Maximising the use and value of soil carbon models in croplands to enable carbon sequestration

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Abstract

Healthy soils support terrestrial life on Earth. Carbon (C) in soils is critical for functional and productive landscapes, and is a key component of the C cycle. To date, human land use has significantly degraded global soils and over 116 Pg soil C has been lost; contributing to greenhouse gas emissions.

There exist opportunities to protect and increase soil C stocks through land management, which would safeguard soil functioning and could remove CO_2 from the atmosphere. A growing number of farmers, businesses, policy makers and standards organisations are hoping to manage soil C to offset greenhouse gas emissions, alongside safeguarding environmental health. Quantifying and predicting soil C storage is critical to the success of such projects, but reliable measurements of soil C stocks and their change are difficult. To provide quantitative predictions of changes, soil C models are critical.

Whilst several well-researched soil C models exist, their intended purposes vary and the predictions they make are uncertain. The complexity of many models reduces their accessibility for field scale soil C prediction. This thesis explores how soil C models can better enable action to benefit soil C stocks, with a focus on decision support for cropland managers. Each analysis chapter addresses known barriers to the use and value of soil C models for on-farm decision support.

Reducing the data requirements of soil C modelling is a key lever for increasing access to useful soil C information. The first analysis chapter in this thesis explores models with very low data requirements. Using an existing dataset, parsimonious regression models for the impact of cover crops on soil C were parameterised and compared to meta-analysis response ratios and the simplest IPCC 'Tier 1' method. The model selection approach combined statistical and practical considerations; a parsimonious model based on unavailable data offers no improvement in accessibility. The results show that cover crop above-ground biomass is sufficient as a single predictor for soil C change after a change to cover cropping in temperate climates. The regression model still works well if cover crop biomass is estimated. Using existing soil C datasets to parameterise simple empirical models can yield methods that are appropriate for predicting change in soil C at a field scale. Such models may not even require measured input data to be used, further improving accessibility for farmers and challenging a focus on precisely measured input data as a precursor to useful model outputs.

Building on the above, another approach to reducing the data burden for farmers is to utilise public databases instead of measured field data. The second analysis chapter compared the outputs of the existing RothC and IPCC Tier 1 models when using primary and secondary data for baseline soil C, soil clay percentage and mean annual temperature. The secondary data varied between negligibly and significantly different from the field measurements. The model results show that the capability of both methods to predict changes in soil C stock is principally dependent on the site, rather than input data source. These results further challenge prevailing emphasis on accurate input data and instead indicate that further calibration steps are needed to ensure that soil C models are generic enough for wide application.

Existing field and modelling studies indicate that impacts of cropland management on soil C are driven by factors that vary from micro to macro in scale. It is therefore understandable that globally applicable models are elusive. In recognition of challenges around model universality and uncertainty, recent updates to Measurement, Reporting and Verification protocols mandate that soil C model predictions must be validated by field measurements, though they provide scant guidance on methods to do this. For land managers, this leaves the process of soil C management uncertain.

The final analysis chapter in this thesis looked at options for employing measured data to improve soil C prediction at a site level. Three modelling methods were applied to time-series datasets. These were the process-led RothC model, Bayesian hierarchical modelling that combined process knowledge with data and data-led Bayesian regression. Results show that none of the modelling approaches was consistently reliable for long-term soil C prediction, but that methods trained on site data can offer some improvement on sub-decadal scales.

Model predictions and soil C measurement both remain uncertain. Future work on clear methods for data assimilation into model predictions is critical to enable the desired role of soil C in both adaptation to and mitigation of climate change.

Lay Summary

Soils are much more than dirt. Healthy soils are home to a diverse range of living organisms and provide a place for plants to grow. This is both because of the physical structure of soil and also because soil contains organic matter and minerals that feed organisms and support plant growth. One of the most important elements in soil is carbon (C).

Soil organic C cycles over time, but inputs and outputs are usually approximately balanced in natural environments. Unfortunately, physical disturbance of soil can drive net loss of soil organic C. This can be through increased decomposition, where organic compounds break down, and increased erosion, where surface soil is moved by wind or water. Some of this C ends up in the atmosphere as carbon dioxide (CO_2). CO_2 is a greenhouse gas: it contributes to climate change by storing extra heat in the atmosphere. Protection of soil C is vital for preservation of soils, ecosystems and the climate. Sequestration means increasing the amount of C in the soil: it is a key consideration for sustainable use of the land.

Agriculture is associated with significant soil C changes because cultivation of the soil is disruptive. Whilst some things that farmers do reduce soil C, there are also choices that can increase the soil C stock (the amount of C in the soil). A growing number of farmers, businesses, policy makers and standards organisations are hoping to manage the C in soils to reduce net greenhouse gas emissions, alongside safeguarding environmental health. Knowing the amount of C in the soil and being able to predict changes in that amount is critical to the success of such projects. However, reliable measurement of soil C stocks and how much they change is difficult. This is because soil C varies over small areas and any changes over time are often small compared to the overall stock. To provide quantitative predictions of changes, soil C models are critical. Models are equations or combinations of equations that can estimate numbers of interest. They might be very simple, or highly complex. Soil C models use statistics and/or knowledge of environmental processes to predict soil C stocks for a given context (for example, a particular farm with particular crops and management actions).

Since these models are mathematical representations of the real world, which is impossible to summarise in a few equations, their estimates do not always match exactly what happens. Whilst several well-researched soil C models exist, their intended purposes vary and the predictions they make are uncertain.

In order to get outputs from a model, data (information) must be input, then the calculations performed. Many models require a lot of information before their calculations can be performed. This reduces their accessibility for farmers aiming to predict soil C changes in their fields. This thesis explores how soil C models can better enable farmers to take action to benefit soil C stocks. Each analysis chapter addresses known barriers to the use and value of soil C models for on-farm decision support.

Reducing the amount of data needed to run a model is a key way of increasing farmer access to useful soil C information. The first analysis chapter in this thesis explores whether models with very low data requirements can be useful at the field scale. I focused on cover crops, which are plants that are grown in seasons where the field is not growing crops to sell, and where the plant material usually stays on the ground rather than being harvested and removed. Using an existing dataset, I built simple models to predict the impact of cover crops on soil C and compared them to two other simple models. To find the model that best met my objectives, I combined statistical and practical considerations because a simple and effective model based on information that is difficult to find would not improve accessibility for farmers. The results showed that cover crop biomass (the mass of plants grown) is sufficient as a single predictor for soil C stock change when a farmer begins cover cropping in temperate climates. This model still works well if estimates for cover crop biomass, rather than precise measured values, are used. This suggests that simple models can be built that are relatively good at predicting soil C change over time. This minimises the amount of information that the farmer needs to be able to use the model, and therefore improves accessibility for farmers. The use of estimated data also raises questions about the usual assumption that measured input data is required to get useful model outputs.

Building on the above, another way to make it easier for farmers to use soil C models is to utilise public databases of information (called secondary data) instead of requiring measured field data (called primary data). In my second analysis chapter, I used two existing models and compared their outputs when using primary and secondary data for baseline soil C, soil clay content and mean (average) annual temperature. The secondary data differed to varying degrees from the measured data. This is to be expected, as the secondary data aimed to represent large areas, whereas measured data was specific to a particular field. The larger the difference in input data, the larger the expected difference in model output, though multiple differences may cancel out. The model results show that the capability of both methods to predict changes in soil C stock is principally determined by site, rather than by the source of data given to the model. This result is important because it suggests, again, that providing carefully measured input data does not guarantee more useful soil C model outputs. Instead, further work is needed to fine-tune models to make sure they are suitable for use across diverse geographies.

Existing research studies that used field experiments and/or models indicate that impacts of cropland management on soil C are driven by many different factors. It is perhaps not surprising that models are not found to be consistently successful in predicting soil C stocks over time in managed landscapes. Recent updates to soil management protocols mandate that soil C model predictions must be confirmed to be reasonable through comparison with field measurements. However, they do not provide clear guidance on how to do this. For land managers, this leaves the process of soil C management uncertain.

The third and final analysis chapter in my thesis looked at ways to use measured soil C data to improve model predictions of soil C at a field level. Three modelling methods were applied to datasets which included multiple measurements of soil C at the same location over time. One model was an existing model based on knowledge of environmental processes (the RothC model), the other two approaches included statistical modelling. These statistical methods combine what we already know about soil together with new measured data to provide updated predictions of soil C over time. The relative weight given to existing soil science knowledge versus new data varies between the two statistical methods in this chapter. The first of the two combined the RothC model with the measured data and tested different values of RothC parameters to improve predictions. The second was a simple equation based on a minimal amount of existing knowledge and giving much more weight to the new data in generating new site-specific parameter values. The results show that none of the modelling approaches was consistently reliable for long-term soil C prediction, but that statistical models trained on site data can offer some improvement on shorter timescales.

Model predictions and soil C measurement are both still uncertain. Future work should look further at how to combine models and measured data. This is critical for soil C protection and sequestration.

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Declaration

I declare that this thesis was composed by myself, that the work contained herein is my own except where explicitly stated otherwise in the text, and that this work has not been submitted for any other degree or professional qualification except as specified.

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HH and JH formulated the research question. HH designed and carried out the analysis and wrote the first draft of the manuscript. SM and MS provided the dataset. All authors discussed findings and reviewed the manuscript.

Helen Hughes

Contents

Abstract ii

Lay Summary iv

Acknowledgements vii

Declaration viii

Figures and Tables xii

Abbreviations and Nomenclature xiv

1 Introduction 1

1.1 Soil functioning and the C cycle . . . 2

1.2 The impact of cropland management on soil C . . . 3

1.2.1 Cover crops . . . 3

1.2.2 Tillage . . . 4

1.2.3 Organic amendments . . . 6

1.2.4 Summary of cropland impacts on soil C . . . 7

1.3 Quantifying the impact of cropland management on soil C stocks . . . 8

1.3.1 Direct measurement . . . 8

1.3.2 Modelling . . . 9

1.4 Farmer and policy context . . . 10

1.5 Current state of soil monitoring research for soil C modelling . . . 12

1.5.1 Data . . . 12

1.5.2 Saturation, equilibrium and model initialisation . . . 13

1.6 Conclusions and aims and structure of this thesis . . . 14

2 Modelling the soil C impacts of cover crops in temperate regions 16

2.1 Introduction . . . 17

2.2 Published paper . . . 18

2.2.1 Methodological clarifications . . . 30

2.3 Conclusion . . . 30

3 **The potential for public databases to increase farmer access to soil C modelling for decision support** **32**
3.1 Introduction 32
3.2 Methods 34
3.2.1 Outline of models applied 34
3.2.2 Primary field data 36
3.2.3 Secondary data sources for model inputs 37
3.2.4 Model runs in R 38
3.2.5 Models generated and naming 41
3.3 Results 42
3.3.1 Differences between measured and estimated input values 42
3.3.2 Rates of soil C change 42
3.3.3 Soil C stocks 47
3.4 Discussion 54
3.4.1 Model parameterisation 54
3.4.2 Model results 55
3.4.3 Implications for decision support applications 57
3.4.4 Implications for modellers 57
3.5 Conclusions 59

4 **Model-data integration: options for employing user data to improve SOC predictions** **60**
4.1 Introduction 60
4.2 Methods 61
4.2.1 RothC 62
4.2.2 Model II: Bayesian Hierarchical Model 63
4.2.3 Model III: Bayesian Regression Model 70
4.2.4 Model testing: prediction 71
4.2.5 Field data 71
4.3 Results 74
4.3.1 Bayesian Hierarchical Model 74
4.3.2 Bayesian Regression Model 79
4.3.3 Model comparison 86
4.4 Discussion 92
4.4.1 Model predictions 92
4.4.2 Soil C data collection 94

4.4.3 Summary of implications for decision support and carbon accounting 95
4.5 Conclusion 96

5 Discussion: what next for cropland soil C management? 97
5.1 Revisiting objectives 97
5.2 Improving soil C models 98
5.2.1 Process-based models need site-level calibration 98
5.2.2 Calibration needs better soil data 99
5.3 Implications for decision support 100
5.3.1 More accessible and accurate field scale modelling is possible, for some applications 100
5.3.2 Predictions are materially affected by model implementation choices, potentially more than input data 101
5.3.3 The need to (re)set expectations around uncertainty 102
5.4 Data vs theory 103
5.5 The role of policies and protocols to enable soil C management 104
5.6 Conclusions 106

Appendices

A.1 Appendix: Supplementary information for Chapter 1 108

A.2 Appendix: Published supplementary information for Chapter 2 110

A.3 Appendix: Supplementary information for Chapter 3 112

A.4 Appendix: Supplementary information for Chapter 4 117

Bibliography 121

Figures and Tables

Figures

2.1 Measured annual soil C change in training and testing datasets 22
2.2 Annual soil C change: observed and predicted, for models shortlisted 23
2.3 RMSE values of soil C change for tested models-with IPCC RMSE as a lower bound . . . 24
2.4 Annual soil C change: observed and predicted, for models with a lower RMSE value than the IPCC factor, using the extended dataset (training data and test data) 25
2.5 Prediction intervals for M1 CC biomass regression model (actual and binned input) 26
2.6 Annual soil C change: observed and predicted, for CC biomass models, using the extended dataset (training data and test data) 28

3.1 Structure of the RothC Model from Coleman and Jenkinson (1987) 35
3.2 Location of sites with SOC stock data and input data for RothC and IPCC T1 models . . . 38
3.3 Primary and secondary model input values for clay, MAT and initial SOC (A-C), and variation in modelled amendment C (D) 43
3.4 Measured and modelled SOC stocks from experiments that reported SOC_{init}, showing model results with various combinations of input data but where organic amendment C equalled measured values 45
3.5 Measured and modelled SOC stocks from experiments that reported SOC_{init}, showing RothC model results where the only estimate was the organic amendment C quantity . . . 46
3.6 Measured rates of SOC stock change compared with the closest modelled rate of SOC stock change 47
3.7 SOC_p for OA treatments from each model 48
3.8 SOC_p for MF treatments from each model 49
3.9 SOC_p for ZI treatments from each model 50
3.10 Total number of models and number of SOC_p results within $\pm$ 1.96 SD of SOC_t. 51
3.11 Model errors normalised by time 53

4.1 Gelman-Rubin convergence diagnostic values across four chains for each site and data subset 76
4.2 BHM parameter priors and posterior distributions for the largest training data subset . . . 77

4.3 Site boxplots for BHM posterior maximum likelihood estimates across training data subsets 78
4.4 Coefficient values for each BRM 80
4.5 BRM predictions for different training data subsets: Boigneville 81
4.6 BRM predictions for different training data subsets: Jabalpur 82
4.7 BRM predictions for different training data subsets: Ludhiana 83
4.8 BRM predictions for different training data subsets: Palampur 84
4.9 BRM predictions for different training data subsets: Rothamsted 85
4.10 RothC, BHM and BRM predictions compared to measured data: Boigneville 87
4.11 RothC, BHM and BRM predictions compared to measured data: Jabalpur 88
4.12 RothC, BHM and BRM predictions compared to measured data: Ludhiana 89
4.13 RothC, BHM and BRM predictions compared to measured data: Palampur 90
4.14 RothC, BHM and BRM predictions compared to measured data: Rothamsted 91

A.1.1 Global Carbon budget (2010–2019), from Canadell et al. (2021) 109

A.3.1 Difference between measured and modelled SOC at the end of experiments 116

A.4.1 BHM predictions using the low and high training data subsets. 120

Tables

2.1 Variables from McClelland et al. (2021) utilised in modelling the impact of cover crops on soil C stocks 21
2.2 Summary of model structures analysed 26

3.1 Site and management information for experiments modelled 40
3.2 Model naming conventions 42

4.1 RothC model parameters allowed to vary in the BHM and their defaults 67
4.2 BHM parameter definitions, prior distributions and proposal distributions 72
4.3 Site and management information for experiments modelled 73

A.2.1 Summary of coefficients for models shortlisted using nested comparison 111

A.3.1 Copy of Table 5.5 from Ogle, Kurz, et al. (2019): Relative Carbon Stock Change Factors (over 20 years) for Management Activities on Cropland 113

Abbreviations and Nomenclature

List of Abbreviations

BHM Bayesian Hierarchical Model

BIO RothC SOC pool: Microbial Biomass

BPF Bootstrap Particle Filter

BRM Bayesian Regression Model

CPM Correlated Pseudo-Marginal

C Carbon

DPM RothC SOC pool: Decomposable Plant Material

FYM Farmyard Manure

GHG Greenhouse Gas

HUM RothC SOC pool: Humified Organic Matter

IOM RothC SOC pool: Inert Organic Matter

IPCC Intergovernmental Panel on Climate Change

MAP Mean Annual Precipitation, mm yr^{-1}

MAT Mean Annual Temperature, ℃

MCMC Markov Chain Monte Carlo

MDA Model Data Assimilation

MH Metropolis Hastings

MLE Maximum Likelihood Estimate

MRV Measurement, Reporting and Verification

NPP Net Primary Productivity

PET Potential Evapotranspiration, mm yr^{-1}

PMMH Particle Marginal Metropolis Hastings

PRI Plant Residue C Inputs *(for RothC)*

RPM RothC SOC pool: Resistant Plant Material

SOC Soil Organic Carbon

SOM Soil Organic Matter

T1 IPCC's Tier 1 methodology for National Greenhouse Gas Inventories

Nomenclature

ΔSC_{yr} annual rate of change in soil carbon stock, Mg C ha^{-1} yr^{-1}

SOC_i measured initial (baseline) SOC stock, Mg C ha^{-1}

SOC_{ref} IPCC reference (native) SOC stock to 30cm depth, Mg C ha^{-1}

Chapter 1

Introduction

Remember that all models are wrong; the practical question is how wrong do they have to be to not be useful
Box and Draper (1987)

Healthy soils support terrestrial life on Earth. A medium for plant growth, water storage and nutrient transfer, they teem with life and play a key role in ecosystem resilience. The ecosystem services provided by soil support biodiversity and feed the world. However, human land use has degraded soils around the world. As climate change, rates of land conversion and agricultural management all continue to intensify, the risk to global soils increases (Montanarella et al., 2016; Smith, Calvin, et al., 2020).

Carbon (C) in soils is critical for functional and productive landscapes and is a key component of the C cycle, but 116 Pg C has been lost from the top metre of soil due to human activities, contributing to net CO_2 emissions (Sanderman et al., 2017). There exist opportunities to protect and increase soil C stocks through land management, which would safeguard soil functioning and could remove CO_2 from the atmosphere. Soil C therefore has a role in both mitigation of and adaptation to our changing climate, as well as protecting biodiversity and food production.

