023.

C.3 Media and press

Podcasts

1. Exploring practical tips for measuring soil carbon: Future Farming Resilience Podcast: ([Hyperlink](#))

2. Aspects of Precision Agriculture and data collection: Future Farming Resilience Podcast ([Hyperlink](#))

Industry articles authored:

1. NIAB landmark: Yield maps – putting decades of data collection to use, March 2021 (see Appendix G)

Industry articles where the research was featured included:

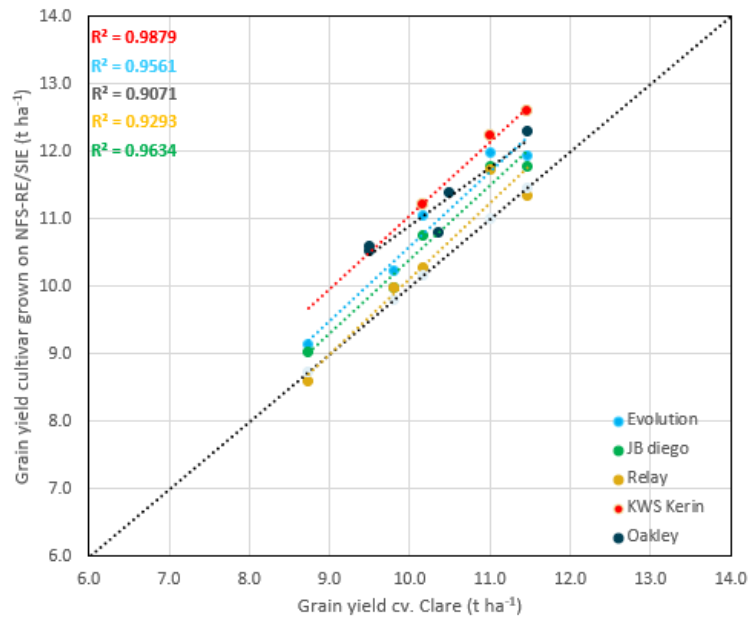
1. Farmers Weekly - How data analytics can help identify marginal farmland, ([Hyperlink](#))

Farmers Weekly - 4 key lessons from the first AHDB Cereals Strategic Farm

Industry articles ([Hyperlink](#))

Appendix D Supplementary material for Chapter 2

D.1 Comparison of yield of cv Clare compared to other varieties grown on the NFS-RE and Straw Incorporation Experiment



Figure_Apx D-1 Yields of cv Clare compared to cv Evolution, cv JB Diego, cv Relay, (2012-2016) , cv Kerin (2014-2016) and cv Oakley (2006-2010) in UK recommended list trials

D.2 Linear functions for the yield and grain protein response to plot ECa from 5 year mean data on NFS-RE

$$p_0 = 8.4158 - 0.1767 \times x$$

$$p_{220} = 11.7311 - 0.1032 \times x$$

$$y_0 = 3.3204 + 0.3272 \times x$$

$$y_{220} = 7.7744 + 0.418 \times x$$

where p_0 and p_{220} is grain protein at 0 and 220 kg N ha fertiliser rates, y_0 and y_{220} is grain yield at 0 and 220 kg N ha fertiliser rates, x is soil ECa.

D.3 Soil parameters used in Sirius

Table_Apex D-1 Soil properties and Sirius parameters for the Low ECa (LEC) and High ECa (HEC) soils

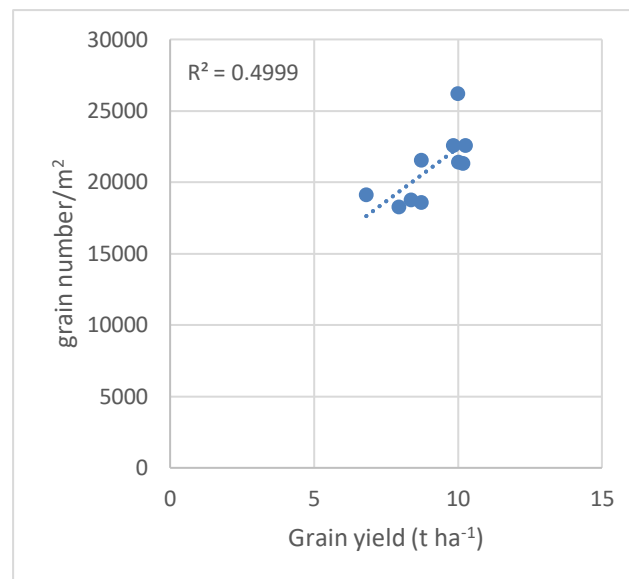
Layer depth (cm)	LEC (2.5-3.5 ms/m)			HEC (7.5-8.5 ms/m)		
	0-30	30-60	60-90	0-30	30-60	60-90
Sand (%)	68.9	65.8	56.6	60.3	49.2	46.7
Clay (%)	16.9	17.7	23.8	20.3	30.8	33.6
Silt (%)	14.2	16.5	19.6	19.4	20.0	19.7
Stone volume (%)	9.0	39.1	44.0	5.4	3.5	9.1
C (%)	0.8	0.3	0.3	0.8	0.5	0.5
N (%)	0.1	0.1	-	0.1	0.1	-
BD ^[1] (g/cm ³)	1.5	1.6	1.6	1.5	1.6	1.6
SLL ^[2]	12.6	10.8	11.1	14.1	21.6	21.0
SDUL ^[2]	24.1	17.3	16.8	26.4	31.5	30.0
SSAT ^[2]	37.9	23.2	21.8	40.2	39.4	37.3
AWC (150cm)	105.4			147.9		
Organic N (t ha 0-45cm)	6.0			7.0		

Appendix E Supplementary material for Chapter 4

E.1 Plant populations and Ear counts for Morley SAMS data used in model evaluation

Site	Year	Plant population (m ²)	Ear numbers (m ²)	Long-term simulation ear numbers
M1	2019	303	671	671
M2	2019	161	536	536
M3	2019	226	428	428
P1	2019	246	631	631
H1	2019	295	281	400
H2	2019	202	524	524
H3	2019	220	482	482
H1	2022	147	231	-
H2	2022	154	305	-
H3	2022	168	336	-

E.2 Yield components for Morley SAMS sites 2019 and 2022



Appendix F Calibration of parameters for cv Skyfall in DSSAT

F.1 DSSAT Cropping System Model

DSSAT emerged as the most frequently used model in the systematic review (Figure Apex B-6), demonstrating a good level of accuracy in simulating within-field spatial variability across diverse crops (Basso et al., 2007; Cammarano et al., 2020; Fry et al., 2017; Thorp et al., 2015). DSSAT's compatibility with the R programming language also allows better integration with optimisation algorithms and spatial analyse software (Alderman, 2020). The subsequent calibration processes were conducted entirely using R (R Core Team, 2023), enhancing the efficiency and flexibility of parameter tuning.

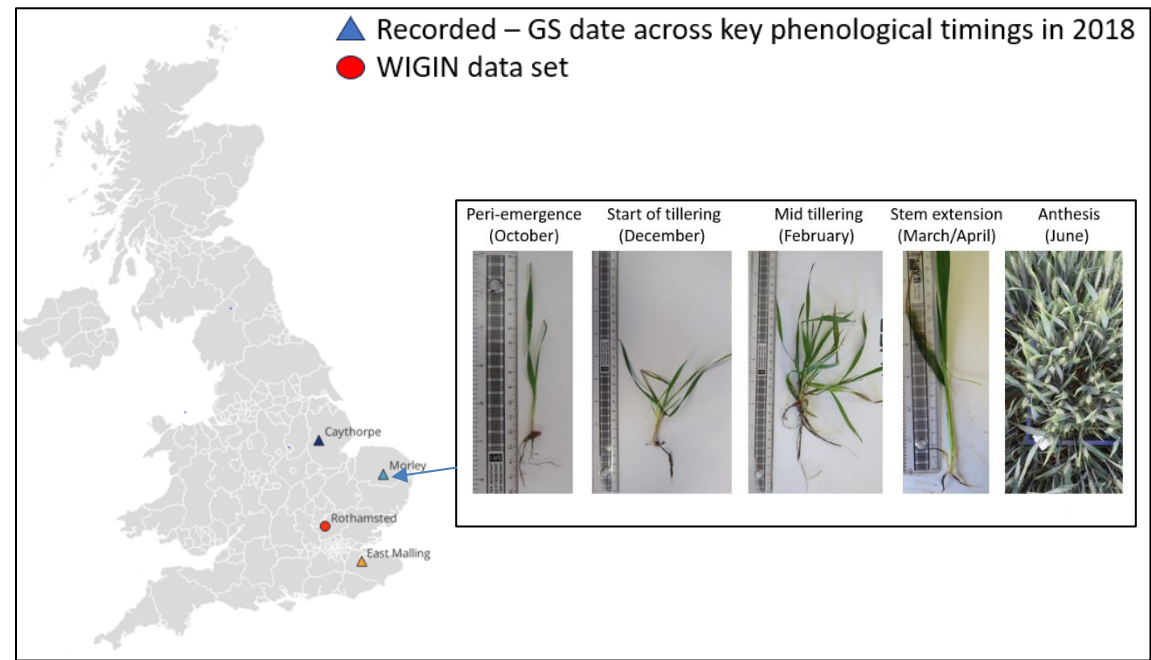
F.2 Calibration of parameters describing phenological development

Accurate parameter estimation requires in-season measurements of phenological stages (He et al., 2017a; Hunt and Boote, 1998; Rosenzweig et al., 2013). The need for high-quality datasets often limits the usefulness of many experimental field trials. For instance, while the NFS-RE dataset (described in

Chapter 2) is suitable for end-of-season nitrogen uptake evaluations, it lacks the necessary growth and development data required to generate cultivar parameters.

Between 2016 and 2018, NIAB conducted a series of "growth and development trials" with the goal of documenting growth stage records across regional trial sites to help local growers with timely pesticide applications. Although these trials were initially intended as a guide, the 2018 season included dissection and canopy photos, which enabled accurate validation of the recorded data, as growth staging is often prone to errors. Furthermore, the 2018 trial was conducted in contrasting geographic locations, including Morley in Norfolk, East Malling in Kent, and Caythorpe in Lincolnshire (Figure_Apx F1).