In this thesis, I ask how we can better enable actions that benefit soil C stocks, with a focus on field-level soil C modelling applications to support people managing land around the world.

This introductory literature review contextualises soil C within ecosystem functioning and C cycling. It then considers cropland management as a driver of soil C change and summarises the latest field evidence for impacts of key practices. The later parts focus on challenges in soil C monitoring, especially for farmers hoping to manage soil C, and summarise the potential for using models to predict soil C. The aims of this thesis conclude the chapter.

1.1 Soil functioning and the C cycle

Soils are formed over thousands of years from bedrock and dead or dying plants and animals (organic matter). As a physical structure and biochemical engine they underpin a large proportion of ecosystem functioning (Paul, 2016). Soils can regulate water, cycle nutrients, buffer pollutants and sustain plant and animal life (Smith et al., 2013). Organic matter is critical for these functions, and the carbon that makes up a major part of soil organic matter (SOM) by mass (Nelson & Sommers, 1996; Pribyl, 2010) is particularly useful. The natural degradation of soil organic C generates compounds that reduce soil density and increase stability (Álvarez et al., 2013). Soil organic C enables soils to retain more water(Manns & Berg, 2014; Weber et al., 2023), increases soil's nutrient holding capacity and reduces loss by leaching (Bot & Benites, 2005).

Earth's soils contain 1,700 Pg C; twice as much as the atmosphere and more than three times as much as vegetation (see Figure A.1.1; Batjes, 2016; Canadell et al., 2021). Change in soil C stock is the balance of biomass inputs and outputs through mineralisation, erosion and leaching (Lal et al., 2015). In natural environments, these fluxes tend to be balanced over time and the soil C stock is stable. However, during land conversion and cultivation, soil erosion tends to increase and the disturbance causes oxidation, driving a net loss of soil and soil C (Abdalla et al., 2020; Lal et al., 2015). Globally, cropland management has driven large soil C losses, intensifying through time (Karstens et al., 2022). By taking management decisions to increase the inputs and/or decrease the outputs of soil C, it is hoped that cropland soils could store more C.

In describing soil C and changes therein, care must be taken with terminology (Chenu et al., 2018; Don et al., 2024). The amount of C in soil is called the *soil C stock*. Don et al. (2024) found that, across published literature, *soil C storage* is used as both a synonym of soil C stock and as a process of increasing soil C stock. Here it is used to refer to a process. Of particular interest to many parties is the idea of sequestering carbon, which refers specifically to the removal of CO_2 from the atmosphere (IPCC, 2001), in this case into the soil. *Soil C sequestration* is therefore relevant to climate change mitigation. As Don et al. (2024) warn, not all soil C accrual is sequestration (Chenu et al., 2018), and some changes in soil C stocks are most accurately described as mitigation of soil C loss.

1.2 The impact of cropland management on soil C

Cropland management decisions including crop choice, fertiliser use, tillage, residue management and water management can affect fluxes of C into and out of soil; ideally increasing C inputs, decreasing C losses or reducing disturbance (Smith, 2008). The magnitude of stock change depends significantly on the preceding conditions, climate and particular management decisions (Lal, 2004; Smith et al., 2008). The potential for significant loss or gain makes cropland a particularly important focus for soil C research. Recent studies have examined how different cropland management practices affect soil C. Below, the research on some management practices is summarised.

1.2.1 Cover crops

Cover crops are grown to cover otherwise un-cropped soil, with a range of potential benefits. As well as reducing soil erosion and increasing biomass production, cover cropping can help manage soil nitrogen levels (Thorup-Kristensen et al., 2003): nitrogen-fixing crops help to meet nutrient requirements for subsequent crops, decreasing the need for fertilisers.

Cash crop residues are often removed from growing sites for use as animal feed or biofuel. This has a negative impact on soil C stocks, increasing with rates of residue removal and over time (Smith et al., 2012). The removal disturbs soil structure, alongside depriving the soil of biomass C inputs. In contrast, cover crop residues provide labile C inputs to the soil, which can increase soil C and subsequent cash crop yields (Finney et al., 2017; Vendig et al., 2023). Whilst cover crops increase emissions from respiration, the net greenhouse gas (GHG) emissions, compared to bare soil, may be reduced due to soil C sequestration and reduced N leaching Abdalla et al. (2019). In addition to providing C inputs, cover crops prevent 40-96% of soil erosion from both wind and water compared to bare soils (Blanco-Canqui et al., 2015).

In a meta-analysis, Jian et al. (2020) found that cover crops drove a global mean increase of 15.5% in soil C stocks, with significant differences between different soil types and climate zones. Clark et al. (2017) found that cover crop growth was highly dependent on climate conditions during their cultivation and Koudahe et al. (2022) flag the need to assess the impacts of cover crops in a greater range of climates and cropping systems.

Poeplau and Don (2015) found a soil C increase rate of 0.24-0.4 Mg C ha^{-1} yr^{-1} under cover cropping in a global dataset with a mean practice duration of 6.8 years, and highlighted that long-term studies of cover crop impacts are rare (Koudahe et al., 2022). Blanco-Canqui et al. (2013) estimated that, under no-till systems, cover crops drive an additional 0.10-1 Mg C ha^{-1} yr^{-1} storage compared to no cover crop. Their meta-analysis suggests time is a key determinant of overall soil C change under cover crops. Some meta-analyses report that changes are not correlated with time, though these are often datasets comprised of short-term experiments of less than 5 years (e.g. Alvarez et al., 2017; McClelland et al., 2021). In short studies, the impacts of cover crops on soil C compared to a no-cover-crop control are often unclear or insignificant (e.g. Clark et al., 2017), in part due to soil heterogeneity making change hard to detect (Blanco-Canqui et al., 2015; Poeplau & Don, 2015).

Impacts of cover crops have also been shown to vary depending on cover crop species (Bai et al., 2019). For example, non-legume crops reduce soil nitrogen content and leaching (Shackelford et al., 2019) whilst legume crops fix soil nitrogen. Species choice can also affect impacts on soil C. Rosolem et al. (2016) found legumes were more beneficial for maintaining a stable C:N ratio, which has a long term benefit for soil C. However, labile soil C is more efficiently increased by grasses than legumes in the short term, due to slower decomposition of grass residue (Blanco-Canqui et al., 2015).

Some studies found cover cropping to have no significant effect or even negative effect on soil C (Abdalla et al., 2019; De Notaris et al., 2021; Jian et al., 2020). This could be related to failed establishment of the cover crop, increased soil disturbance during cover crop management, or to soil-related mechanisms such as microbial priming, whereby additional C inputs change the rate of SOM mineralisation by microorganisms (Siles et al., 2022). Liang et al. (2023) found negligible effects overall, but identified a threshold for cover crop C input, above which soil C accrual was considerable (see Chapter 2).

The impacts of cover crops on soil C and GHG emissions vary depending on the choice of crop, as well as the climate and environment they are planted in. Not discussed here are the impacts of termination method. Overall, whilst some published meta-analyses have drawn statistically significant conclusions about the direction and magnitude of soil C change due to cover crops, the key drivers identified vary.

1.2.2 Tillage

Tillage practices are often categorised into conventional till, reduced till or no-till. Though these terms are used across the literature, the definitions applied to them vary between papers (Bai et al., 2019): meta-analyses tend to apply their own definitions when categorising the datasets used, but mapping from the source data definitions is not always simple.

In the 1990s, investigations into tillage options focused on the benefits of no-till for reducing soil erosion (Ogle, Alsaker, et al., 2019). Studies looking at soil C concluded that no-till was beneficial for carbon storage in comparison with conventional till, as the latter increases soil surface area and disturbs aggregates, driving decomposition (Paustian, Andrén, et al., 1997). The conclusion that no-till could sequester soil C was taken up by many modellers and soil C quantification methodologies, including the Intergovernmental Panel on Climate Change (IPCC) guidelines for National Greenhouse Gas Inventories (Eggleston et al., 2006). More recently, mixed results have led to this claim being re-examined. The pattern built in the earlier studies is thought to be linked to the depth of soil C measurements, which often did not extend to the full plough layer, and to a lack of focus on accounting for bulk density changes (Ogle, Alsaker, et al., 2019).

Management activities such as tillage reduce soil bulk density in the plough layer and can raise the soil level without the addition of new material (Ellert & Bettany, 1995). Therefore, measurements of soil C in tilled and non-tilled soils should not be compared on the basis of depth alone. Studies aiming to quantify soil C stock changes across managements (particularly including tillage) must account for density changes by explicitly measuring bulk density and controlling for mass equivalency (Ogle, Alsaker, et al., 2019; Smith, Soussana, et al., 2020). Newer meta-analyses control for mass equivalency, but at a cost: in Meurer et al. (2018), the most common reason for excluding a study was issues with bulk density measurements or depth making the data incomparable.

Building on analysis by Haddaway et al. (2017), Meurer et al. (2018) controlled explicitly for mass equivalency using the approach by Ellert and Bettany (1995), and confirmed that soil C stock benefits of no-till and reduced till were limited to the surface soils. Ogle, Alsaker, et al. (2019) also controlled for mass equivalency and found that soil C stock is higher under no-till from 0-20cm depth, but higher under full-till at depths below 20cm. Angers and Eriksen-Hamel (2008) found that soil C stocks under no-till were on average 4.9 Mg C ha^{-1} higher than full-inversion tillage and that the benefit of no-till increased slightly, but significantly, over time. However, their meta-analysis did not require a mass equivalency approach to be taken in the comparison between no-till and full-inversion tillage.

In tillage action, residue and plant material on the soil surface is redistributed within the soil profile. This slows its decomposition compared to material on the surface and means that an important consideration for the different impacts between full- and no-till is the C inputs: Virto et al. (2012) found that greater crop C inputs explained 30% of the stock differences between no-till and full-inversion till.

The impact of tillage may be different depending on climate and soil type, though uncertainties are large (Tiefenbacher et al., 2021). The benefits of no-till have been found to be greater in warmer and wetter climates due to better potential physical protection (Haddaway et al., 2017; Ogle, Alsaker, et al., 2019). Conversely, Sun et al. (2020) found that changing to no-till had different impacts on crop yield and soil C depending on climate, with dry regions showing increased yield and soil C stocks and cold regions showing potential for soil C loss. Ogle, Alsaker, et al. (2019) found that the impact of tillage in warm climates was less deep in sandy soils than loamy, silty or clayey soils. These apparently differing conclusions indicate the importance of considering tillage's impact on (surface and subsurface) micro-environmental conditions which influence decomposition rates (Chenu et al., 2018).

Taken together, recent studies and meta-analyses suggest that the soil C impact of no-till compared to conventional till is not clear cut and that site characteristics must be considered (Sun et al., 2020; Tiefenbacher et al., 2021). Any soil C stock benefits are likely restricted to the surface layers and may be reversed below 15-20cm. Over the whole soil profile, the change may be negligible (Luo et al., 2010) as tillage acts to redistribute C more evenly: disrupting the normally steep drop off in C stocks with depth. Across studies, uncertainties in quantification of these relationships are large and Ogle, Alsaker, et al. (2019) conclude that no-till is best regarded as a physical resilience method rather than managing for soil C sequestration.

1.2.3 Organic amendments

Organic amendments are added to soil for purposes including nutrient management and improving soil structure. A wide range of materials of plant or animal origin can be applied as organic amendments, including crop residues, manure, compost, wood chips and biochar. Chenu et al. (2018) identified the poor characterisation of organic amendments as a limitation to assessing the impact of a range of management options. Rubin et al. (2023) summarised the evidence for soil C sequestration, soil GHG emissions and life-cycle emissions for organic amendments and found that impacts, their magnitude, and the level of evidence for these varied between amendment types. In a regional synthesis for Southeast Asia, Tan and Kuebbing (2023) found that soil C benefits of compost and manure can be offset by increases in emissions of other GHGs such as methane and nitrous oxide.

Fertilisers can be organic or mineral in origin: studies focused on fertiliser management often include both. Use of fertiliser can increase soil C accrual, which may be maximised by a combination of mineral and organic fertilisers (Hijbeek et al., 2019). Several papers found differences with depth: Tautges et al. (2019) highlight different net soil C stock changes at shallow depths compared to the whole profile. Campbell et al. (2000) focused on shallow soil C and found the greatest increase in stock was associated with adequate application of N and P in fertiliser. Fertilisers are often chosen to manage nutrient availability. Significant correlations are observed between increase in attainable yields and increase in soil OM when organic inputs are provided, though any potential yield benefit of organic amendments can be negated if mineral fertiliser has supplied sufficient nutrients (Hijbeek et al., 2017).

Han et al. (2016) undertook a global meta-analysis of soil organic carbon (SOC) change under different fertiliser management, finding that the SOC benefits of different manure management relative to initial SOC were not consistent across climates or time. In most climates, manure is more efficient at C storage than straw, with the difference most clear in warm temperate climates and the first decade: manure application sequestered 0.36 g kg^{-1} yr^{-1} and straw 0.13 g kg^{-1} yr^{-1} (Han et al., 2016). The rate of SOC change was negatively correlated with initial SOC. Cool temperate climates tended to take longer to reach a soil C equilibrium compared to tropical sites (Han et al., 2016). Whilst short-term soil amendment C retention rates vary between amendment types (Angers et al., 2022), long-term retention rates are similar (Smith et al., 1997).

Many options for organic amendments are similar materials in a different part of a potential 'lifecycle'. For example, plant biomass is the major component of crop residues, straw, compost and herbivore manure. Studies have assessed the difference in soil C stock response to fresh, digested or composted materials: in the long term (decades to centuries) Cardinael et al. (2015) found that the impact of straw did not change whether it was fresh or composted, while Thomsen et al. (2013) found that the storage of C did not vary significantly whether inputs were fresh or digested, having accounted for C losses in processing. Recent studies seem to suggest that, counterintuitively, the more labile organic amendments contribute more to SOM in the long term, with several proposed explanatory mechanisms including greater carbon use efficiency in microbial processing of labile inputs and protection of soluble compounds in soil through movement to mineral surfaces (Chenu et al., 2018). It has also been shown that below-ground inputs (such as roots, or amendments buried by soil fauna) are retained at much higher rates than above-ground inputs (such as plant litter or amendments remaining on the soil surface) (Jackson et al., 2017).

1.2.4 Summary of cropland impacts on soil C

Overall, evidence suggests that the impacts of cropland management practices on soil C depend on a wide range of factors. There is a lack of consensus on these drivers (Derrien et al., 2023; Lin et al., 2023) combined with a lack of data in some agro-environmental contexts (Chenu et al., 2018). In addition, research studies often focus on one practice comparison at once, whereas farmers are undertaking combinations of practices (Bradford et al., 2023). In some cases, these combinations may be referred to as "conservation agriculture" or "regenerative agriculture", which have clear objectives in terms of soil, but are not completely prescriptive in terms of practices.

Given that soil C stock changes depend on climate, environment, soil characteristics and land use, it is necessary to quantify soil C at field level to understand the impact of management.

1.3 Quantifying the impact of cropland management on soil C stocks

1.3.1 Direct measurement

The concentration (%) of soil C in a soil sample can be assessed using a range of laboratory methods (including wet oxidation, loss-on-ignition and dry combustion); the choice of method can affect the results (Roper et al., 2019). To measure stocks of soil C (Mg C ha^{-1}) accurately requires volumetric samples, because the bulk density of the soil must also be calculated. As stocks of soil C change through the soil profile, measurements of soil C should be given for a particular sampling depth.

There are a number of pertinent challenges to measurement of soil C, particularly for assessing change over time. These are underpinned by the heterogeneity of soils, constant fluctuations in soil C stocks and the small scale of management-driven changes relative to the background levels of soil C (Smith, Soussana, et al., 2020; Stanley et al., 2023; Wiesmeier et al., 2019).

Spatial and temporal aspects of sampling strategies should be designed with these challenges in mind, typically increasing costs (Campbell & Paustian, 2015; Minasny et al., 2017). Sample numbers should increase with heterogeneity and each should be analysed separately in the same laboratory (Stanley et al., 2023), particularly if aiming to detect relatively short term changes in soil C.

To accurately account for changes in soil C stock in managed soils, where practices can change the bulk density and height of the soil, the need to take a mass equivalency approach is an additional complication for measurement (see Section 1.2.2; Ellert & Bettany, 1995; Fowler et al., 2023).

The need for such robust sampling makes relying solely on measurement of soil C for monitoring and decision support infeasible for many (Campbell & Paustian, 2015), particularly considering the cost of sampling compared to the value of soil C stored (Smith, Soussana, et al., 2020). Even with a careful sampling strategy, soil C measurement can have significant uncertainty.

If soil C measurements are to be used to inform management decisions, there remains a challenge for predicting future change from past measurements, particularly for new management options that have not yet been sampled. Modelling of soil C can help to reduce the need for direct measurement and can be used to compare the potential soil C impact of a range of practices over time.

1.3.2 Modelling

Over recent decades, interest in parameterising soil processes for various purposes has led to the development of soil models that provide predictions of soil C stock evolution over time.

Modelling approaches can be based on a scientific understanding of the environment, a statistical interpretation of observed data or a combination of both (Derrien et al., 2023). Process-based models represent known environmental interactions as equations, whereas statistical models are based on parameterised links in observed data, and therefore are not rooted in the physics of the Earth system. These approaches have different strengths and weaknesses (Blagodatsky & Smith, 2012). Due to being based only on data provided to generate them, statistical models are not applicable outside the calibration space. By representing physical interactions, process-based models are often applicable across environmental settings. Whilst they are underpinned by a lot of theory, process-based models require relatively little data for generation and can be flexed or added to as new knowledge develops. Statistical models require significant amounts of data to generate and can only be applied to the modelled ‘problem’. The principal advantage of statistical models is the ability to represent relationships that are too complex, or have too many unknowns, to be represented reliably by mechanistic models. They cannot be built on, but can be re-parameterised with new data.

In process-based models, the use of several soil C "pools" is a common approach to modelling the range of different decomposition rates that occur in soil materials (Smith et al., 2012), and this has been the dominant approach for several decades (Campbell & Paustian, 2015). However, these pools are defined by decomposition concepts, rather than measurable chemical or physical fractions. This can make them hard to compare to measurements and challenging to parameterise (Stockmann et al., 2013). Abramoff et al. (2018) applied the concept of pools to measurable soil C fractions instead, and compared the outcomes with the CENTURY model - a well-regarded soil C model that includes pools (Parton et al., 1988). The comparison indicated many areas of similarity in output between the two models but also indicated divergence in soil C stock change when multiple influences were involved.

Acceptable assumptions in models depend on their intended use: for example, the IPCC provides methods for national inventories, which need to be able to represent a broad range of environments on a consistent basis, rather than work to represent specific environments in great detail (Eggleston et al., 2006). The spatial scale of soil C assessment leads to differing conclusions about what is an important dependency (Manzoni & Porporato, 2009): plant to field level drivers are often based on soil chemistry and texture, whereas regional to global relationships are better described by climate and vegetation, leading to separate indicators being required in models (Blagodatsky & Smith, 2012; Wiesmeier et al., 2019). The temporal axis is important, since soil C stocks fluctuate naturally and short-term changes in overall stocks can be hard to discern. Longer-term models must also consider the context of soil C equilibrium and saturation (see Section 1.5.2), which takes place over time-spans of decades (Don et al., 2010; Klumpp et al., 2017).

Chenu et al. (2018) identify key difficulties in using process-based models for soil C dynamics at the local scale. These can be split into two categories. The first is challenges in providing the input data needed by the models, i.e. the unknown equilibrium status of the soil at the start of the model run, initialising the modelled SOC pools and estimating the actual C inputs to the soil. The second source of difficulty is shortcomings in model ability to explicitly represent observed drivers of local soil C patterns, such as representation of soil types, subsoils and the impact of practices on decomposition rates. This means that model validation and calibration are critically important in soil C modelling (Campbell & Paustian, 2015; Le Noë et al., 2023; Smith, Soussana, et al., 2020).

Model calibration means *"fitting model parameters to best reproduce some empirical data"*, whilst validation refers to testing model abilities to reproduce observations on which it was not calibrated (Le Noë et al., 2023). For both, good data are required, which is discussed further in Section 1.5.1.

1.4 Farmer and policy context

A growing number of farmers, businesses, policy makers and standards organisations are looking to manage soil C for environmental health, food (production) security and/or reducing net greenhouse gas emissions. The European Union has adopted its first soil monitoring law (European Parliament, 2024) and many net zero pledges rely on soil carbon sequestration (Smith et al., 2022). Quantifying and predicting soil carbon storage is critical to the success of such projects, but, as discussed, reliable measurements of soil carbon stocks and their change are difficult.

For farmers, any change in practice represents a risk, through impacts on productivity, costs, or both. This understandably makes the uncertainty of soil C management unattractive, particularly as the economics of farming becomes increasingly challenging. De-risking these transitions for farmers is pivotal to turning the tide on soil degradation and soil C loss.

Financial return is one option to reduce risk for farmers changing practices. This underpins the idea of carbon markets, where carbon is traded at prices subject to supply and demand market dynamics. Carbon markets are a mechanism to reduce net GHG emissions by polluters paying for "carbon credits" from projects that store carbon, counting the sequestered carbon as a negative emission to offset their continued positive emissions. Trading carbon for money offers an incentive for projects to sequester carbon. However, some main principles for effective carbon credits are that the carbon is measurable, stored permanently and is additional to any change that would have happened without the project. These guarantees are hard to make in soil C management projects. When there is uncertainty, carbon credits are usually discounted (Black et al., 2022); reducing the return on investment for carbon sequestration projects. The reduced financial benefit of selling carbon credits from soil C management may, then, not be worth the burden of the restrictions that the project places on land managers or even cover the costs of undertaking the project.

Whilst a growing number of countries have environmental policies that incentivise more sustainable farming practices, the absence of specific policy for soil C sequestration means the market for (outcome-based) carbon credits has tended to operate in a private or NGO space (Black et al., 2022; Phelan et al., 2024). This landscape, combined with carbon accounting challenges, has led to inconsistencies between different standards and protocols which drive uncertainty in the equivalency of credits between markets (Oldfield, Lavallee, et al., 2022).

For soil C sequestration projects, measurement, reporting and verification (MRV) protocols must outline how soil C stock changes are to be quantified. Currently, many protocols allow the use of models, often in combination with measurements to verify (or re-calibrate) model predictions, though guidance on how to use models and data in this way is sparse (Oldfield, Lavallee, et al., 2022).

Some socio-economic barriers to adoption of soil carbon management and carbon credits are still not well understood (Davidson, 2022), and are probably difficult to generalise. However, recent research around farmer perceptions and willingness to engage in carbon markets highlights challenges. Farmer confidence in crediting mechanisms is undermined by inconsistencies between schemes, administrative complexity and a lack of methodological transparency (Phelan et al., 2024, and references therein). There are also critical incongruities between the demands of carbon crediting methods and the realities of farming (Amin et al., 2023). An important example here is timescales. Carbon crediting requirements must ensure appropriate permanence of soil C accrual and (as discussed in Section 1.2) practices must be guaranteed to be undertaken for a number of years in order to have a clear impact. The business case for agreeing to these requirements has to be compelling and science cannot always provide clear answers with a palatable level of uncertainty (Oldfield, Lavallee, et al., 2022).

Decision support tools have a role in tackling key challenges for effective soil C management. By presenting relevant information in a way that is accessible to non-experts, they can simplify some of the mechanistic complexity described in Section 1.2 and improve farmer understanding of soil processes. By facilitating prediction of multiple scenarios before any investment is made, risks can be examined and reduced. By consolidating and standardising scientific understanding and management information, decision support tools can also aid collaboration between actors. As discussed, there are a variety of drivers behind soil C management, including resilience, direct financial incentive and optimising resource use. Different tools are targeted towards particular drivers; they must apply appropriate soil C models and report outputs responsibly, including uncertainty.

Farmers are knowledgeable about their work and soil (Eze et al., 2021) and peer-to-peer learning has a role for expanding the uptake of practices to improve soil (Mattila et al., 2022). The roles for scientists in overcoming these challenges include translating scientific knowledge into useful information (Phelan et al., 2024) and improving models, including by generating datasets to test and refine them (Oldfield, Lavallee, et al., 2022). The complexity of models and burden of data provision is a barrier to farmers being equipped with useful information to enable soil C sequestration (Dechow et al., 2019).

1.5 Current state of soil monitoring research for soil C modelling

This section draws attention to two topics shaping the recent discourse on soil C modelling. The first is data quality and quantity. The second is evidence for soil C saturation and equilibrium, which informs potential for soil C sequestration and common assumptions during model initialisation.

1.5.1 Data

As identified in Section 1.3.2, good soil C datasets are needed for model calibration and validation, and to build understanding of soil C dynamics. Many recent studies highlight shortcomings in data for properly assessing soil C: this includes lack of data at or below the plough depth and missing bulk density measurements which are crucial in assessing practices with a significant impact on soil structure (like tillage) (Raffeld et al., 2024). In a meta-analysis Poeplau and Don (2015) warned that soil C stocks or bulk density (to calculate soil C stocks) were only reported in 13 studies (30%) and only 3 studies included data below typical plough depth. Tautges et al. (2019) conclude that ignoring changes in soil C at depth may result in false conclusions about the impact of management. Though soil C stocks are estimable through pedotransfer functions and mass equivalency, this represents a weakness in conclusions drawn by resulting meta-analyses.

Harden et al. (2018) state that many data useful for measuring soil C change at annual scales are rarely consolidated and highlight opportunities of large soil datasets; including generating empirical models. Todd-Brown et al. (2022) and Malhotra et al. (2019), among others, also outline how consolidating soil data could drive progress across a number of soil research areas. However, the myriad ways in which soil data has been collected, logged and stored are a significant barrier to dataset consolidation, meaning that a community standard on data collection and management is required (Todd-Brown et al., 2022).

1.5.2 Saturation, equilibrium and model initialisation

As understanding of soil mechanisms developed, the idea of an upper limit on soil C stocks (saturation point) in a given soil emerged (Lal, 2008; Stewart et al., 2007). The discourse on whether there is a limit and what the limit would be continues. Begill et al. (2023) found no upper limit in a broad analysis of German soils; a conclusion that is challenged by Six et al. (2024) who identify six key principles necessary to draw reliable conclusions about saturation levels on the basis of soil type. The existence of an upper limit on soil C stocks means that soils further from saturation can store more C and that all sequestration potentials are finite. Therefore baseline (or initial) soil C stocks are relevant to assessing the long-term potential impact of management (Stewart et al., 2007). This has been found in many field experiments, though is also true that the appearance of greater C storage in soils with low C compared to those with high C can be driven by statistical artefacts (Slessarev et al., 2022), so care must be taken. Overall, most managed soils are far from saturation, but it remains important to consider in long-term soil C modelling (Six et al., 2024).

In addition to an absolute limit, there is also the idea that soil C stock reaches an equilibrium under consistent conditions (natural or managed). In such a steady-state, inputs to soil C are balanced with outputs over time (Paustian, Collins, & Paul, 1997). Most soil C models include equilibrium dynamics (Stewart et al., 2007), though time periods over which equilibrium is reached vary from decades (Don et al., 2010; Jensen et al., 2022; Nayak et al., 2019) to centuries (Wutzler & Reichstein, 2007).

As mentioned in Section 1.3.2, many process-based models are based on conceptual pools of soil C characterised by different decomposition rates. In order to perform a forward run of the model, the initial pool sizes must be given: a challenge for these unmeasurable quantities. This initialisation step therefore often requires an assumption. The most common approach is a spin-up run (Herbst et al., 2018; Taghizadeh-Toosi et al., 2020). This refers to running the model in reverse to establish pool values, and assumes soil C stocks are in some equilibrium at the start of the forward run. Other suggested initialisation methods either map measurable fractions to conceptual fractions (e.g. Zimmermann et al., 2007), or account for long-term land use history - which requires data (Don et al., 2010; Taghizadeh-Toosi et al., 2020). Whilst these alternative methods have been shown to have benefits for model prediction in some cases, their higher data needs are often hard to meet (Klumpp et al., 2017; Yeluripati et al., 2009).

The validity and impact of the spin-up equilibrium assumption is somewhat unclear. Wutzler and Reichstein (2007) concluded that a spin-up run is only valid where the model is calibrated for a similar disturbance history. Herbst et al. (2018) warn that the assumption of equilibrium for long-term arable sites can cause errors. Foereid et al. (2012) and Yeluripati et al. (2009) found that modelled rates of change were sensitive to initialisation method whilst Dimassi et al. (2018) found that the role of initialisation in soil C projection uncertainty (using the CENTURY model) was negligible. Klumpp et al. (2017) compared RothC model initialisation approaches and found the most effective method to be adjusting spin-up C inputs so that the modelled SOC matches measured initial total SOC, rather than assuming equilibrium. This approach is also pragmatic in avoiding the need for extensive historical data.

Overall, soil C modelling must consider equilibrium and saturation dynamics. Model implementation decisions must be appropriate for the scenario to be represented.

1.6 Conclusions and aims and structure of this thesis

Sustainable and resilient agriculture requires fertile soils, which require carbon (Lal, 2004). It is critical to issues of ecosystem health, food security and climate change to understand and be able to predict how agricultural management affects soil C and, in particular, which options can sequester or retain soil C. The impacts of cropland management on soil C are varied, uncertain and context specific, with drivers spanning spatio-temporal scales. Soil C models are a key tool to handle this complexity. However, for land management applications, their data requirements are an obstacle, vague or wide uncertainties are a risk and the resulting information is not always what is needed to support decisions. There is a need for greater attention to provision of meaningful decision support that achieves maximum accuracy with minimum complexity, despite continuing debate in soil science (Derrien et al., 2023).

Therefore, the overarching aim of this thesis is to enable useful soil carbon modelling at field scale to support cropland management decisions. This means reducing the data burden of modelling and/or increasing the value of model outputs. Specific objectives are:

1. **Establish useful empirical models for soil C prediction with cover crops as a focus practice:** *Chapter 2*

2. **Understand the impact of using public datasets instead of measured data as model inputs:** *Chapter 3*
3. **Explore methods to combine models with site data:** *Chapter 4*
4. **Reflect on implications for soil science, land managers and protocols:** *Chapter 5*

Chapter 2 has been published, and Chapters 3 and 4 are structured in a paper style. Chapter 5 draws together the findings from the earlier chapters and concludes the thesis.

Chapter 2

Modelling the soil C impacts of cover crops in temperate regions

Chapter 2 has been published as:

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With the following author contributions:

HH and JH formulated the research question. HH designed and carried out the analysis and wrote the first draft of the manuscript. SM and MS provided the dataset. All authors discussed findings and reviewed the manuscript.

2.1 Introduction

As introduced in Section 1.2, cover crops are planted as an alternative to bare soil between cash crop production seasons. The motivations for this include physical protection of the soil, increased organic matter input to the soil and increased plant biodiversity which all support ecosystem productivity and resilience (Schipanski et al., 2014). Cover crop biomass provides C to soil, so the practice is proposed as a way to protect and increase soil C stocks. The growing evidence base for cover cropping impacts on soil C suggests that stocks can increase at rates of 0.1 to 1 Mg C ha^{-1} yr^{-1} (Blanco-Canqui et al., 2013; McClelland et al., 2021; Poeplau & Don, 2015), with impacts varying by climate, environment and management characteristics.

As a potential multi-benefit practice that has resource and time costs, understanding the impact of cover crops is of value to farmers and land managers. Many soil C predictions require a baseline soil C value because rates of change in soil C are believed to be related to existing stocks; as either a function of existing stocks or of a perceived deficit in existing stocks compared to potential stocks (Slessarev et al., 2022; Stewart et al., 2007). However, measuring soil C is challenging. Establishing a reliable baseline value for comparison requires particular rigour; it is important to contextualise it with land use and management history and for it to be valid across the intended area of use, meaning that sufficient sampling is key.

This published chapter utilised existing data to parameterise parsimonious regression models for the soil C impact of cover cropping in temperate climates without using a baseline soil C stock figure. We compared the predictive ability of these to meta-analysis response ratios and the simplest IPCC 'Tier 1' method. The response variable used was the annual change in soil C (ΔSC_{yr}). Not only is this appropriate for the intended application of these models on farms, where decisions are taken on daily to yearly scales, it also removes the requirement for any existing soil C measurement.

The model structures are simple and the methodology for model selection combines statistical and practical considerations, since a parsimonious model that utilises unknown input data remains inaccessible.

2.2 Published paper

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Modelling the soil C impacts of cover crops in temperate regions

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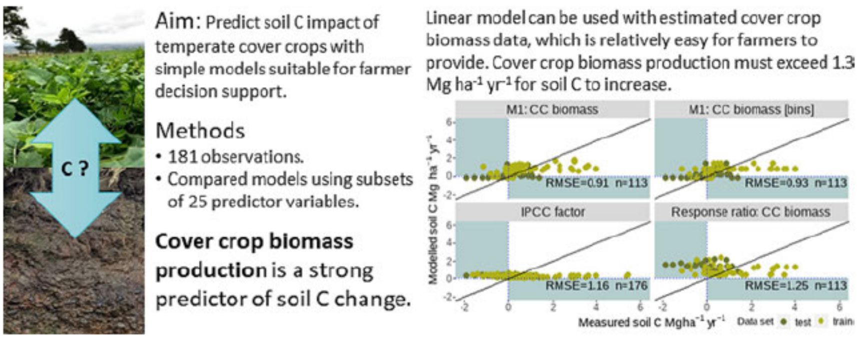
HIGHLIGHTS

- Belowground carbon (C) storage for both ecosystem health and greenhouse gas management is of growing interest to farmers.
- Farmer decision support for soil C management must have low data cost.
- We compared regression models, IPCC factors and meta-analysis response ratios for soil C impacts of temperate cover crops.
- The most suitable model to predict soil C change was based on cover crop biomass.
- We predicted an increase in soil C stocks with cover crop biomass over 1.3 Mg ha^{-1}.

GRAPHICAL ABSTRACT



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ABSTRACT

CONTEXT: Agricultural land management decisions are based on numerous considerations. Belowground carbon (C) storage for both ecosystem health and greenhouse gas (GHG) management is a growing motivation. Observed heterogeneity in soil C storage in croplands may be driven by various environmental, climatic and management factors. Farm system models can indicate which practices will drive C storage, provided the practice is well parameterised and the land manager can provide necessary input data.
OBJECTIVE: We aimed to predict soil C impacts of temperate cover cropping using simple models suitable for broad farmer use and decision support.
METHODS: The dataset used was initially compiled for a meta-analysis (McClelland et al., 2021) to quantify soil C response to cover crop treatments relative to a non-cover cropped system. It contains 181 data points from 40 existing studies in temperate climates. Environmental, climatic and management indicators were regressed pairwise to predict annual soil C stock change under cover cropping relative to no cover cropping. We also included the IPCC tier 1 methodology and meta-analysis response ratios in our model comparison.
The ease of reliable measurement and monitoring across the modelled indicators was also considered because the best-correlated relationships are squandered if data constraints risk decision-makers being unable to use the model.
RESULTS AND CONCLUSIONS: Using an extended test dataset to consider priorities for model users, several regression models outperformed the IPCC tier 1 methodology. In particular, two regression models reliably

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predicted negative changes in soil C, which IPCC and meta-analysis factor approaches could not. A single variable regression model based on cover crop biomass (dry matter) production was the best combination of statistical power, biological relevance and parsimony. In temperate climates, we predicted an increase in soil C stocks as long as cover crop biomass production exceeded 1.3 Mg ha^{-1} yr^{-1}.

SIGNIFICANCE: Our final model can be applied with estimated user input data, and avoids the need for baseline soil C as an input; this makes it relatively accessible for farmers. Parsimonious models for soil C change under land management practices can be effective and are an opportunity to increase access to soil C management information for farmers.

1. Introduction

Carbon (C) sustains soil health by increasing water and nutrient retention, supporting resilient soil structures and the soil microbial community (Nieder and Benbi, 2008; Lal, 2018). It is a crucial element of functioning ecosystems, both managed and natural. Globally, the impact of historical land conversion to cropland and cropland management on soil C stock has been substantial and detrimental. Due to greater direct physical and chemical disruption of soils, cropland is associated with higher rates of soil C loss than grazing or forestry management (Lal, 2004). Net loss of soil C impacts ecosystem function and contributes to greenhouse gas (GHG) emissions that are driving ongoing climate change (Lal, 2014).

Globally, a soil C sequestration rate of 0.4% per year would offset 20–35% of anthropogenic GHG emissions; this target is the centre of a major initiative, “4 per mille”, for agricultural soils to tackle the climate crisis (Minasny et al., 2017). To achieve this emissions benefit, alongside protecting ecosystems and ensuring sustained crop yields, crop management decisions can be taken to decrease soil C losses, increase soil C additions or both (Lal, 2004). As an opportunity to tackle net GHG emissions, soil C sequestration and storage are likely to have lower impacts on land, water and energy, and cost less than other negative emission technologies (Smith, 2016). The principal limitations are that the soil C sink capacity is limited, and any storage of C is easily reversible (Smith, 2016). For arable land managers to consider soil C stocks, the ability to monitor them reliably at appropriate spatial and temporal scales is critical.