The lack of end of season measurement other than grain yield meant that there use for calibration other than phonological parameters was limited. However, it is



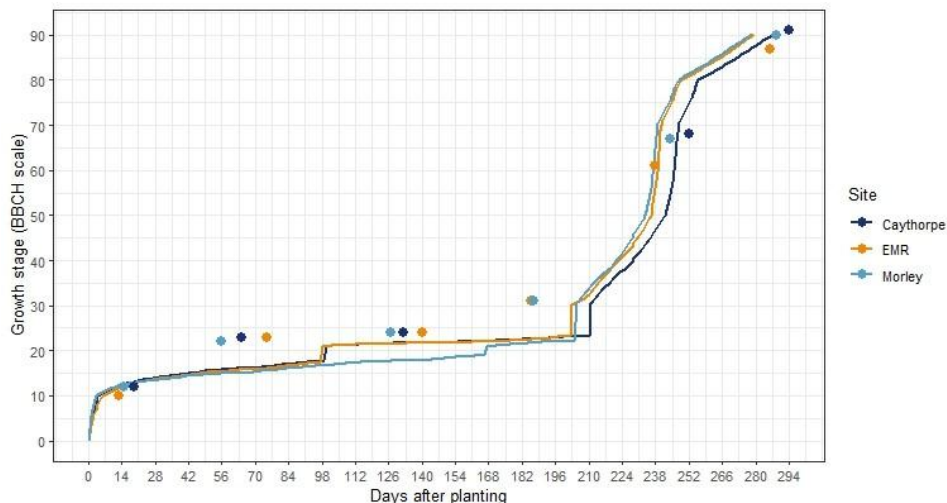
Figure_Apx F2 Experiment locations for first stage testing of cultivar parameters for cv Skyfall in DSSAT. Triangles represent locations of NIAB growth and development trials; Red circle is Rothamsted (WGIN data set). Example of photos used to validate growth stage recordings at Morley.

standard practice to calibrate cultivar parameters in stages: first focusing on

phenological development, followed by biomass, grain yield, and quality (Seidel et al., 2018).

To begin, a representative soil profile for each trial site was parameterised in DSSAT. The parameters for M1 site (described in Chapter 4) were used for Morley, as it had a representative electrical conductivity (ECa) for the 2018 field. Since no recorded profile data were available for East Malling or Caythorpe, the representative soil series for each site were utilised (Cranfield University, 2023). Weather data were sourced from the nearest COSMOS stations (Cooper et al., 2021). DSSAT's default parameters for the cultivar Maris Funden, a variety used in UK climate change impact studies (Cho et al., 2012), were used as a baseline. The model was run using the observed planting date, nitrogen fertiliser applications, and weather conditions for each site, with the simulated days after planting (DAP) compared to the observed DAP for six key growth stages in the 2018 season (Figure_Apx F2). This comparison highlighted poor agreement between the default parameters and observed growth stages at Morley. Although accuracy improved for key stages such as anthesis and maturity (GS60-70 and 89, respectively), a root mean square error (RMSE) of 14.4 days was observed for growth stages beyond stem extension (GS >30). This underscores the need for better cultivar parameter calibration before wider model application for UK wheat.

To calibrate these parameters using the NIAB growth and development trials data, the simplex optimisation algorithm (Nelder and Mead, 1965) was employed. This method is a recommended optimisation procedure for cultivar parameter calibration (Wallach et al., 2021). The parameters selected for calibration were those previously identified by Attia et al (2016). Since post-GS30 stages are critical for accurate crop growth simulation N uptake and water limitations, the optimisation function was weighted to prioritise the relative RMSE (RRMSE) for these stages (with a 0.7 to 0.3 ratio compared to earlier stages).



Figure_Apx F3 Comparison between simulated (lines) and observed (dots) growth stages for the cultivar parameters for Maris Funden at Morley, East Malling (EMR) and Caythorpe.

F.3 Calibration of parameters describing crop growth and yield

The WGIN dataset, compiled at Rothamsted between 2004 and 2019, focused on the response of modern and historic wheat varieties, as well as additional genetic material, to varying N rates (0, 100, 200, 350 kg N ha⁻¹). Data collected included grain yield, yield components (grain number and individual grain weight), straw yield, and grain nitrogen concentrations measured at harvest. Anthesis and maturity dates were also recorded in some years. For this study, DSSAT was parameterised using a sampled soil profile from Blackhorse Field (Avery and Catt, 1995), this field was used in the 2016 trials A comprehensive weather dataset for the trial years was compiled from the COSMOS weather station at the site (Cooper et al., 2021). Additionally, soil nitrogen contents measured during the spring were used to set initial soil N concentrations. These measurements were supplemented with an estimated 30 kg N ha⁻¹ to account for nitrogen uptake by the crop at the time of sampling.