Soil C stocks are heterogeneous at all spatial scales and measurements are time consuming, costly and often unreliable (Campbell and Paustian, 2015). Given this, and the increasing focus on protecting and improving soil C stocks, models for soil C change have been developed over the last four decades. Available methods range from process-based (RothC (Coleman and Jenkinson, 1996), CENTURY (Parton et al., 1988), DAYCENT (Parton et al., 1998), DNDC (Li et al., 1992)) to empirical (IPCC National GHG inventories (Eggleston et al., 2006), Smith et al., 1997), with varying data requirements and underlying assumptions. Depending on the intended application, modelling minimises the need for soil C measurement over time and can also indicate potential impacts of land management decisions *ex ante*. Since these models were developed, evidence for the impacts of management practices on soil C has expanded and available modelling methods have evolved (Smith et al., 2020).

This paper focuses on the practice of cover cropping and its influence on soil C. Cover crops are grown to cover otherwise un-cropped soil in time and/or space. The most common application of cover crops is planting between cash crop seasons, i.e. instead of a fallow field (Poeplau and Don, 2015). However, cover cropping can also refer to planting alongside the main crop, called ‘companion cropping’ or ‘intercropping’. Here, cover crops are plants grown where the residues are not harvested, unless otherwise specified.

Previous research indicates that soil C stocks respond positively to cover cropping, though magnitudes vary. Poeplau and Don (2015) found a soil C increase rate of 0.24–0.4 Mg C ha ^{1} yr ^{1} under cover cropping, in a dataset with a mean practice duration of 6.8 years. Blanco-Canqui et al. (2013) estimated that, in no-till systems, cover crops drive an additional 0.10–1 Mg C ha ^{1} yr ^{1} storage compared to no cover crop. McClelland et al. (2021) found an average increase of 1.11 Mg C ha ^{1} across their dataset on temperate cover crops over a range of time periods. If annualised, this gives an estimate of 0.21 Mg C ha ^{1} yr ^{1}, albeit the authors note that time since cover crop introduction was a poor predictor of soil C response.

Soil C sequestration takes place over years to decades, whilst land management decisions are made by farmers on a daily basis. Tools to support farmer consideration of GHGs must include those management options that have an impact on soil C. Additionally, input data must be reliably retrievable by users, processes should be comprehensible and outputs must be valuable information to aid decisions. The Cool Farm Tool (CFT) is an example of a tool developed using these principles and prioritises farmer usability alongside peer-reviewed methods (Hillier et al., 2011). Many soil C calculations within the CFT are underpinned by Intergovernmental Panel on Climate Change (IPCC) ‘Tier 1’ methods for GHG inventories, which apply default factors to estimate the impact of a management change on existing soil C stocks, based on climate, land use and practices (Eggleston et al., 2006). The impact is applied for 20 years after the practice change, at which point soil C stocks are assumed to be at equilibrium. The IPCC methods were parameterised through synthesis of peer-reviewed research into the GHG impacts of land use and are designed for use at a national scale. By requiring only current soil C and management information, the IPCC Tier 1 methods have a particularly low data cost and are therefore ideal for resource constrained or non-expert users. The global applicability of the IPCC and CFT makes them more easily comparable across sites and supply chains than localised approaches. The IPCC methodology does not have a specific cover crops factor, so the CFT uses the C input factor to represent the impact of a change in cover cropping.

At the time of writing, no further information on practices or environment is required from users for the CFT to estimate the impact of a change in cover cropping. However, the impact of cover crops on soil C is observed to vary across environments and with management decisions. It depends on whether the cover crop is a grass, legume or non-legume (Shackelford et al., 2019;Rosolem et al., 2016; Blanco-Canqui et al., 2013; Abdalla et al., 2019; Finney et al., 2017), on climate conditions (Clark et al., 2017) and growing season (Poeplau and Don, 2015; Alvarez et al., 2017; Amado et al., 2006). In short-term studies, the impacts of cover crops on soil C compared to a no cover crop control are often unclear or insignificant (e.g. Clark et al., 2017), in part due to soil heterogeneity making change hard to detect (Blanco-Canqui et al., 2015).

Evidence suggests that cover crops provide an opportunity for farmers to protect or improve soil C stocks in their fields, but that the impact depends on some combination of environmental and management factors. The recent meta-analysis by McClelland et al. (2021) showed that cover crop aboveground biomass production, climate, cover crop growing season and soil clay content were the most powerful indicators for the impact of cover cropping on soil C. Using their existing dataset, this analysis parameterised a number of simple (parsimonious) regression models for the annual change in soil C under cover cropping in temperate topsoils (0-30 cm), employing a range of biological, environmental and management indicators. It then aimed to select the best available structure for predicting field-scale soil C changes under cover cropping.

2. Methods

2.1. Data

The collation and initial manipulation methods for the dataset used in this analysis are set out in McClelland et al. (2021). The dataset includes information from 40 papers (181 observations) comparing a cover crop experiment to a no cover crop control. The dataset is focused on temperate and sub-tropical climates, with 27/40 studies reporting on sites in the USA. The complete dataset includes 58 applicable indicators for each study site: location, climate, environmental and soil indicators and crop information, alongside some descriptive statistics. The most common cash crops in the dataset were cereals (maize, wheat, sorghum), soybeans, cotton and tomatoes. Cover crop species included were roughly evenly split between legume, non-legume and a mix of both (57, 67 and 57 observations, respectively).

Several characteristics of the McClelland dataset are noted here. Firstly, not all indicators were available in each study. Secondly, where possible, indicators were standardised and gaps were calculated as follows: soil carbon data were standardised to 0-30 cm depth using the methods set out by Jobbagy and Jackson (2000), as measurements ranged from 0-2.5 cm to 0-100 cm. When bulk density measurements were not available, site locations were used to extract the data from the USDA soil survey 'SSURGO' (Soil Survey Staff, 2017) for sites in the U.S. A. For studies outside the U.S.A., study authors were contacted directly for these data. These steps were necessary due to a lack of standardisation in soil C measurement and reporting.

2.2. Preparation for modelling

Analysis was completed in R (version 4.1.0). Prior to analysis, the following steps ensured that the parameterisation was applied to the most relevant data from the McClelland et al. (2021) dataset.

The basis for comparison was an experiment (cover crop) plot and a control (no cover crop) plot. The impact of having a cover crop can be described as the difference between the experiment and control outcomes at the end of the experiment. The response variable was annual soil C stock change in Mg ha^{-1} yr^{-1} (ΔSC_{yr}) calculated using Eq. (1).

$$\Delta SC_{yr} = \frac{(SC_{exp} - SC_{cont})}{yrs} \tag{1}$$

Where yrs = years since cover cropping began, SC_{exp} = mean soil C in the experiment plot (Mg ha^{-1}), SC_{cont} = mean soil C in the control plot (Mg ha^{-1}).

The few cases with calculated $\Delta SC_{yr} > 15$ Mg ha^{-1} yr^{-1} ($n = 2$) were removed as outliers and deemed to be beyond the scope of our model. This rate of sequestration from cover cropping alone, in excess of approximately 30 Mg ha^{-1} yr^{-1} of organic dry matter, is infeasible, and an order of magnitude greater than published average sequestration rates (e.g. Poeplau and Don, 2015; Blanco-Canqui et al., 2013). In addition to this, points where ΔSC_{yr} exceeded the total above-ground cover crop (CC) biomass (Mg dry matter ha^{-1} yr^{-1}) ($n = 7$) were excluded as unrealistic based on the following rationale. Cover crop biomass is expected to be the primary source of additional C in experimental plots. Though above-ground biomass excludes root biomass and rhizosphere contributions to soil C, only approximately half of biomass is C. A majority of biomass C inputs to soil mineralise rapidly (Angers et al., 2022; Berthelin et al., 2022); Villarino et al. (2021) and Castellano et al. (2015) suggest that only approximately 30% of input biomass C is successfully incorporated into the soil. With these balancing factors, we consider above-ground biomass produced as a sensible upper bound for ΔSC_{yr}.

We excluded studies of only one year in length ($n = 26$) as they were deemed unreliable for considering soil C change over time (Blanco-Canqui et al., 2015). Finally, studies with cover crops present year round ($n = 14$) were excluded: these are likely to better reflect perennial systems, which we also consider to be beyond the scope of our model. Given some overlap, these steps removed 34 data points in total, leaving 147 available for regression analysis.

The comparison between experiment and control is most valid where the two plots have the same environmental characteristics and have been identically managed during the cash crop season(s), as the cover crop is then assumed to be the driver of any soil C stock difference between the two sites. In this dataset, the environmental characteristics of the experiment and control sites are well matched in this way. In terms of management, 83% (122/147) of sites are appropriately matched and the remaining 17% have a difference in tillage or fertiliser (presence, type or amount). A grouping variable '*Ref*' was created based on the study the data came from and any within-study difference in how the control and experiment plots were managed.

Fertiliser quantities were standardised to kg N ha^{-1}.

Indicators were excluded where their coverage was not adequate for modelling cover crops across all temperate cropping scenarios. This principally applied to categorical variables and there were two main issues: categorical completeness (e.g. not all countries represented) and data density (sparse data in certain categories). Three indicators were excluded on this basis: country, cash crop type and cash crop fertiliser type.

Following the exclusions described, the dataset contained 24 relevant indicators with $n \geq 5$ observations that could be included in a model to explain the impact of cover crops on soil C (see Table 1). Since C input is a key driver of soil C change, we added a 25th indicator-'additional C input'- categorising whether the experiment plot had any other organic C amendments (e.g. compost, manure) and whether this was additional to the control plot.

2.3. Regression modelling

As ΔSC_{yr} was approximately normally distributed across our dataset, linear regressions were fitted using the R functions 'lm' and 'lmer' from the lme4 package (Bates et al., 2015). As the models were to be compared across different fixed effects, those with random effects were fitted with maximum likelihood rather than residual maximum likelihood. The first linear regressions used each of the 25 variables in turn as a single predictor variable for ΔSC_{yr}: in the form of M1 (lm) and M1r (lmer) (Eqs. (2) and (3)). For categorical variables, slope coefficients were calculated for each unique level. The *Ref* grouping variable was modelled as a random intercept; included because it was assumed that some of the variance in data was driven by between-study variance, as

Table 1
Variables from McClelland et al. (2021) utilised in modelling the impact of cover crops on soil C stocks.

Numeric variables		Categorical variables	
Label	n	Label	n
Experiment duration	147	CC frequency	147
Mean control plot SOC	147	CC frequency [group]	147
Bulk density	147	Ag. System	147
Soil pH	87	Experiment tillage	147
Percent (%) sand in soil	138	Soil texture	146
Percent (%) silt in soil	138	Agro-ecological zone (AEZ)	147
Percent (%) clay in soil	138	CC season	136
Mean annual temperature (MAT)	147	CC termination method	138
Mean annual precipitation (MAP)	147	Cash crop system	147
CC biomass (aboveground)	84	CC type	147
CC C:N ratio	57	CC system	147
Cash crop fertiliser amount	81	CC mix	147
		Additional C input	147

n = number of observations, CC = cover crop. All variables refer to the experiment plot unless otherwise indicated.

well as sampling error. In this study, the random effect was modelled with a random intercept only to simplify the application of these models to out-of-sample data- i.e. for prediction.

Multiple mixed effects linear models were generated using lmer for each pair of variables using M2r and M2ri (Eqs. (4) and (5)). These models extended to include two predictive variables and their interaction (as fixed effects). Using Cook's distance with a threshold of 1 (Cook and Weisberg, 1982), points with an excessively strong influence on the model were omitted and the model re-parameterised without them.

$$\mathrm{M1} : \Delta SC_{yr} \sim var1 \tag{2}$$

$$\mathrm{M1r} : \Delta SC_{yr} \sim var1 + (1|Ref) \tag{3}$$

$$\mathrm{M2r} : \Delta SC_{yr} \sim var1 + var2 + (1|Ref) \tag{4}$$

$$\mathrm{M2ri} : \Delta SC_{yr} \sim var1 + var2 + var1 : var2 + (1|Ref) \tag{5}$$

2.3.1. *Initial regression model selection*

Applying each of Eqs. (2)–(5) to the 25 candidate variables generated 650 regression models. The Generalised Variance Inflation Factor (Fox and Monette, 1992) was used to test for significant multicollinearity. Models including a term with $GVIF^{\frac{1}{2*df}} > 4$ (analogous to $VIF > 16$) were removed from consideration: this removed two models from M2r and 141 from M2ri.

An initial selection amongst of nested models was performed before considering their prediction performance with test data where nested means that the larger of two models contains all the terms from the smaller, with at least one additional term. Therefore, all four model structures are nested for each var1 and var2 pair. Given the different data (densities) amongst the parameterised models, model comparison is easier amongst nested models than non-nested models (e.g. comparing across models M1). For comparing nested regression models, marginal R^2 (R^2_m) calculated using the MuMin package (Barton, 2019) was used; R^2_m focuses on the variance explained by fixed effects. This left 300 unique models.

The 300 models were then evaluated using three criteria: R^2_m, Akaike Information Criterion (*AIC*, Burnham and Anderson, 2002; Akaike, 1998), and the intercept *p*-value (p_{int}). We used the lmer package to calculate *p* values by the Satterthwaite method, which is a preferred method (Luke, 2017). The 10 models with the lowest *AIC* values which also satisfied R^2_m>0.1 and $p_{int} < 0.05$ were retained for testing.

2.4. *Other models*

A variety of model structures is available to estimate the impact of cover crops on soil C. Here, we follow the principle of parsimony and focus on simple models, which have the benefit of low data cost. Two additional model structures and an input simplification were included for comparison with our selected regression models. First, the response ratios calculated from the same dataset in McClelland et al. (2021), and secondly the IPCC Tier 1 approach (using factors from Ogle et al., 2005). The latter is globally applicable and widely used, and is designed for national level inventories rather than field scale estimations. Ogle et al. (2005) factors are the result of a meta-analysis and a parsimonious approach to estimating soil C stock change; they are used here as a benchmark for other models.

We adapted these models for annualised soil C stock change as follows:

- McClelland et al.:

$$\Delta SC_{yr} = mean.c * \frac{(e^{lnRR} - 1)}{5.2yrs}$$

where 5.2 yrs is the average duration of training dataset and $lnRR = ln\left(\frac{X_{CC}}{X_{NCC}}\right)$ where X_{CC} is the mean SOC value for cover crop treatments, and X_{NCC} is the mean SOC value for no cover crop controls.

- Ogle factor:

$$\Delta SC_{yr} = mean.c * \left(\frac{\frac{1}{0.91} - 1}{20}\right)$$

where 0.91 is the response ratio for a change from medium to low input in a moist climate (Ogle et al., 2005). This method is the current approach used in the Cool Farm Tool (Hillier et al., 2011). In 2019, an update to the earlier IPCC factors was published (IPCC, 2019); the relevant factor difference is slight and would not affect the evaluation of the relative merits of the models described here.

- Input data bins: some models were also tested with the input data binned into stated ranges; a common approach when users can only estimate the value required. The models then calculated the response variable using the mid-points of the bin ranges rather than a specific measurement.

1.1. Model testing

We compiled a supplementary set of independent test data (Fig. 1), comprising 29 data points from eight studies (Bhardwaj et al. (2019), Blanco-Canqui et al. (2011), Blanco-Canqui et al. (2013), Constantin et al. (2010), Parkin and Kaspar (2006), Rochester (2011), Ruis et al. (2020), White et al. (2020)). These eight sources were not included in the final dataset of McClelland et al. (2021) but were, or would have been, identified using the initial search protocol set out in McClelland et al. (2021) and could be supplemented where necessary.

The test data were applied alongside the training data to test the shortlisted models. Like any out-of-sample data, the new test data does not have an applicable value for the regressions' random effect, and the mean intercept is taken. For testing, the random effects in the training data were also treated as unknown. The models are therefore applied to both subsets of the available data as they would be to any new, out of sample prediction.

Prediction intervals for input data were calculated using R functions predict() and predictInterval() from the merTools package (Knowles and Frederick, 2016).

3. Results

Out of 300 combinations of two variables, 278 nested comparisons found two variable models (M2r or M2ri) that performed better than single variable alternatives (M1 or M1r). Of these, 117 included an interaction (M2ri) and 161 did not (M2r). Of the 22 single variable models found, 19/22 included the random effect (M1r).

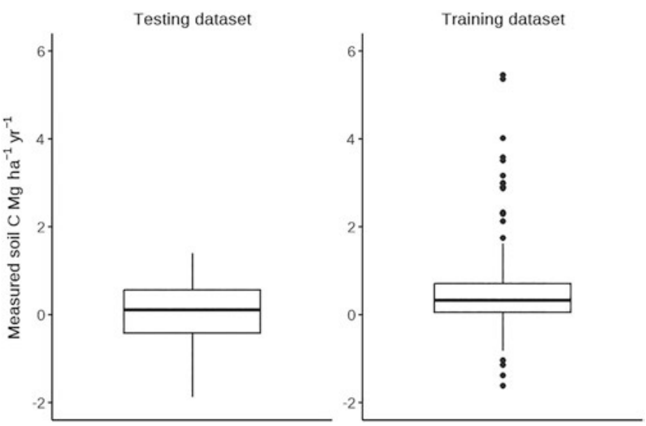

Fig. 1. Measured annual soil C change in training and testing datasets.

Focusing on the strongest 300 models, 54 met the criteria of having both $R_m^2 > 0.1$ and $p_{int} < 0.05$. We then shortlisted the following 10 models as having the lowest *AIC* values. All were two-variable models and three included interaction terms.

M2r: Bulk density & CC biomass
M2r: CC C:N ratio & % clay in soil
M2r: CC C:N ratio & % silt in soil
M2r: CC C:N ratio & Experiment duration
M2r: CC C:N ratio & MAP
M2r: CC C:N ratio & MAT
M2r: MAP & Soil pH
M2ri: AEZ & CC C:N ratio
M2ri: CC C:N ratio & Tillage
M2ri: CC season & CC biomass

Fig. 2 shows the model predicted change in soil C against the measured change in soil C for each shortlisted model (further model statistics in Supplementary Table 1). Seven of these models include the C:N ratio of the cover crop, which has positive coefficients indicating that a higher C:N ratio leads to greater soil C sequestration; studies have found that a higher C:N ratio reduces SOM decomposition (Thomsen et al., 2008). In all seven models including cover crop C:N ratio, either the intercept or the second variable included a negative coefficient. Where the other variable had a negative sign, cover crop C:N ratio limits the negative impact of that indicator on soil C; this is true for subtropic AEZs, percent silt in the soil, MAP, MAT and experiment duration. Over the 10 models, 12 variables were represented, nine of which are numerical. Due to data gaps not all models were assessed using the same number of data points, with the range in number of data points for each model from 53 to 79 out of a potential 147.

Having used nested comparison, R_m^2, p_{int} and *AIC* to identify the 10 strongest regression models based on the training dataset, we turned to testing. All types of model were applied to the extended testing dataset. Models tested were the 10 shortlisted regression models, their constituent one variable regression models (all with random effects assumed unknown), the response ratios from McClelland et al. (2021), the IPCC factor, the CFT approach and two one-variable regression models with input data in bins.

We examined RMSE values, using the IPCC Tier 1 methodology (based on Ogle et al., 2005) as a lower bound for acceptable RMSE values: since this method is for national GHG accounting, reasonable models for field scale prediction of soil C change should outperform the IPCC factor in this application.

RMSE values for the extended dataset indicate several models perform better than the IPCC tier 1 method (Fig. 3). Despite not being analytically shortlisted, several one-variable regression models have competitive RMSE values.

Our dataset has an interquartile range of measured ΔSC_{yr} of 0.013–0.682 Mg C ha ^{1} yr ^{1}, and overall range between 1.863 and 5.457 Mg C ha ^{1} yr ^{1} (Fig. 1). Fig. 4 shows that many regression models with favourable RMSE values predict a similar ΔSC_{yr} across the range of input data and thus do not capture this variation. Three models amongst those with strong RMSE values predict some of the observed negative changes: M2r CC C:N ratio & % silt in soil, M1 CC biomass and M2r Bulk density & CC biomass. The latter two models, including CC biomass, successfully predict the direction of change for the majority of points with observed negative ΔSC_{yr}.

M1 CC biomass (Eq. (6)) models a decrease in soil C stock of 0.27 Mg C ha ^{1} yr ^{1} if no CC aboveground biomass is present, increasing by 0.21 Mg C ha ^{1} yr ^{1} for each Mg of dry matter produced. The 95% confidence intervals for model predictions of ΔSC_{yr} for M1 CC biomass (Fig. 5) are approximately ± 2 Mg C ha ^{1} yr ^{1}.

M2r Bulk density & CC biomass (Eq. (7)) suggests that greater bulk density (within the range modelled, 1.01–1.77 g cm ^{3}) and biomass production are both valuable for carbon sequestration. Carbon

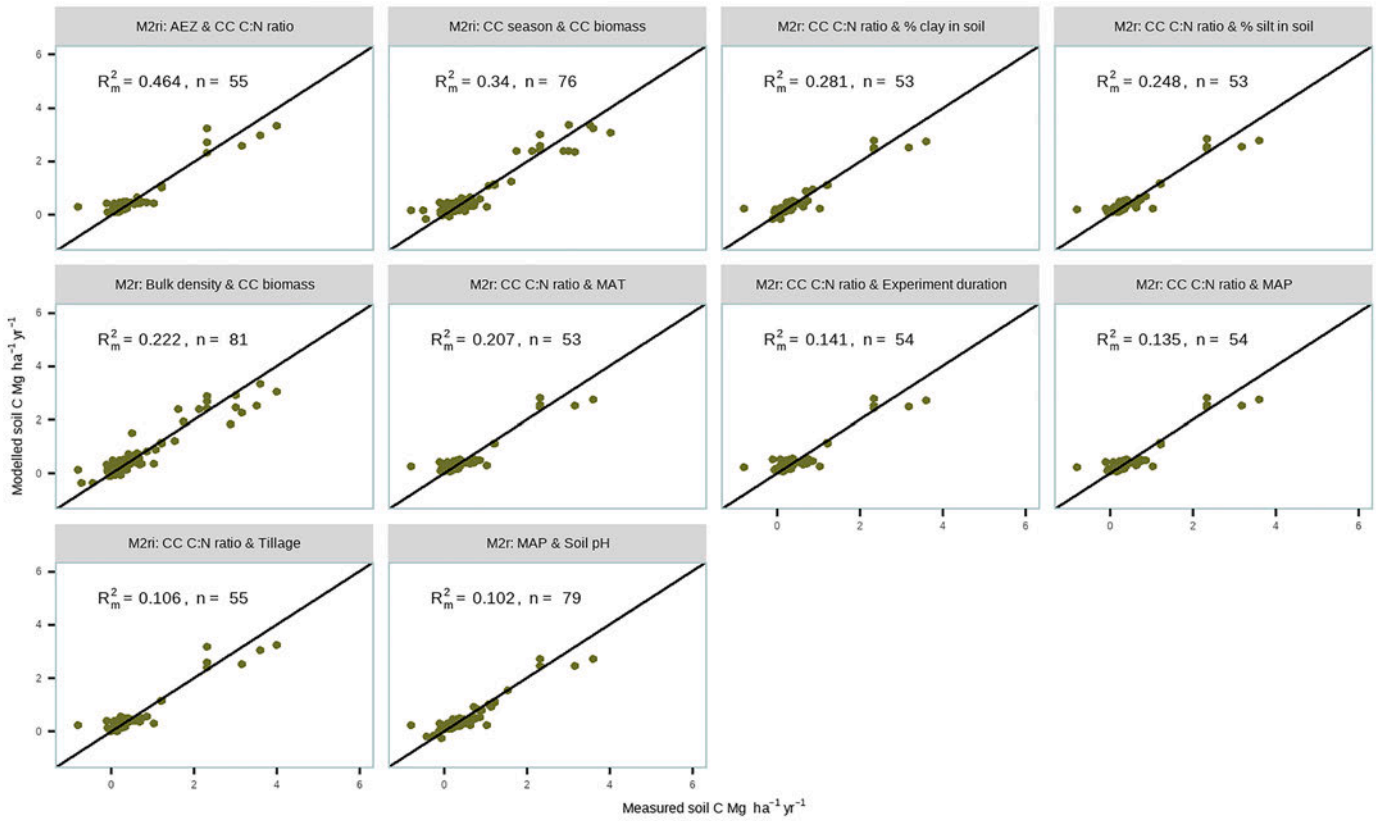

Fig. 2. Annual soil C change: observed and predicted, for models shortlisted using nested comparison, R_m^2, p_{int} and *AIC* combined, using the training dataset. The line y x is shown, which represents perfect prediction, n number of observations modelled. R_m^2 indicates the variance explained by fixed effects in each model.

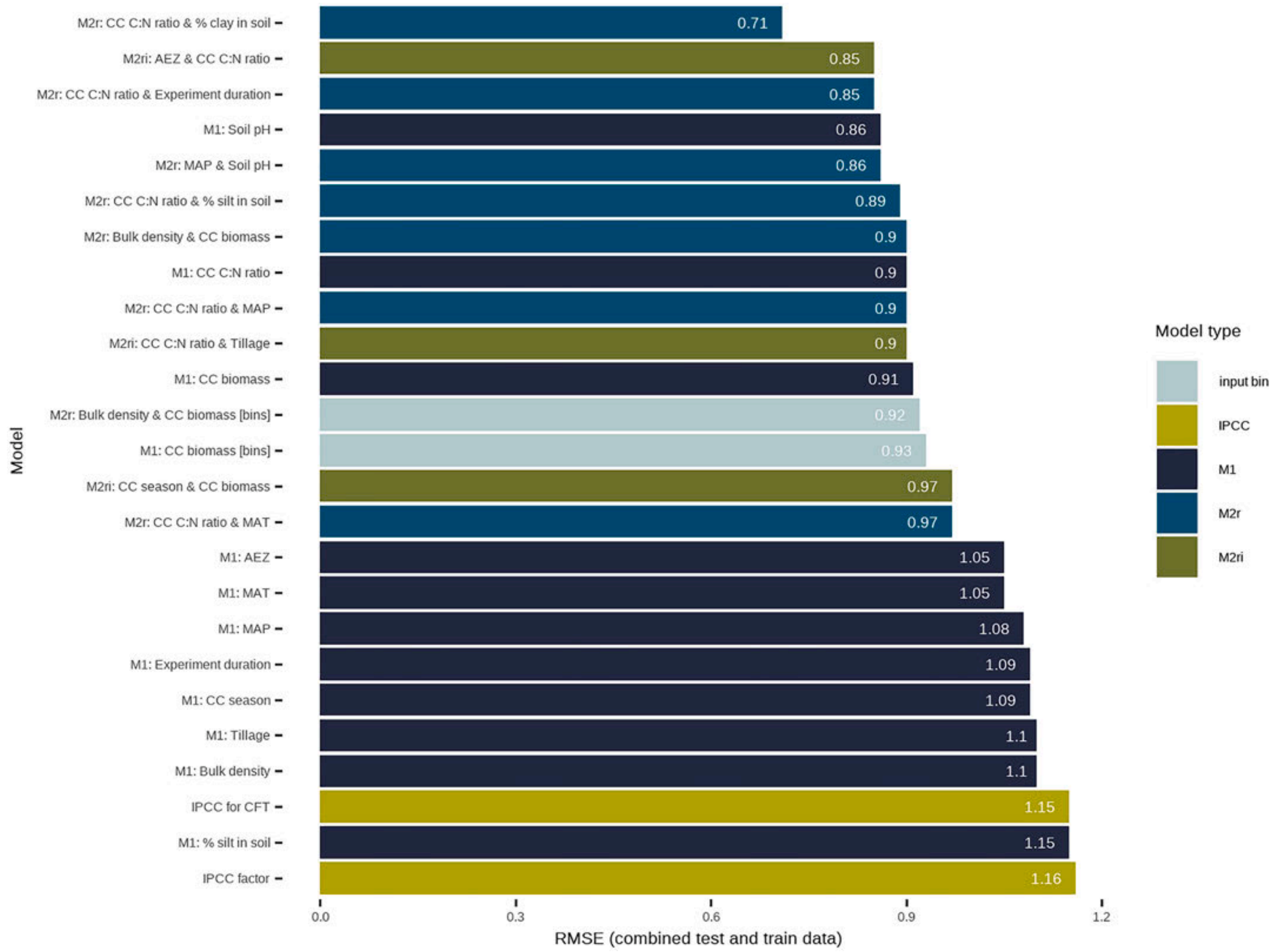

Fig. 3. RMSE values of soil C change for tested models-with IPCC RMSE as a lower bound.

sequestration would be predicted with a bulk density over the mean of 1.41, regardless of CC biomass production. With a low bulk density, significant CC biomass production is needed to reach positive C storage.

$$\text{M1 CC biomass}: \Delta SC_{yr} = 0.273\,[\quad 0.801, 0.255] + 0.213\,[0.106, 0.320]*CC\ biomass \tag{6}$$

$$\text{M2r Bulk density\&CC biomass}: \Delta SC_{yr} = 3.361\,[\quad 6.409, \quad 0.313\,] + 2.391\,[0.268, 4.5141]*Bulk\ density + 0.145\,[0.070, 0.220]*CC\ biomass \tag{7}$$

4. Discussion

4.1. Statistical model selection

In general, two variable regression models explained more variance in soil C storage under cover cropping than one variable models, and interaction terms were often useful. The best performing models often combined an environmental indicator (climate, soil characteristics) and a cover crop indicator (C:N ratio, biomass). Although tillage and mixing of residues within the soil are known to affect crop residue decomposition, these indicators appeared rarely in top performing statistical models; they added little in the context of more important explanatory variables. Cover crop termination method, whether the cover crop was incorporated into the soil or not, was not part of a regression model that explained ΔSC_{yr} well, despite being considered important (Potter et al., 2007). The descriptor of whether additional organic C (beyond CC inputs) was provided to the soil was also not part of the best performing models, which implies that cover crops may be able to increase soil C in systems already using organic amendments.

All of these models are relatively parsimonious. This is congruent with the aim to identify a simple and widely applicable model for the impacts of temperate cover cropping on soil C at the field scale. In any case, the dataset size ($n = 147$) makes parameterising regression models with many variables impossible and effectively rules out backwards model selection.

The initial model selection steps in this analysis were statistical, further selection steps focused on model prediction and sought to bring together statistical metrics with priorities for model use. The choice of AIC as the final statistical selection criterion had a significant impact on the models selected. Compared to selection based on the best R_m^2 the AIC calculation leads to selection of more numerical variables, and often those models with fewer data points. The 10 highest R_m^2 values overlap 50% with the lowest AIC values, and, had we used R_m^2 as the basis for our selection we would have selected five different models that all include CC season with $\geq$138 data points, three of which have a second categorical variable. In spite of this, it is important to note in the following that, although the discussion is specific to our use of the AIC criterion, the final conclusions are unaffected by this choice.

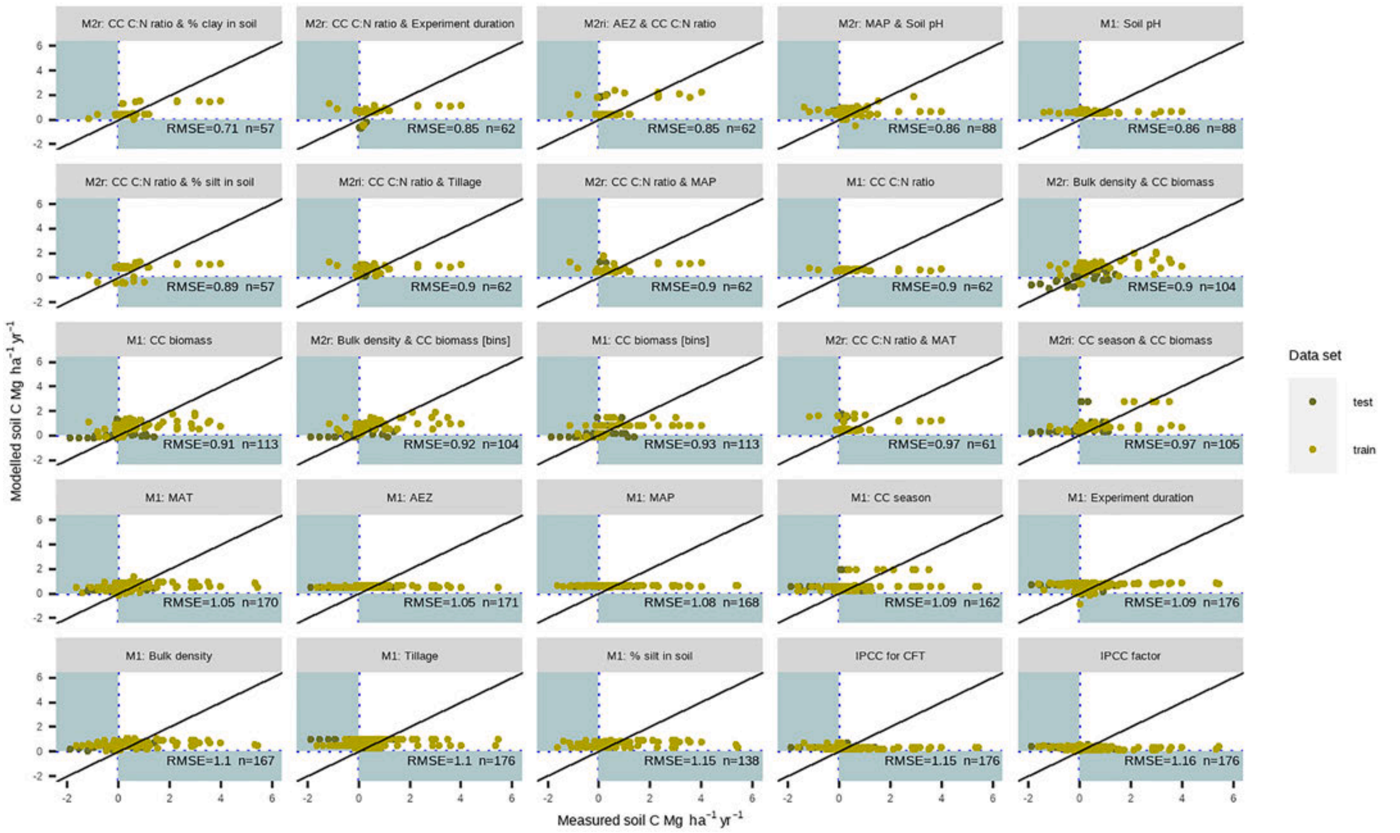

Fig. 4. Annual soil C change: observed and predicted, for models with a lower RMSE value than the IPCC factor, using the extended dataset (training data and test data). The line y x is shown, which represents perfect prediction.

4.2. Soil depth

In initial modelling, a strong sensitivity to soil depth measurement was observed. Whilst the papers in this dataset measured soil C to depths between 2.5 and 100 cm, McClelland et al. (2021) standardised the dataset to 0-30 cm using a method from Jobbagy and Jackson (2000). While vertical soil C density profiles vary (Sun et al., 2020), we perform standardisation with the intention of removing this sensitivity from our data and regression models. To test the standardisation equation, we assessed the difference between applying the standardisation and actual soil C stock using the subset of studies that had taken soil measurements at multiple depth increments. The soil C stock numbers from a.) the Jobbagy and Jackson (2000) standardisation formula applied to the topmost layer of soil and b.) the sum across measured layers were compared, assuming that the latter is the 'true' value.

For studies measuring multiple increments between 0 and 30 cm ($n = 39$, 7 studies), the median discrepancy between standardisation and sum is 3%, though the overall range is between 27% and + 11%. When including the two further studies where summing and standardisation are both required (i.e. there are multiple layers, but not to exactly 30 cm depth), the range of difference is much greater, up to 100%. Though these differences are not marginal, no clear relationship (linear or polynomial) could be easily identified in this dataset, except some evidence of similar discrepancies between measurements from the same study, which is used as a grouping effect. Another function for calculating soil C to a given depth was also tested in this way (Feliciano et al., 2018- based on Smith et al., 2000) and the differences between summed and standardised stocks were similar. This, along with the other gap-filling and standardisation steps set out in the methods, demonstrates the limitations of collating soil C data from an evidence base with no standardised best practice. This is familiar in soil C review studies: Poeplau and Don (2015) found that soil C stocks or bulk density (to calculate soil C stocks) were only given in 30% of studies, and that only 7% of studies included data below typical plough depth.