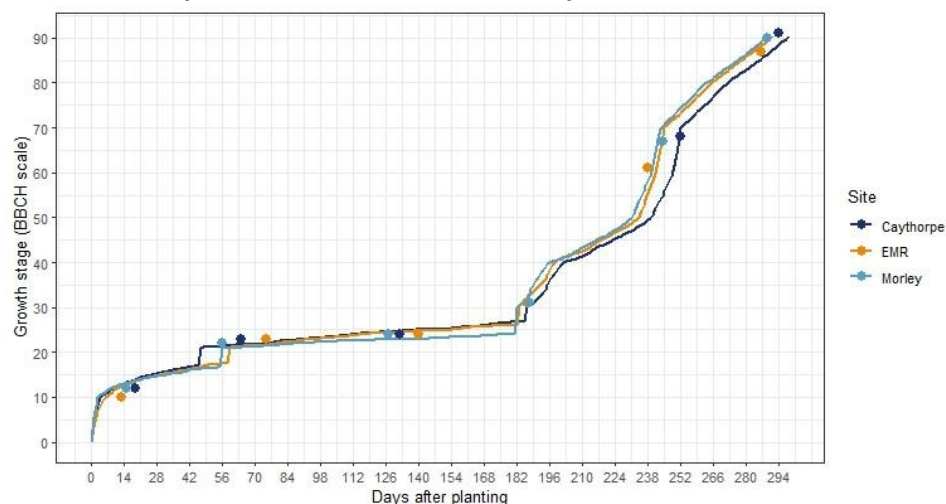
Skyfall was grown in the experiment during 2015, 2016, 2017, and 2018. However, the 2018 season was excluded from calibration due to low yields and high disease pressure. Initially, updated phenological parameters for Skyfall were

assessed by comparing simulated anthesis and maturity dates with the observed data.

A total of ten parameters, describing crop growth and yield, were calibrated using data from the three years across the four N rates for cv. Skyfall. The objective function, based on the relative root mean square error (RRMSE), included variables such as grain yield, grain weight, grain number, grain N concentrations, and straw weight. The Nelder-Mead optimisation algorithm was applied to optimise the fit of these parameters.

F.4 Updated parameters for cv. Skyfall for DSSAT

The calibration of parameters for cv. Skyfall substantially improved the simulation accuracy of growth stages across all sites in the NIAB growth and development experiments, reducing the RMSE for GS >30 to 2.5 days. Notably, the delayed flowering at the northernmost site, Caythorpe, was accurately simulated (Figure_Apx F3). A small evaluation using anthesis and maturity dates from the WGIN dataset (2015-2017) showed that anthesis was well-simulated, capturing year-to-year variation. However, while trends in longer growing seasons were captured, maturity dates were consistently simulated later than observed

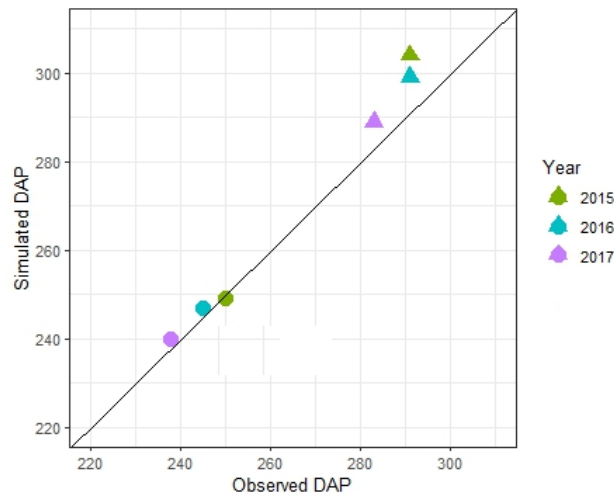


Figure_Apx F4 Comparison between simulated (lines) and observed (dots) growth stages for the calibrated cultivar parameters for cv. Skyfall using the growth and development data from Morley, East Malling (EMR) and Caythorpe.

(Figure_Apx F4). Anthesis was simulated well with the variation across years

captured. While the trend of longer growing seasons in 2016 and 2015 was captured, maturity date was simulated consistently later than the observed date.

For growth and yield parameters, the errors were within acceptable ranges, with RRMSE for yield, grain number, grain weight, grain nitrogen, and straw weight at



Figure_Apx F5 Observed against simulated anthesis (circles) and maturity (triangles) for the 2015, 2016 and 2017 WGIN Skyfall data set at 200 kgN ha⁻¹.