4.3. Response variable

The choice of response variable, ΔSC_{yr}, is driven by target applications for the model, rather than determining a precise estimate of soil C change over superannual timescales. Many land management decisions are made on a yearly basis and GHG monitoring is often based on this timescale; an annual C stock change suits these uses and allocation of impacts to single crops in the context of crop-based C footprinting. We do note that studies have found that the early impact of any practice change is hard to disaggregate (Smith et al., 2020) and that time is not a good predictor of overall soil C stock change measured in cover crop studies, which are often only a few years in length (McClelland et al., 2021). Additionally, whilst microbial priming effects of organic C inputs can be significant in croplands (Mo et al., 2022) and priming effects of cover cropping can have a negative effect on SOC storage (Camarotto et al., 2020), these are not disaggregated parameters in our model. Finally, soil C sequestration rates are rarely linear and not limitless; equilibrium and, possibly, saturation will be reached (Smith, 2008). The database does not include time series data and has an average measurement duration of 5.2 years, which is shorter than the 20 year time horizon applied by the IPCC. These factors increase uncertainty in the models and the models should therefore be used with this context in mind.

4.4. Baseline model skill

Whilst the IPCC factor approach is globally applicable and has low data requirements, it is parameterised for national scale GHG inventories. In theory, field-scale parameterisations allow for assessment

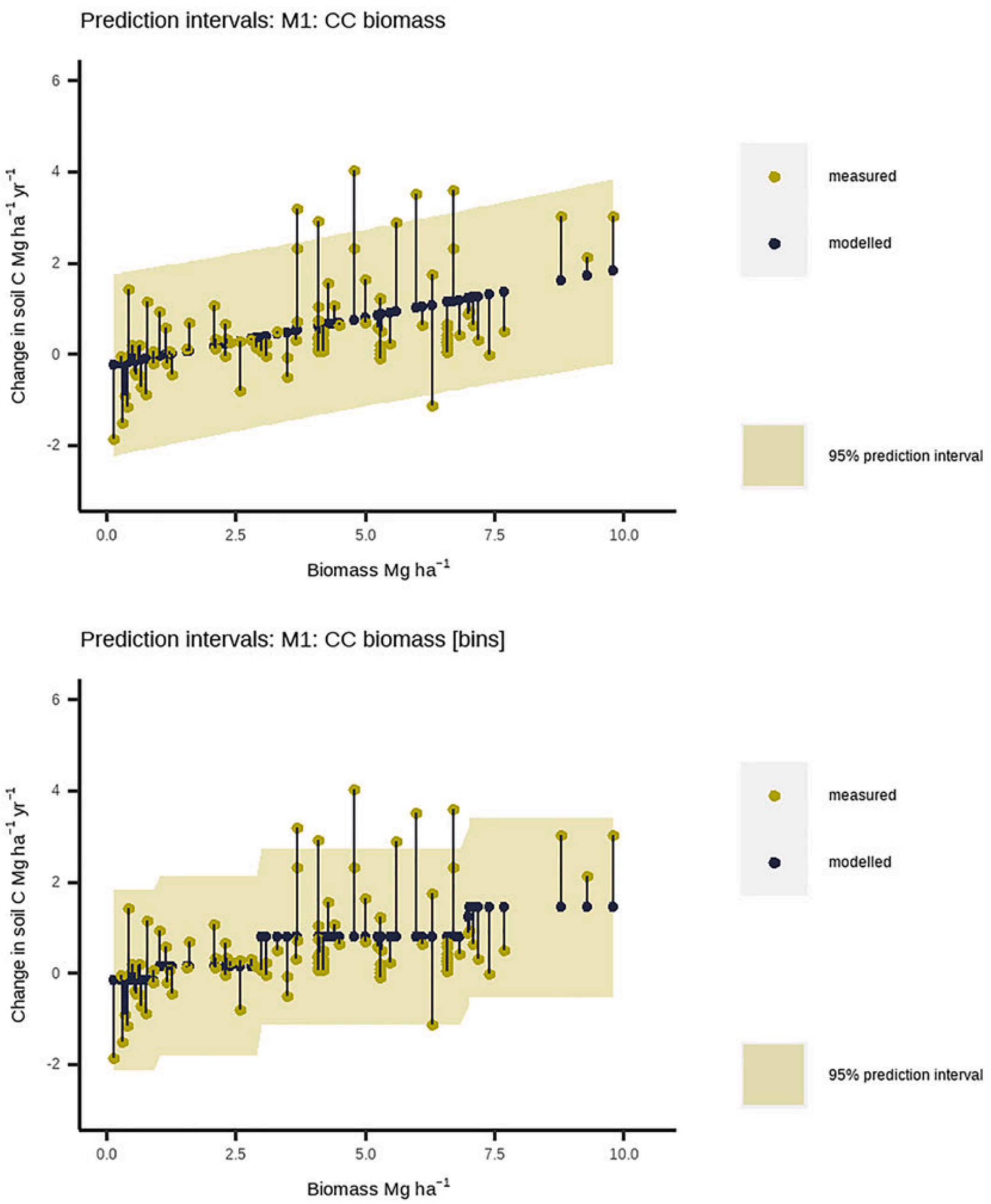

Fig. 5. Prediction intervals for M1 CC biomass regression model (actual and binned input).

that is more precise. The tested response ratios from McClelland et al. (2021) had lower RMSE values than the IPCC method. Structurally, the response ratios are equivalent to the IPCC methodology: the reference (control) soil C value is multiplied by a factor that represents a rate of change. These models are better suited for estimating long-term stock change factors when a baseline and management change is known, whilst the regression approach is better for our criteria.

Several regression models with two variables have much lower RMSE results than the IPCC methods. Considering the data cost of these different models (Table 2), it is also notable that several one variable regression models represent an improvement.

Table 2
Summary of model structures analysed.

Model category	Baseline soil C	Total number of data points required
Regression model	Only where used as an indicator	1–2
McClelland RRs	Yes	2–3
IPCC/Ogle factor	Yes	1
Bin	(Inherited)	1–2 as estimated range, exact measurement not required.

4.5. Direction of change in soil C stocks

The IPCC factor predicts a modest positive change in soil C stock in the first 20 years of cover cropping. Whilst cover crops have a positive impact on soil C stocks on average, this is not universally true. A principal function of models for soil C storage change is indicating direction of change. Fig. 4 shows that insensitivity in our models often results in observed negative ΔSC_{yr} (soil C storage reduction) being modelled as positive (C sequestration). The majority of our statistically selected models do not have the ability to predict a negative change in soil C, despite observations.

The models that successfully predict some negative change within the extended dataset seem to support existing environmental evidence. The M1 CC biomass model requires a minimum of 1.3 Mg ha ^{1} aboveground biomass production to reach a positive ΔSC_{yr} (sequestration) associated with cover cropping. This suggests that if the cover crop is not productive (e.g. poorly established or otherwise unsuccessful) there is insufficient carbon being added to the soil to offset soil C turnover from disturbance associated with its cultivation. It further supports the consensus that plant C inputs are a primary requirement for soil C sequestration (Minasny et al., 2022; Janzen et al., 2022). If aiming to increase soil C, increasing net primary productivity through cover cropping and the subsequent delivery of cover crop biomass to the soil should be prioritised.

The M2r Bulk density & CC biomass equation suggests that greater bulk density and biomass production are both valuable for carbon sequestration. A significant amount of CC biomass production is required to offset C loss in a lighter soil, whilst a reasonable bulk density can ensure some C sequestration.

4.6. Data requirements

In this study, we selected for parsimonious models with potential for broad application. Whilst models that are more complex may yield more predictive power, they also risk over-parameterisation and can exclude certain application where limited data are available. For field scale soil C management, farmers are the primary user group. They bring a wide range of contexts and are (mostly) non-modellers. To have value, decision support tools must have attainable input requirements, comprehensible processes and relevant outputs. The IPCC factor model requires baseline soil C stock, which remains hard to measure. On the other hand, for example, for a given location, climate data is often publicly available. Some decision support tools looking at soil C tackle data limitations using GIS and existing databases to supplement user inputs, for example COMET-Farm (Paustian et al., 2017). COMET-Farm relies on detailed management inputs and specific field locations to parameterise its process-based model, drawing on available soil and climate data. This may result in more accurate outputs, but limits geographical use to areas with supporting data.

In the absence of reliable measurements, growers can often provide a reasonable estimate of conditions on their farm. For example, CC biomass is not always measured, but is observable aboveground and so estimable. To assess the impact of estimating input data, binning approaches were applied to the IPCC factor, M2r Bulk density & CC biomass and M1 CC biomass. We binned CC biomass input data according to approximate quartiles (Table 3), and rounded bulk density values to the nearest of a low, medium, high level (1.3, 1.5, 1.7 g cm ^{3}). In the CC biomass approach, this allows the user to select a range within which their value sits, rather than providing a specific value. The model then approximates the true value to be the mid-point of the range. A qualitative assessment, such as a low, medium, high assessment of bulk density is often simpler for users.

In the three models tested here, binning input data does not have a material impact on overall RMSE, and the regression approaches both retain their ability to model soil C reduction at low CC biomass or bulk density levels. For M1 CC biomass, the resulting concentration of output values reduces model performance most for biomass between 3 and 7 Mg ha ^{1} (Fig. 6). A greater number of bins could tackle this, provided that the ranges are not too narrow for growers' estimates.

Table 3
Binning approach tested for the M1 CC biomass regression model.

Biomass range Mg ha ^{1}	Biomass value used Mg ha ^{1}	ΔSC_{yr} Mg ha ^{1} yr ^{1}
$0 \leq x < 1$	0.5	0.167
$1 \leq x < 3$	2	0.153
$3 \leq x < 7$	5	0.793
$x > 7$	8	1.432

4.7. Final model selection

Model testing highlighted differences in model suitability across several criteria key for decision support. Having shortlisted statistically explanatory models, the main considerations are data requirements from the user and geographical applicability. The lower the resources required for data collection, the wider the reach of the decision support tool can be. IPCC Tier 1 methods are globally applicable and have low data requirements, so any proposed model must represent an improvement to that.

There are multiple models that have an RMSE lower (better) than the IPCC methods, but only two can reliably capture negative soil C change- a specific improvement on the IPCC factor approach. Using the binning approaches outlined, both M1 CC biomass and M2r Bulk density & CC biomass perform well if the input data is estimated, rather than measured. However, as discussed above, bulk density is notoriously heterogenous across time and small spatial scales, and therefore harder for non-experts to estimate at a field scale.

The performance of M1 CC biomass represents the best value for input data. The proposed linear relationship between CC biomass production and soil C stock change is environmentally valid across climates. If re-parameterised for tropical climates, we might expect the regression coefficients to reflect the faster soil C turnover in warmer, wetter conditions (Paustian et al., 1997). The lower soil C benefit of each unit of biomass input may be balanced where overall biomass production is higher. To some extent, the intercept reflects the role of cover crops in preventing soil erosion, so this may become more negative in geographies with high erosion risk (for example dry, steep or windy areas) where the soil C cost of bare soil is greater.

5. Conclusions

Cropland soil C stocks must be preserved or increased for continued productivity, ecosystem health and GHG management, but direct measurement remains impractical for numerous reasons. To establish a simple model suitable for farmers to predict the impact of cover crops on temperate soil C stocks, this analysis parameterised a large number of linear regression models. Omitting soil C saturation and equilibrium dynamics, these models are suitable for use over medium timescales following practice change. The statistically prioritised models tended to combine environmental and cover crop information, which reflects conclusions drawn in the literature. We then tested the statistically selected models against simple meta-analysis response ratios and the IPCC Tier 1 method, considering user contexts. The single variable model using CC biomass data best satisfied our criteria for a fit-for-purpose predictive model.

Though models selected through statistical methods may have significant explanatory power, models for more global use must be considered in the context of user access and value. For modelling soil C impacts of land management, identifying the direction of C stock change and reliably accessible input data are key, as well as meaningful representation of practices on the ground. The M1 CC biomass model predicts negative soil C stock change at low biomass production, as less C is delivered to the soil. In severely data limited scenarios, total CC biomass production can be estimated without the need for averaging across complex heterogeneity at micro scales. We found that using estimated input data did not materially affect model performance, though care should be taken that defined bins retain key model characteristics.

Against a backdrop of measurement challenges and significant

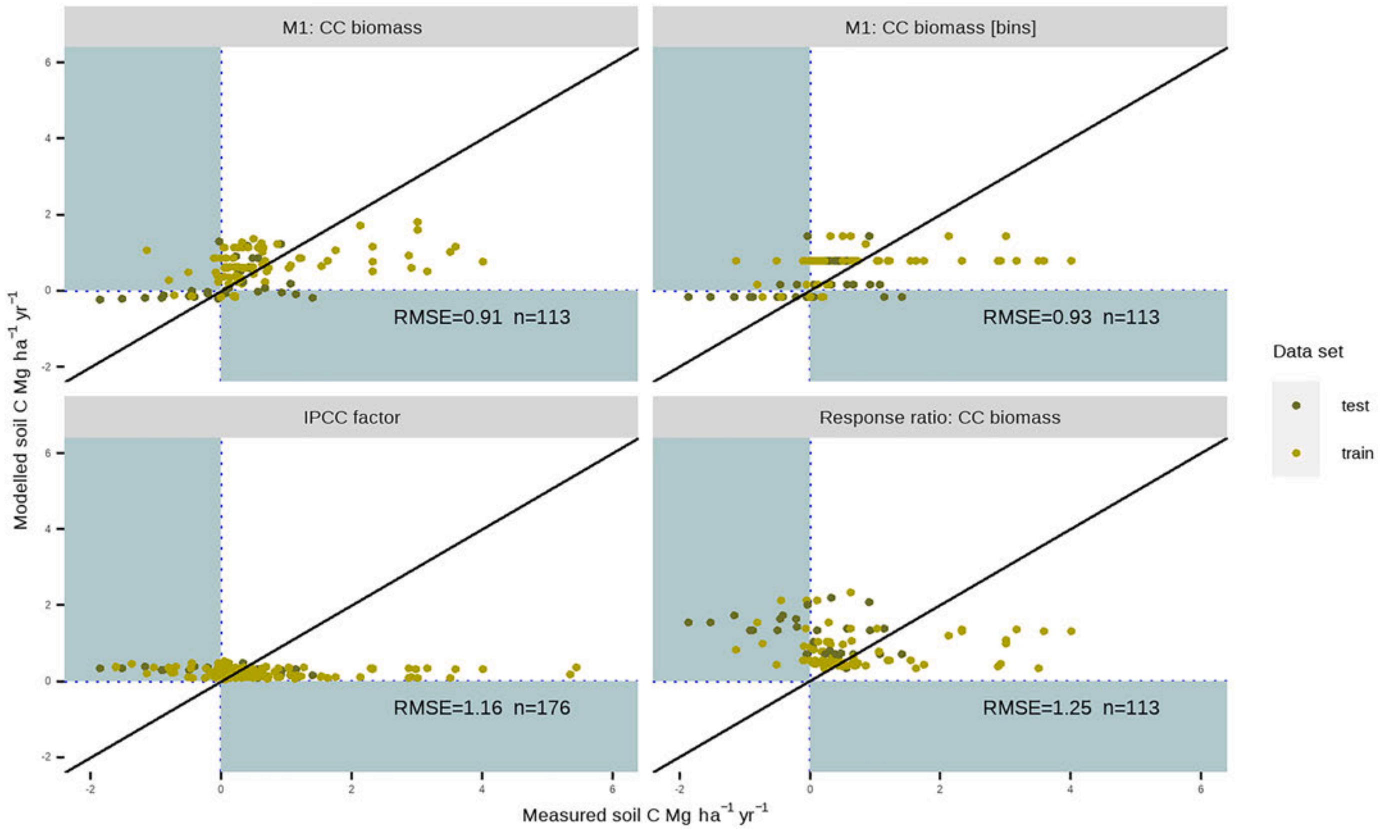

Fig. 6. Annual soil C change: observed and predicted, for CC biomass models, using the extended dataset (training data and test data). The line y x is shown, which represents perfect prediction.

prediction uncertainty, we have parameterised new parsimonious models for soil C change under cover cropping with no loss of effectiveness. Unlike other common methods, prediction based on CC biomass does not require an estimate of baseline soil C, which many making management decisions struggle to provide. This model is suitable for wide application in temperate climates as a representation of known environmental processes, but also due to its minimal input data requirements.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.agsy.2023.103663.

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2.2.1 Methodological clarifications

1. The statistical evaluation criteria were chosen to combine consideration of relative predictive accuracy between models (AIC) with explanatory power of the fixed effects (R^2_m). The criterion $p_{int} < 0.05$ reflects evidence that use of a non-zero intercept in the model is useful.
2. In Section 2.4 of the paper, the calculations for ΔSC_{yr} for cover crops from McClelland et al. (2021) and the IPCC (Ogle et al., 2005) are led by the fact that these sources present proportional soil C impacts which must be combined with a baseline soil C stock value. In these cases, therefore, the mean control (no cover crop) soil C stock is multiplied by the annualised net change factor. In the McClelland et al. calculation, the expected proportional change of cover crops is the overall meta-analysis response ratio minus 1, annualised by dividing by the average length of experiment in the dataset. In the IPCC case, the expected proportional change is the SOC impact of changing from low to medium C inputs minus 1, annualised by dividing by the IPCC default time period of 20 years.
3. Test data were selected to closely match the criteria of the McClelland et al. (2021) search and to fulfill the data needs of models to be tested, but were not selected systematically due to resource constraints. It was important to compile an independent test dataset since in McClelland et al. (2021) the entire dataset was included in calculating the $lnRR$ values subsequently used in this analysis and so could not be split into training and testing subsets.

2.3 Conclusion

The results here show that models with extremely low data requirements can give useful indications of the soil C impacts of cover cropping.

Successful establishment and growth of cover crops underpins all the potential benefits that the practice can have. This is reflected in the final selection of cover crop biomass as the most useful explanatory variable in predicting ΔSC_{yr}. Indeed, biomass production is the main difference between the non-cover crop control and cover crop treatments in the dataset. The model is applicable to a change to cover cropping over short to medium timelines ($<$ 20 years) in temperate climates.

The focus on estimating change in soil C stocks over medium timescales due to a single specific practice change contributes to the effectiveness and validity of these parsimonious models. The regression models are based on comparing two soil C stock values, and are not aiming to construct a time series of soil C evolution. This means that some context of the site (such as temperature, precipitation, soil type) can be somewhat stripped out of the models. Avoiding predicting total soil C stock evolution under the complexity of multi-practice management means that factors known to be important in soil processes can be omitted from the models without fundamental loss of predictive skill.