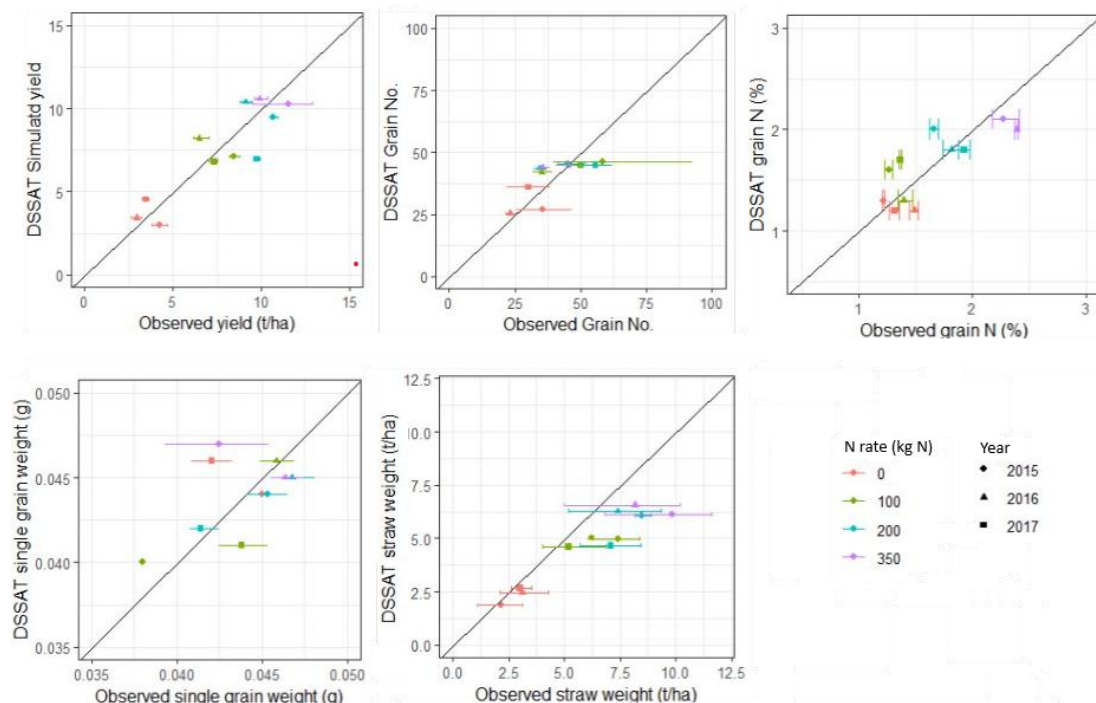
518%, 7%, 18%, 14%, and 14%, respectively. generally, variation between observed data across years and nitrogen rates was notable, simulated results generally fell within the observed range (Figure_Apx F5).

In this preliminary study, crop cultivar parameters for cv. Skyfall were calibrated for the DSSAT model using available experimental data. However, a major limitation was the restricted number of years for calibration, which required using all the data and prevented independent validation. Independent evaluation is essential to ensure the model's robustness and reliability in new conditions. Without it, there's a risk the model may be overfitted and not generalise well across varying environmental or management scenarios (Wallach et al., 2006).

To address this, future research will expand the evaluation datasets. In 2024, a new trial began in the 12x36m plots of the NFS-CE experiment, with several modern and historic wheat varieties, including cv. Skyfall, to explore interactions

between cultivation and N rates. This, along with other historic datasets such as the CINTRIN data set (NIAB, 2024b), will support further calibration, including parameters for other CSMs such as APSIM and WOFOST, which are compatible with R (de Wit et al., 2019; Miguez, 2024).

In summary, while the calibration has improved model performance for cv. Skyfall for DSSAT, the lack of independent validation remains a limitation. Upcoming experiments will provide diverse data for both evaluation and refinement of the parameters to support the wider application of a diverse range of CSM to support managing spatial variation in UK wheat.



Figure_Apx F6 Observed against simulated grain yield, grain number, grain N concentrations, single grain weight and straw weight for the best calibrated crop growth and yield parameters in DSSAT for the data for cv Skyfall from the WGIN data set. Error bars represent the range of observed data between experiment replicates (n3).

Appendix G Landmark article (March 2021)

Yield maps – putting decades of data collection to use

THE MORLEY
AGRICULTURAL FOUNDATION

AHDB

CENTA



British
Geological
Survey



The spatial recording of agricultural productivity has been practiced directly and indirectly, for millennia. The Domesday Book, completed in 1086, recorded the number of plough teams in each English parish, fertile lands supporting up to four ploughs per square mile with less fertile lands requiring up to eight times fewer.

I once read that 80% of the land cultivated at the beginning of the 20th century was cultivated in 1086. If this is true it is fair to assume that the variation in productivity seen across farms today has been causing management headaches for growers for centuries and in some places likely a result of differences in historic management. No-one can argue that we have not got better at recording spatial variation in crop growth. Since the 1990s yield monitors on combines have become commonplace. Satellites have allowed periodic monitoring of crop growth through the season, and even more recently, drones and other sensors are being employed to map variation in crop and soil properties.

Many farms have been collecting spatial data such as yield maps for a number of years. It is much more recently, however, that these datasets have become temporally rich enough to start doing meaningful analysis with. Using a five-year rotation of oilseed rape, winter wheat, sugar beet, spring barley and winter barley at Morley Farms in Norfolk as an example; it took over a decade of yield mapping to acquire multiple years of data for each crop. Now, with 13 seasons of yield mapping each field has on average three years of wheat yield data, allowing for a cross-year analysis to better understand drivers of spatial and temporal variability and how this could be managed.

Trusting the data

Before anything useful can be done with yield map data we have to trust the data is a true representation of yield. Data points that are not representative of actual crop yield can occur through a number of mechanisms, most notably swaths not filling the header or running over previously combined areas. These

inaccuracies make meaningful analysis difficult, and can lead to misconceptions that the whole dataset is inaccurate. Therefore, although some scepticism in interpretation is useful it should not prevent us from trusting values from points we are confident have been collected in normal combine operation.

Fortunately, there are techniques that allow us to find and remove data points that are not representative of actual performance. Behind each combine yield point is data, including the speed at which the combine was moving. So, quite easily, points that are outside normal operation speed can be removed. Anything outside the threshold of the field average yield, plus or minus three times the standard deviation, is considered unrealistic of actual performance and can also be removed. These steps will not remove all errors, particularly in fields with high levels of variability, so we have to be a bit more creative.

A technique I like, for its conceptual simplicity as well as its efficiency, is the Local Moran Statistic. Local Moran identifies local spatial outliers, i.e. it tests whether a yield



point is significantly different from its neighbours. This algorithm then provides a value for each point, if the number is above zero (positive Moran) it indicates that the feature has neighbours with similar high or low yields. If the value is less than zero (negative Moran) this indicates the yield point is dissimilar to the values around it and therefore is an outlier. If the significant value (p-value) is also small enough (<0.05) the point can be removed.

Identifying patterns

One key theme in the literature is a list of methods for analysing patterns of yield variability over time. This allows fields to be divided into zones in which points within that zone can be expected to perform the same in a given season. These zones could provide spatial constraints to adjust inputs based on crop demands (variable rate) or through targeted soil sampling or using farmer knowledge to ascertain what is driving yield variability. A lot can be learned from this, by identifying factors responsible for increased yields in high yielding zones growers can then work to replicate this across farm.

A popular method in the literature is cluster analysis. Clustering attempts to find patterns in datasets, a simple example is the K means cluster. Figure 1 shows an example dataset in which we have yields for specific areas of a field in 2011 and 2013 plotted against each other. A clustering algorithm can cluster these into groups that perform similarly in both years, i.e. orange areas are low and red areas high-yielding in both years, whereas blue areas fluctuate between high and low in 2011 and 2013 respectively.

The most popular clustering algorithm used in yield map analysis is the Fuzzy K-Means clustering; AHDB Project Report No. 565 provides a good description with examples. To do this, yield maps are normalised to a 10-20 m² grid, providing a mean yield for that grid cell in each year.

Morley – using yield maps and targeted soil sampling to understand spatial variation in productivity

The use of yield maps to quantify

variation and its drivers and how this might be better managed at Morley Farms started in 2018 with the Morley Soil and Agronomic Monitoring Study (SAMS), set-up by The Morley Agricultural Foundation. 30 sites of interest were identified through combining ten years of yield maps into gridded long-term performance. A mixture of high, low and fluctuating yield sites were selected as well as a number of headland sites across farm. Each receive annual soil and agronomic measures to better explain variation across farm as well as how properties are changing over time with modern agricultural best practice. Figure 2 shows the soil organic matter contents at each site measured in baseline testing in 2019.

Although variation in soil type does have an impact there appear to be more influential drivers, such as historic land use. During and after World War II the RAF compiled aerial maps of the country,

many of which are now available to view online for free. The two fields, Home Pasture (HP) and Perownes (P), whose sites have much higher soil organic matter look to have been in grass pasture in 1946 compared to arable cropping in other fields. A second aerial survey compiled in 1988 showed both fields in arable cropping, suggesting they have been part of an arable rotation for at least 30 years. The higher organic matter is not surprising. The Rothamsted Ley Arable experiment has demonstrated that after converting long-term pasture to arable cropping, soil organic matter levels still have not returned to an equilibrium (compared to long-term arable) after 40 years. Whether current practices on-farm at Morley, which involve rotational ploughing for sugar beet and the use of farmyard manure, are enough to maintain these higher soil organic matter levels at a point above the equilibrium of

Figure 1. Example of a clustering algorithm clustering two years of yield data

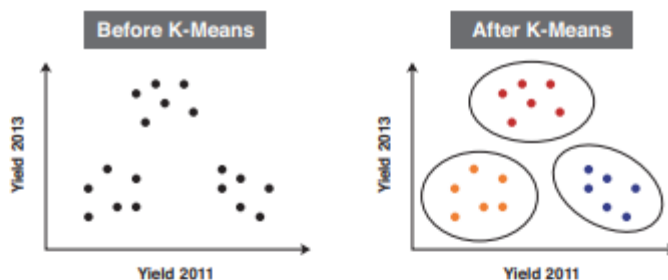
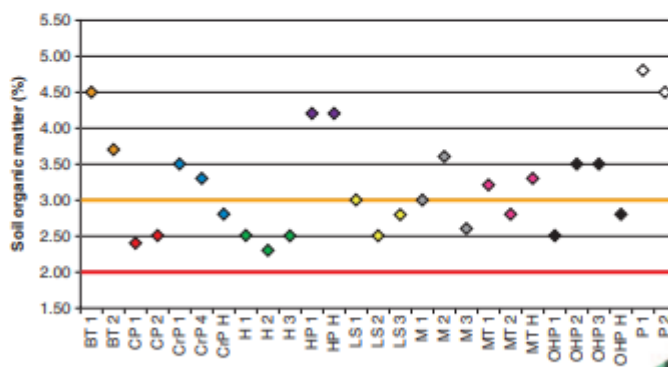


Figure 2. Morley soil organic matter (%) tested by loss on ignition, 2019. Colours indicate sites in the same field

Orange line indicates target threshold, below which soil function may be reduced, red line is very low threshold (Soil Biology and Soil Health Partnership 2018)



the rest of the farm will hopefully be captured in the Morley SAMS dataset.