The 95% confidence intervals for the M1 cover crop biomass model are wide compared to the predicted ΔSC_{yr}. The width of the confidence intervals indicates an uncertain estimate and that there is variation in the data not explained by the variables used. In soil C management, this is particularly important where the interval crosses zero and means that soil C could be lost or gained, though wide uncertainties are common, for example IPCC (2019) has $\pm$50% for many T1 soil C factors. A larger training dataset may have led to narrower confidence intervals.

The loss of soil C with low cover crop biomass production shown in this analysis was also found by Liang et al. (2023), who found a similar threshold of 0.7-1.1 Mg dry matter ha^{-1} and identified a switch from positive to negative soil organic C priming.

The use of estimated input data for some of the more statistically explanatory models did not have significant impacts on their predictive capability. The application of estimated data was carefully matched to the model, for example ensuring representation of the negative ΔSC_{yr} rates associated with low cover crop biomass production. This finding prompts questions about the relative importance of accurate, measured input data specific to the site to be modelled. A focus on accurate input data is common in environmental modelling and is another facet of the data cost burden for users.

Chapter 3

The potential for public databases to increase farmer access to soil C modelling for decision support

3.1 Introduction

Soil organic carbon (SOC) is a pivotal part of ecosystem health and productivity, as well as a consideration for the C balance of agriculture. As part of a dynamic system, it is widely believed that soil C stocks tend to decrease under conventional cultivation and achieve a new equilibrium when carbon inputs to the soil equal outputs due to soil loss and decomposition (Don et al., 2024; Stewart et al., 2007). To protect or increase the soil C stock, management action can aim to reduce soil C loss or to increase soil C input. A common approach to the latter is to provide additional organic C through amendments in the form of plant residues, farmyard manure (FYM), compost or similar (Crystal-Ornelas et al., 2021). A wide variety of different amendments are used in practice and short-term retention of amendment C in soils varies between amendment types (Angers et al., 2022; Dechow et al., 2019), although at longer timescales a fairly similar proportion is stabilised (Smith et al., 1997; Thomsen et al., 2013). As well as stabilising or increasing soil organic C stocks, organic amendments provide nutrients which benefit crop yields in a similar way to mineral fertilisers (Celestina et al., 2019; Oldfield, Bradford, et al., 2022). Since organic amendments are a finite resource, we need to know when and where their application will have the desired effect of building soil organic matter (SOM).

Key drivers for farmers and land managers to seek support for soil management decisions include avoiding the cost and challenges of regular SOC sampling and measurement, and an interest in understanding the potential impact of management before committing resources to a change. For a decision support tool to be accessible to a potential user, its input data requirements must be feasible for them to fulfill. For the tool to be of value, output data must be accurate, easily interpreted and related to available actions with relevant outcomes. In the case of soil C, the challenge of bridging accurate modelling and in-field decisions centres on the spatio-temporal complexity of the processes being parameterised. The evolution of the overall soil C pool over time depends on myriad factors, including management, environment and climate influencing soil physical, biological and chemical properties and their interactions (McClelland et al., 2021). Decisions at the field scale are accounting for soil processes operating from microscopic to landscape scales (Wiesmeier et al., 2019) and, to achieve accurate outputs, models must emulate the same. To enhance the real-world impact of SOC modelling on ecosystem functioning, the accuracy of model outputs must be maximised whilst the user cost of the input data is minimised (Dechow et al., 2019).

Model input data requirements vary; as a rule, the more granular the modelled scope, the more data are required to run the model, with process-based models typically requiring more data than empirical models (Sykes et al., 2019). Process-based models often use several conceptual pools of SOC to parameterise decomposition dynamics (Jenkinson et al., 1990; Parton et al., 1994). Typical data requirements include a baseline SOC measurement, quantified C inputs, management information, climate and soil measurements for the site. Simpler empirical methods have been designed to estimate national and regional SOC stocks and changes (Ogle, Kurz, et al., 2019; Smith et al., 1997); accepting that the approach works for a statistically 'average' field. In these cases, a subset of similar information may be used, and broad categories (e.g. climate zone, soil type) can be applied to reduce the need for site measurement.

Among the options that exist to enable accurate modelling of soil carbon stock in relation to management, two approaches have been widely attempted to date:

1. **Maximise value of model results by targeting models to user requirements**
   User purposes for a soil decision support tool can vary across benchmarking, reporting, monitoring, and comparison (Arulnathan et al., 2020). Each SOC model is designed with a particular purpose in mind, and has limitations and assumptions that should be considered by the user (Le Noë et al., 2023; Paustian et al., 2019). A farmer may need to quantify SOC stocks for the purpose of carbon credits, to compare the (real or potential) impact of multiple management options or to estimate the rate of change of SOC storage to understand the impacts of management on soil health. The goal in this case might be to achieve quantitative predictions of SOC change which are; (i) conservative in nature, (ii) accurate, (iii) directionally correct.
2. **Minimise cost to run models by utilising secondary datasets**
   Some adaptations to minimise input data cost are already in use: the Cool Farm Tool (Hillier et al., 2011) allows the user to select a quantitative range or qualitative category for inputs that would be harder to measure, then translates this into the necessary model input. Hughes et al. (2023) showed that well-parameterised binning of input data can still lead to reasonable model outputs. Whilst providing extensive measured data remains a challenge, recent data science

developments provide opportunities for instant public access to global spatial datasets containing, for example, climate and soil information for latitude-longitude pairs. Whilst spatial resolution of these datasets is coarser than field scale, they are typically built from observed data and can be updated regularly. It may be that these are acceptable substitutes for primary measured data.

This chapter investigates the impact of secondary data inputs on two SOC models often used at farm scale, the Intergovernmental Panel on Climate Change (IPCC) Tier 1 (T1) methodology and RothC, when applied to a dataset of field studies where organic amendments have been applied and SOC measurements recorded. It assesses where model data requirements can be streamlined with minimal loss of model performance and relates this to farmer decision support needs.

3.2 Methods

3.2.1 Outline of models applied

IPCC Tier 1

The IPCC T1 soil C method for mineral soils is an empirical approach used as part of the Guidelines for National GHG Inventories (IPCC, 2019). It is based on multiplicative factors derived from extensive meta-analyses (Ogle et al., 2005; Ogle, Kurz, et al., 2019). Whilst IPCC T1 was designed for national inventories, the method has often been utilised for field-level estimates (e.g. Hillier et al., 2011; Peter et al., 2016). It is a useful benchmark here because it has very low data requirements, supported by its broad classifications for environment and management.

The IPCC T1 calculations predict new equilibrium SOC stocks to 30 cm depth from reference SOC stocks based on SOC stocks under native vegetation (SOC_{ref}), and factors based on land use, management and inputs. SOC_{ref} depends on the site's climate and soil type. If initial SOC has been measured, the T1 method can be adapted to predict SOC stock change using this as a baseline (i.e. instead of reference SOC), taking care to choose the correct factors, see Equation 3.1 (adapted from Equation 2.25 in Ogle, Kurz, et al. 2019). The IPCC approach assumes that equilibrium is reached after 20 years. For experiments undertaken for less than 20 years the intermediate SOC stock can be calculated using Equation 3.2.

In Equation 3.1 and 3.2, SOC is the soil organic carbon stock to 30 cm depth (Mg C ha^{-1}), t and T are the time point and experiment duration in years, c is the IPCC climate zone and s is the IPCC soil type for the site, F_{LU}, F_{MG} and F_I are SOC change factors for land use, tillage and inputs respectively (applied factors from Ogle, Kurz, et al. 2019 are shown in Table A.3.1).

$$SOC_{t\geq 20_{c,s}} = SOC_{t=0_{c,s}} \cdot \left(F_{LU_{c,s}} \cdot F_{MG_{c,s}} \cdot F_{I_{c,s}}\right) \tag{3.1}$$

$$SOC_{t=T_{c,s}} = SOC_{t=0_{c,s}} + \left(SOC_{t\geq 20_{c,s}} - SOC_{t=0_{c,s}}\right) \cdot \frac{T}{20} \quad for\, T < 20 \tag{3.2}$$

RothC

The RothC model is a process-based model for SOM decomposition with five conceptual SOM pools which differ in their decomposition rates and patterns (Figure 3.1). It was used here since it has been widely applied in scientific research, but also for decision support and SOC verification (e.g. Black et al., 2022; Woollen et al., 2017). RothC data requirements are considerably higher than IPCC T1, though lower than some other process-based models (e.g CENTURY, Parton et al. 1988).

Decomposition rates are based on the clay % of the soil, site temperature, precipitation, potential evapotranspiration (PET) and soil cover. The user must also provide values for organic C inputs (FYM and plant residues). Organic C inputs are split into the pools depending on how resistant or decomposable the material is. Plant residues are split into DPM and RPM pools (see Figure 3.1), using a ratio of 1.44 in crops and improved grassland (Coleman & Jenkinson, 1987). FYM is split DPM 49%, RPM 49% and HUM 2% (Coleman & Jenkinson, 1987). The RothC model, as originally set out, does not explicitly include physical disturbance (e.g. tillage) as a consideration.

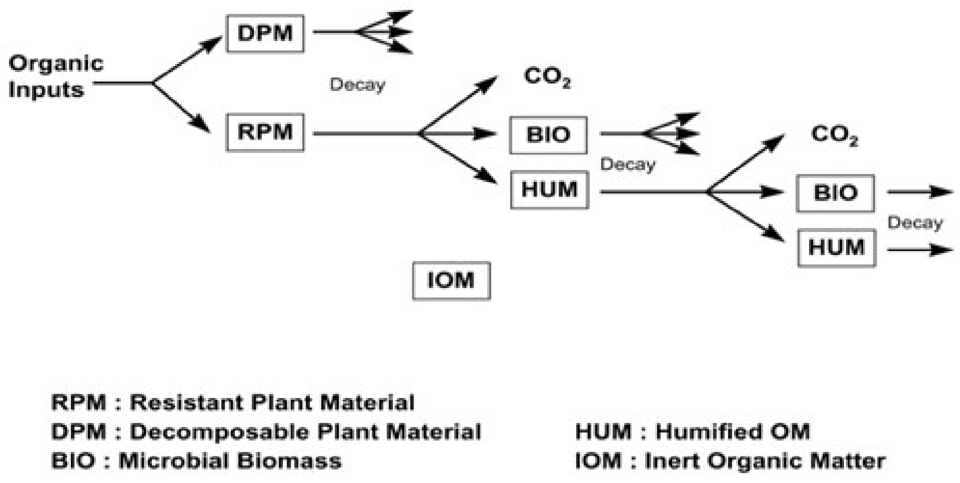

Figure 3.1: Structure of the RothC Model from Coleman and Jenkinson (1987)

3.2.2 Primary field data

This analysis used the dataset from Foster et al. (2020), collated through a systematic review of agricultural experiments quantifying the soil C impacts of organic amendments. In brief, the dataset includes peer-reviewed studies of field experiments including organic amendments with a control and replicates (Foster et al., 2020). In the dataset, experiment managements are labelled as organic amendment (OA), chemical fertiliser only (CF) or zero input (Cmin). These have been relabelled as OA, MF (mineral fertiliser only) and ZI (zero inputs). Any management including an organic amendment is labelled OA; it may also include mineral fertiliser (Table 3.1).

For the aim of this chapter, I required SOC stock measurements. Therefore, I ignored other variables in the dataset, including SOC concentration data without associated bulk density data. This left 68 experiments from 25 studies.

Standardisation and preparation of primary data

To comply with the IPCC framework, I standardised the soil C stocks to 30 cm using the methods set out by Jobbágy and Jackson (2000) as described by Abdalla et al. (2019), see Equation 3.3.

$$SOC_{30} = \left(\frac{1-\beta^{30}}{1-\beta^{d_0}}\right) \cdot SOC_{d_0} \tag{3.3}$$

Where 30 and d_0 relate to soil depths (cm). SOC_{30} is the soil C stock to 30 cm depth (Mg ha^{-1}), SOC_{d_0} is the soil C stock to depth d_0 reported in the study (Mg ha^{-1}), β has a value of 0.9786 and is the relative rate of decrease in soil C with depth (Abdalla et al., 2019).

Where multiple layers of soil C were measured, these were summed to the interval closest to 30 cm before standardisation. The same intervals were used for initial SOC and final SOC stocks. Where two intervals were equidistant from 30 cm (e.g. 20 cm and 40 cm), the deeper increment was included so that the standardisation was based on as much information as possible. Whilst the Foster et al. (2020) dataset included available land use, mean annual precipitation (MAP) and mean annual temperature (MAT) data, it did not include potential evapotranspiration (PET) data, which was required for RothC modelling and IPCC climate zone classification. PET data were extracted from CRU TS 4.06 for 1980-2010 (Climatic Research Unit et al., 2022).

Additional management data not included in Foster et al. (2020) are required to run RothC: whether the soil is bare or covered and the clay % of the soil. I extracted these from the subset of studies in the dataset that reported them (Figure 3.2).

Of the organic amendments listed in Table 3.1, FYM and poultry litter were categorised as a manure-type C input to RothC. Straw, residues, mulch, biosolids and sulphitation pressmud were categorised as plant residue C inputs.

3.2.3 Secondary data sources for model inputs

I ran the IPCC T1 and RothC models with different combinations of primary (measured) and secondary input data. Most secondary data used are publicly available and spatially or environmentally determined. Spatially determined data are lower resolution than measured data, and the primary and secondary values might be a close match or very different: this study is not a sensitivity analysis.

Initial SOC

IPCC SOC_{ref} values based on climate and soil type were used as secondary initial SOC in both IPCC and RothC model runs.

Clay

Clay % of soil was extracted from the Harmonised World Soil Database (HWSD) (Wieder et al., 2014) using the hwsdr package (Hufkens, 2021).

Mean Annual Temperature

RothC requires monthly average temperatures. Most often, studies publish MAT. Monthly average temperatures were extracted from CRU TS 4.06 for 1980-2010 (Climatic Research Unit et al., 2022) and used as secondary data. To generate monthly average temperatures from primary MAT values, the difference between the CRU MAT and the measured MAT was added to the CRU monthly average temperatures. Thus, the distribution of monthly average temperatures is identical, but adjusted to the primary MAT value.

Input Organic C

Measured values for organic C inputs from both organic amendments were varied by $\pm$ 25% to simulate over- or under-estimation by the user.

Table 3.1 summarises the eight studies (20 experiments) with sufficient primary and/or secondary data to run RothC in SoilR.

3.2.4 Model runs in R

IPCC Tier 1

IPCC climate zones were determined using Figure 3A.5.2 from IPCC (2019) and the data extracted from CRU TS 4.06 (Climatic Research Unit et al., 2022). The lack of reported PET data precluded the use of primary climate data to determine IPCC climate classes; mixed data sources would have led to erroneous conclusions, particularly in the MAP:PET ratio utilised in the classification approach. The IPCC soil type for each site was extracted from the HWSD (Wieder et al., 2014) using the hwsdr R package (Hufkens, 2021).

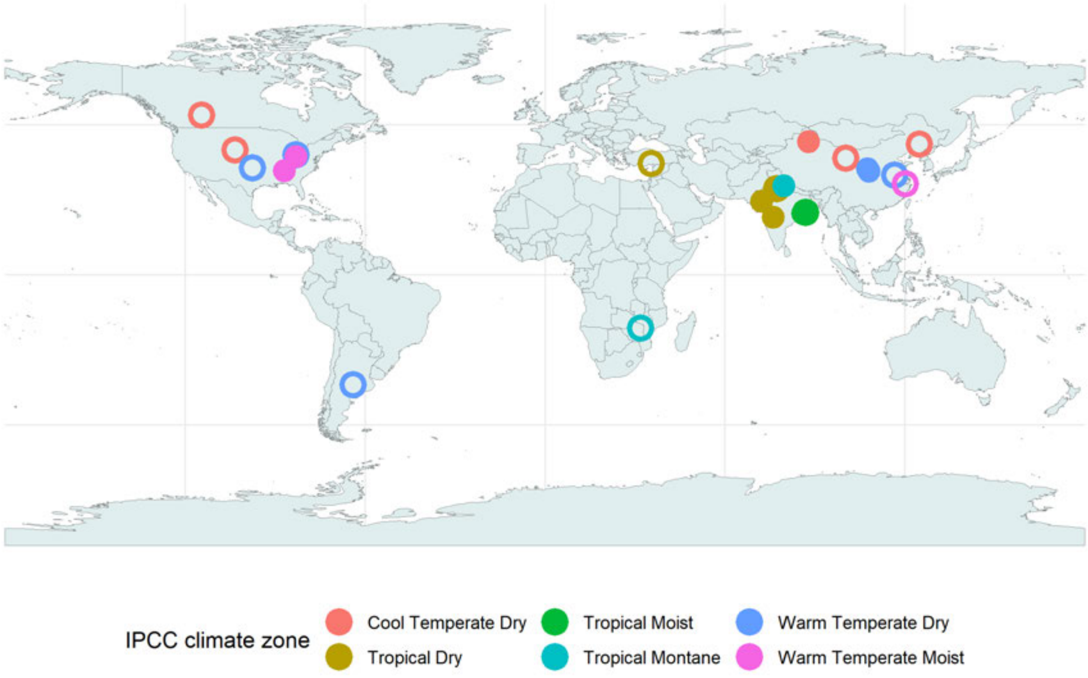

Figure 3.2: Location of sites with SOC stock data and input data for RothC and IPCC T1 models. Colours reflect the IPCC climate zone of the site. Filled circles are sites with sufficient data to run RothC, open circles are sites with SOC stock data but insufficient data to run RothC.

IPCC Input factor levels were matched as follows; OA: high with manure, MF: medium input, ZI: low input (see Table A.3.1). These factors have a significant impact on the predicted change in SOC. Default factors for 'low input' indicate a reduction in SOC, 'medium input' has no SOC change and 'high input' indicates SOC increase. Irrigation and other practices had no impact on the choice of input factor.

RothC

The RothC model was applied using the SoilR R package (Sierra et al., 2012). A critical limitation of the SoilR package is that soil cover (1 or 0) is stated for the entire run of the model, rather than by month of the year. I ran the SoilR RothC function with soil bare when soil was not cropped for more than half of the year (S601- bare all year, S686- bare seven months, S781- bare eight months) and covered otherwise: in this dataset, sites modelled with covered soil had at least eight months of plant cover. Residues left in the field after harvest did not affect the bare/covered assessment of soil.

To spin-up the RothC model to equilibrium at the start of the experiment, plant residue inputs (PRI) were optimised to reach the desired initial SOC (either SOC_{init} or SOC_{ref}). This involved iterating over possible PRI values between zero and 20 Mg ha^{-1} yr $^{-1}$ and identifying the PRI quantity that results in the closest RothC prediction of initial SOC; similar to the method used by Jordon et al. (2022). Klumpp et al. (2017) found this method of RothC initialisation performed best in terms of matching observed SOC stocks. Forward runs assumed that the only change in C input came from the organic amendments applied. PRI was set at spin-up levels and was not varied: the implications of this are explored in the Discussion section of this chapter.