Using guidelines published in AHDB's 'Soil Biology and Health Partnership' project summary, 44% of sites across Morley Farms may see an improvement in soil function from an increase in organic matter. Figure 3A shows the fields Manns (M) and Perownes (P) in 1946 with the north corner of Manns and Perownes in pasture. Following cluster analysis using the Fuzzy K-Means algorithm a high yielding zone (cluster 1) can be seen at the bottom of a slope in the south side of Manns, SAMS site M1 sits inside this. However, this zone is featured heavily inside the old pasture field boundary of 1946. It recorded a mean yield 0.7 t/ha and 1.0 t/ha higher than the next best zone in the 2011 spring wheat (Figure 3C) and 2013 winter wheat crop respectively (Figure 4). These were both challenging seasons with spring and summer 2011 being one of the driest on record in east England. Potentially the higher organic matter levels improved water availability to the crop in this area compared to the areas around it. Supporting the guidelines set out in AHDB's 'Soil Biology and Soil Health Partnership' – some sites might see an increase in soil function if soil organic matter levels were raised to that of Perownes. Soil textural classification at P2 and M2 shows there is little difference in soil texture (Figure 3D), suggesting differences in soil organic matter levels are a result of historic management not underlying variability.

Through a Central England NERC Training Alliance (CENTA) PhD with Cranfield University, NIAB and the British Geological Survey (BGS) we hope to develop these methods over the next three years to help better understand spatial and temporal variability in productivity at Morley and how this can be better managed.

AHDB Strategic Farm East – using yield maps to identify marginal land

The Environmental Land Management Scheme (ELMS), due to be rolled out in 2024, will see farmers paid for delivering public goods such as clean air and water, thriving plants and wildlife and protecting against environmental hazards among others. As well as

Figure 3. **A** SAMS sites and 1946 aerial field layout, **B** current field layout with area in grass in 1946 highlighted by red polygon, **C** 2011 yield map showing higher yields in old pasture field, **D** soil texture for P2 (circles) and M2 (triangles) at 10 cm (red), 30 cm (green) and 55 cm (blue) soil depths

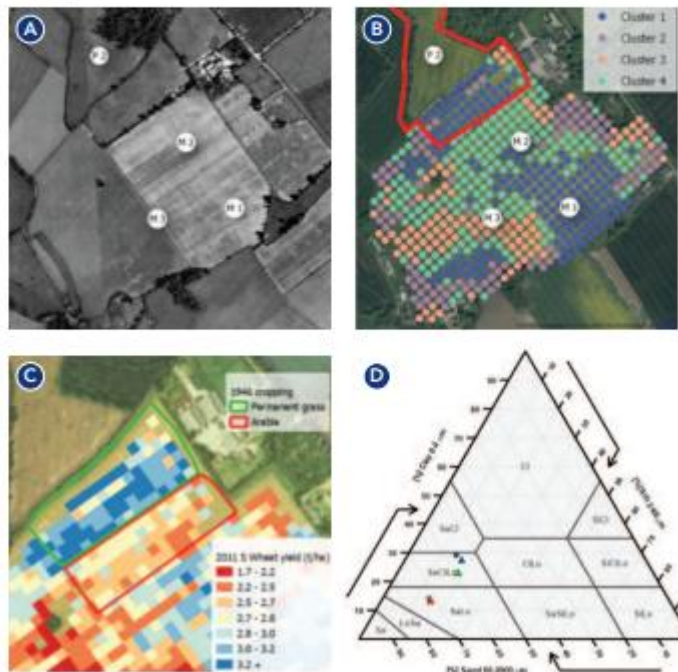
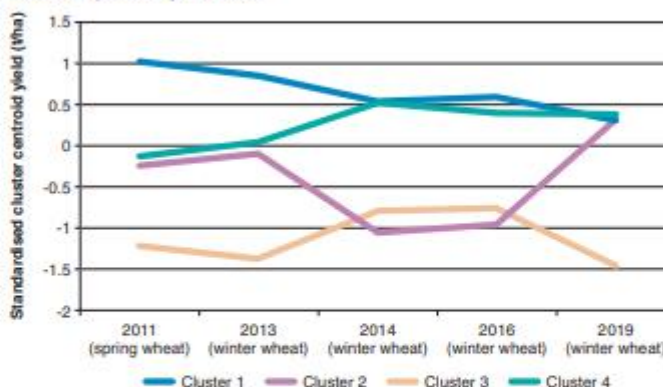


Figure 4. Normalised yield for Cluster centroid means identified at Manns from five years of yield data



supporting farm husbandry that supports the environment it is expected that areas of land currently used for food production will be taken out of production to deliver these services. Being able to identify

areas of the farm that perform poorly for a given crop will allow for the more targeted use of Tier 1 (e.g. wild flower strips) ELMS schemes with the smallest impact on farm business in that year. Alternatively areas



identified that perform poorly consistently across the rotation will be best suited for long term schemes such as woodland and habitat creation.

AHDB Strategic Cereal Farm East, managed by Brian Barker near Stowmarket in Suffolk, has 10 years of

yield map data and field level fixed and variable costs. An AHDB project, led by NIAB, will use the methods described above across the farm to identify areas of land that could be classed as marginal and therefore potentially best suited for ELMS schemes. These areas are likely to

have the smallest economic impact on farm business as well as providing accurate estimates of lack of revenue from converting areas to ELMS. The project is due to conclude in autumn 2021, hopefully providing a framework that can be implemented on other farms.

Appendix H Soil carbon through management zone sampling (Poster) presented at Wageningen Soils conference 2023



world-class experience, skills and resources

Incorporating yield data analysis to capture spatial soil carbon variation on farm

D.E Clarke*, J. Martlew, E.A Stockdale

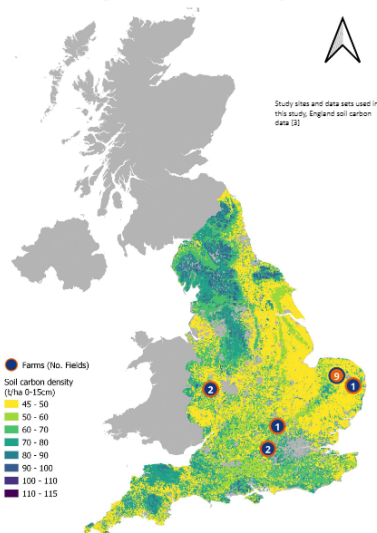
NIAB, Farming Systems, Cambridge UK, CB3 0LE

*David.Clarke@niab.com

Introduction

Monitoring soil health and evaluating management practices for building and maintaining soil carbon (C) are increasingly important for growers and ecosystem sustainability. This enhances soil management and offers potential compensation through ecosystem services. Yet, precise soil carbon measurement is costly, hindered by within field and across farm heterogeneity. Strategic methodologies for targeted on-farm monitoring are required.

Aim: This study aims to employ Fuzzy k-Means Clustering^[1] to identify management zones and strategically sample representative sites for soil carbon assessment through a horizon-based sampling approach^[2].



Study sites - This study employed two distinct datasets.

- The first dataset originated from the Bayer Carbon Farms Pilot, incorporating 4 farms, collectively comprising 6 fields across England.
- The second dataset was sourced from the Morley SAMS study, providing a valuable platform for method demonstration. Within this dataset, 9 fields from a single farm were examined, benefiting from prior whole-farm yield mapping efforts.

By harnessing these datasets, our study enabled the practical application of the methods across a variety of arable agricultural landscapes.

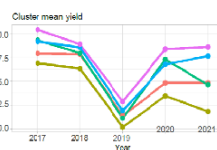
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Methods

- Using 5-9 years of field-specific yield data, Fuzzy k-Means Clustering identified 3-6 homogeneous yield zones within each field, from which 2-4 zones were sampled.

Smoothed yield clusters

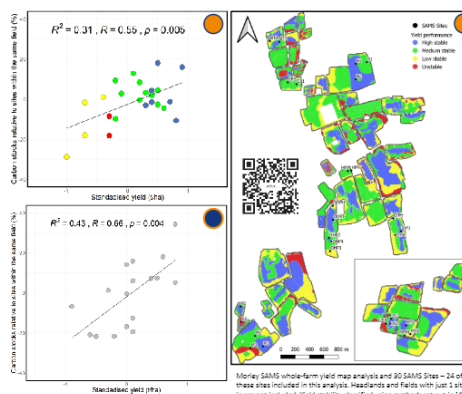


Example of clustering results for a field from the Bayer carbon farms data set and sampling sites within clusters

- A single site per zone was chosen based on robust cluster membership. Horizon-based sampling recorded depths guiding bulk density and soil C measurements. Stone content was estimated, and smaller stone volume measured from bulk density cores.
- Regression analysis was used to quantify the relationship between standardised yield and field relative soil carbon stocks



Results and Conclusion



- A significant correlation between standardized yield performance of management zones and soil carbon stocks is recorded in both the SAMS and Bayer Carbon Farms datasets, explaining 31% and 43% of the variability, respectively.
- Soil properties conducive to soil carbon storage, such as clay content, soil depth, and low stone content are factors commonly associated with higher yields in rainfed agricultural systems. This yield-carbon relationship is likely reinforced by larger crop residue inputs in high-yield zones.
- Integrating yield map analysis offers a practical solution to capture soil carbon variability within fields and across farm.

Acknowledgments

- The Bayer Carbon Farms data set was supported by Bayer Crop Science, thanks to the participating farms and Nick Duncan and Greg Cattle from Bayer CropScience
- The Morley SAMS project is supported by The Morley Agricultural Foundation



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