Table 3.1: Site and management information for experiments modelled. SOC stocks to 30 cm depth. Sources: 363: Sainju et al. (2008); 445: Bhattacharyya et al. (2010); 601: Lenka and Lal (2013); 624: Liu et al. (2013); 651: Li et al. (2013); 655: Sun et al. (2013); 686: Srinivasarao et al. (2014); 781: Yucel et al. (2015); 890: Das et al. (2017); 926: Shahid et al. (2017); 1036: Datta et al. (2018). AN = ammonium nitrate, DAP = diammonium phosphate, ND = no data, SPM = sulphitation pressmud.

#	Site location	Duration (years)	IPCC climate zone	MAP (mm)	MAT (°C)	*CRU MAT (°C)*	Measured clay (%)	*HWSD clay (%)*	IPCC soil class	SOC_{init} (Mg ha^{-1})	*SOC_{ref} (Mg ha^{-1})*	Crops	Treatment name	OA	MF	ZI	OA - MF comparison	Reps	IPCC till code	Irrigated	OA C (Mg ha^{-1} yr^{-1})
363	Alabama, USA	10	Warm Temperate, Moist	1177	16	16	27	25	LAC	52.5	55 ± 8%	cotton, rye, maize	S363_5-CT_100	Poultry litter	AN	-	Constant N	3	Full till	Yes	1.7
													S363_7_MT_100	Poultry litter	AN	-	Constant N	3	Low till	Yes	1.7
													S363_9_NT_100	Poultry litter	AN	-	Constant N	3	No till	Yes	1.7
445	Uttarakhand, India	30	Tropical Montane	1043	18	22.9	6	47	HAC	22.5	51 ± 10%	soy, wheat	S445_NPK+FYM	FYM + NPK	NPK	Yes	Additional	6	Full till	No	1.6
601	Ohio, USA	15	Warm Temperate, Dry	1016	11	10.8	ND	21	HAC	ND	24 ± 5%	wheat	S601_mulch_16	Mulch	-	Yes	-	3	No till	ND	6.8
													S601_mulch_8	Mulch	-	Yes	-	3	No till	ND	3.4
624	Gansu, China	29	Warm Temperate, Dry	540	9.8	10.1	ND	19	HAC	ND	24 ± 5%	maize, soy, wheat	S624_FYM	FYM	-	Yes	-	3	Full till	ND	0.4
													S624_NP+FYM	FYM + NP	NP	Yes	Additional	3	Full till	ND	0.4
													S624_NP+S	Straw + NP	NP	Yes	Additional	3	Full till	ND	2.5
651	Xinjiang, China	20	Cool Temperate, Dry	164	6.9	9.7	ND	23	HAC	ND	43 ± 8%	wheat	S651_N2P2R	Straw + NP	NPK	Yes	Additional NP, constant K	4	Full till	Yes	2.1
													S651_NPKR	Straw + NPK	NPK	Yes	Additional	3	Full till	Yes	1.0
655	Guanzhong Plain, China	6	Warm Temperate, Dry	600	12.9	12.5	27	ND	HAC	26.0	24 ± 5%	maize, wheat	S655_CT+SR	Straw + urea + DAP	Urea + DAP	-	Additional	3	Full till	Yes	4.9
													S655_NT+SR	Straw + urea + DAP	Urea + DAP	-	Additional	3	No till	Yes	4.8
													S655_RT+SR	Straw + urea + DAP	Urea + DAP	-	Additional	3	Low till	Yes	4.9
													S655_SST+SR	Straw + urea + DAP	Urea + DAP	-	Additional	3	Low till	Yes	5.1
686	Gujarat, India	18	Tropical, Dry	550	ND	27.3	11	ND	HAC	ND	21 ± 5%	millet, bean, castor	S686_50 % F + 50 % FYM	FYM + urea	Urea	Yes	Constant N	4	Full till	No	1.5
													S686_50 % FYM	FYM	Urea	Yes	Constant N	4	Full till	No	1.5
													S686_Farmers	FYM	-	Yes	-	4	Full till	No	0.5
781	Ohio, USA	13	Warm Temperate, Moist	950	13.6	11.3	23	21	HAC	ND	64 ± 5%	maize, soy	S781_25	Biosolid + PK	PK	-	Additional	4	No till	ND	0.9
890	Meerut, India	18	Tropical, Dry	823	ND	25	10	21	HAC	ND	21 ± 5%	rice, wheat	S890_NPK+CR	Straw + NPK	NPKZn	Yes	Constant N	3	Full till	Yes	4.2
													S890_NPK+FYM	FYM + NPK	NPKZn	Yes	Constant N	3	Full till	Yes	1.3
													S890_NPK+GR	Residue + NPK	NPKZn	Yes	Constant N	3	Full till	Yes	0.7
													S890_NPK+GR+FYM	Residue + FYM + NPK	NPKZn	Yes	Constant N	3	Full till	Yes	2
													S890_NPK+SPM	SPM + NPK	NPKZn	Yes	Constant N	3	Full till	Yes	1.1
926	Cuttack, India	41	Tropical, Moist	1500	27.6	27.5	31	10	LAC	23.9	38 ± 5%	rice	S926_FYM	FYM	-	Yes	-	3	Full till	Yes	0.9
													S926_N+FYM	FYM + N	N	-	Additional	3	Full till	Yes	0.9
													S926_NPK+FYM	FYM + NPK	NPK	-	Additional	3	Full till	Yes	0.9
1036	Maharastra, India	28	Tropical, Dry	847	ND	26.3	30	55	HAC	ND	21 ± 5%	sorghum, wheat	S1036_NPK+FYM	FYM + NPK	NPK	Yes	Constant N	3	Full till	Yes	4.3

3.2.5 Models generated and naming

The maximum number of model scenarios per experiment was 26 (two IPCC models with two initial SOC options and 24 RothC models comprising each permutation of two initial SOC options, two clay options, two MAT options and three amendment C options). RothC model runs used between zero and four substitute data values (initial SOC stock, clay, MAT, amendment C), whilst IPCC T1 estimates varied only the initial SOC stock.

Due to missing data in both the experiment measurements and the public datasets used to estimate data, not all model permutations could be run for all experiments (Table 3.1). Critically, some studies did not publish SOC$_{init}$ values or any other time series data. Not only does this mean that models cannot be run using known starting SOC stocks, it also means that measured ΔSC_{yr} cannot be calculated and compared with model results.

Experiment names

To aid traceability, studies (i.e. sites) are referred to using the reference number assigned by Foster et al. (2020), e.g. S363. Experiments are similarly referred to by their names from Foster et al. (2020); see Table 3.1. To keep comparison between treatments clear, experiment names are related to the OA treatment and are not altered when referring to the related MF or ZI treatments: references to particular treatment classes are made clear in the text and figures. Where multiple OA treatments at a site are matched with the same MF and ZI controls these duplicate model results are only counted once in summary statistics.

Model codes

Given the large number of models analysed, the models are referred to by the concatenated names of the input data used. Table 3.2 lists the names used for this purpose. For example, values from $RothC\_refC\_HWSD\_MAT\_0.75$ refer to the RothC model run with secondary initial soil C and clay data, primary MAT data and the organic amendment C input adjusted to 75 % of the measured total.

Table 3.2: Model naming conventions

Input data	units	Primary data name	Secondary data name
Initial soil C at start of experiment	Mg C ha^{-1}	initC	refC
Soil clay %	%	mclay	HWSD
MAT	℃	MAT	CRU MAT
Organic C input factor	-	1	0.75 *or* 1.25

3.3 Results

3.3.1 Differences between measured and estimated input values

Across the whole Foster et al. (2020) dataset (i.e. before restricting to studies with SOC stocks and model data), the mean difference between measured and HWSD clay data was 1 % (n.s.) and the mean difference between measured and CRU MAT data was -0.83 ℃ (95% CI: -1.50, -0.16 ℃, significantly different from zero with $p < 0.05$).

Within the modelled subset, the secondary data differed to varying degrees from the measured data (Figure 3.3). For example, CRU MAT for S445 was almost 5 ℃ higher than the measured MAT, while HWSD clay was 41% higher than measured clay (Panels B and A, respectively, Figure 3.3). The primary and secondary MAT values were within 0.5 ℃ of each other for study sites except S445, S651 and S781.

For two studies reporting SOC$_{init}$ data, the absolute difference between SOC$_{init}$ and SOC$_{ref}$ was under 2.6 Mg C ha^{-1} (Table 3.1; Panel C, Figure 3.3). For S926, SOC$_{ref}$ was 14 Mg C ha^{-1} larger than SOC$_{init}$ and for S445 SOC$_{ref}$ was 28 Mg C ha^{-1} higher: more than double the measured SOC$_{init}$.

The variation in OA amendment C was proportional to the measured amount of amendment C applied (Figure 3.3, Panel D).

3.3.2 Rates of soil C change

Figure 3.4 shows RothC model trajectories were generally similar across different OA treatments within a site, though measured changes varied. Regardless of the input data used, RothC tended to underestimate the rate of change in SOC stocks (ΔSC_{yr}) in experiments with < 2 Mg C ha^{-1} yr^{-1} organic amendment applied ($p < 0.001$). The largest underestimations of ΔSC_{yr} in OA treatments by RothC were seen in longer experiments with lower amendment C input that also included inorganic fertilisers (e.g.

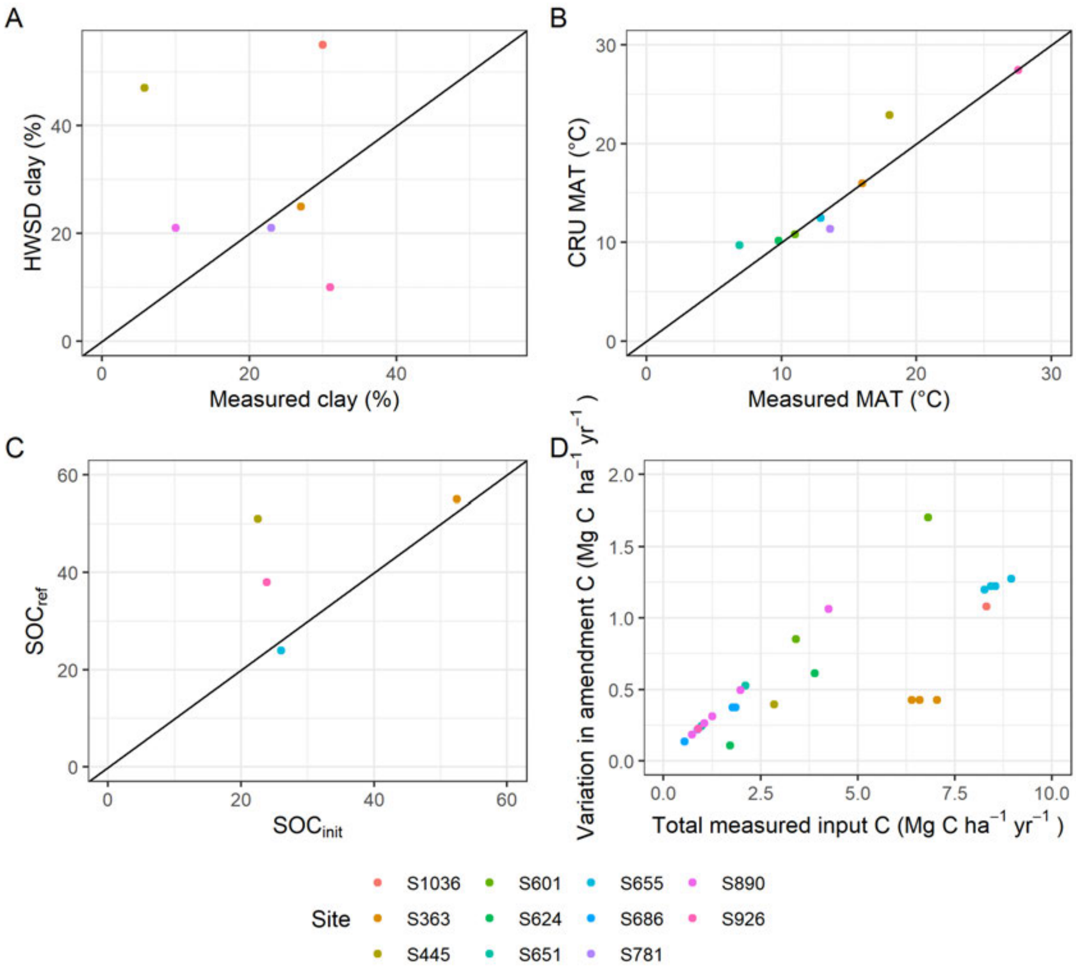

Figure 3.3: A, **B** & **C**: primary and secondary model input values for clay, MAT and initial SOC, respectively. **D**: total measured C input and variation in modelled amendment C. Colours denote sites.

S445_NPK+FYM, S926_N+FYM, S926_NPK+FYM). Particularly given the RothC spin-up assumptions used here, the amount of amendment C is a key determinant of RothC's modelled ΔSC_{yr} at a given site. In some cases, overestimating C input by 25 % still resulted in RothC underestimating ΔSC_{yr} (Figure 3.5).

In experiments reporting SOC$_{init}$, both OA and MF managements had a discernible impact on SOC stocks, despite a range of land use histories and environmental contexts (Figures 3.6). In MF scenarios, RothC and/or IPCC predicted little or no change in SOC stock over time. For RothC, because the model started at equilibrium SOC and the associated equilibrium PRI is included in the forward run, predicted ΔSC_{yr} will be small in the absence of a change in C input. Figure 3.6 shows that whilst measured ΔSC_{yr} is typically greatest when management includes addition of organic C, chemical fertilisers can prompt significant ΔSC_{yr} in some situations.

With all other parameters held equal, RothC projects (to practical precision levels) the same ΔSC_{yr} regardless of whether SOC$_{init}$ or SOC$_{ref}$ was used at the start of the model (Figure 3.4). IPCC T1 factors are multiplicative, and the implied rates of change in stock are therefore determined by the initial SOC value.

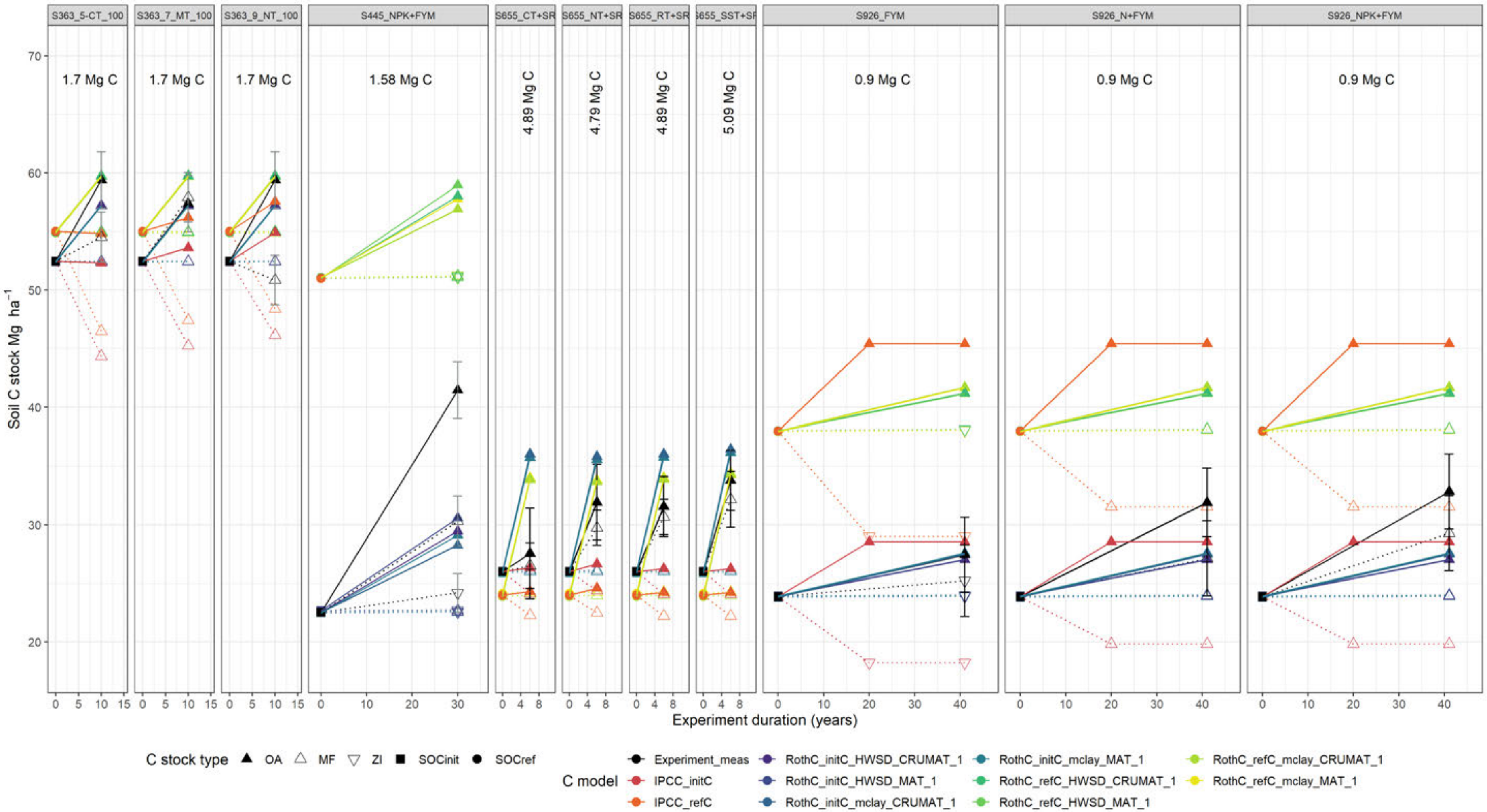

Figure 3.4: Measured and modelled SOC stocks from experiments that reported SOC_{init}, showing model results with various combinations of input data but where the amendment C quantity equalled measured values. Annual measured amount of organic amendment C added is shown. Colours refer to measurement (black) or different models. Point shapes indicate the soil C type (SOC_{init}, SOC_{ref}, OA, MF, ZI). Standard deviation (SD) ranges are shown for measured soil C values: black bars were reported in the study, grey bars are the dataset weighted mean (see Wiebe et al. 2006)

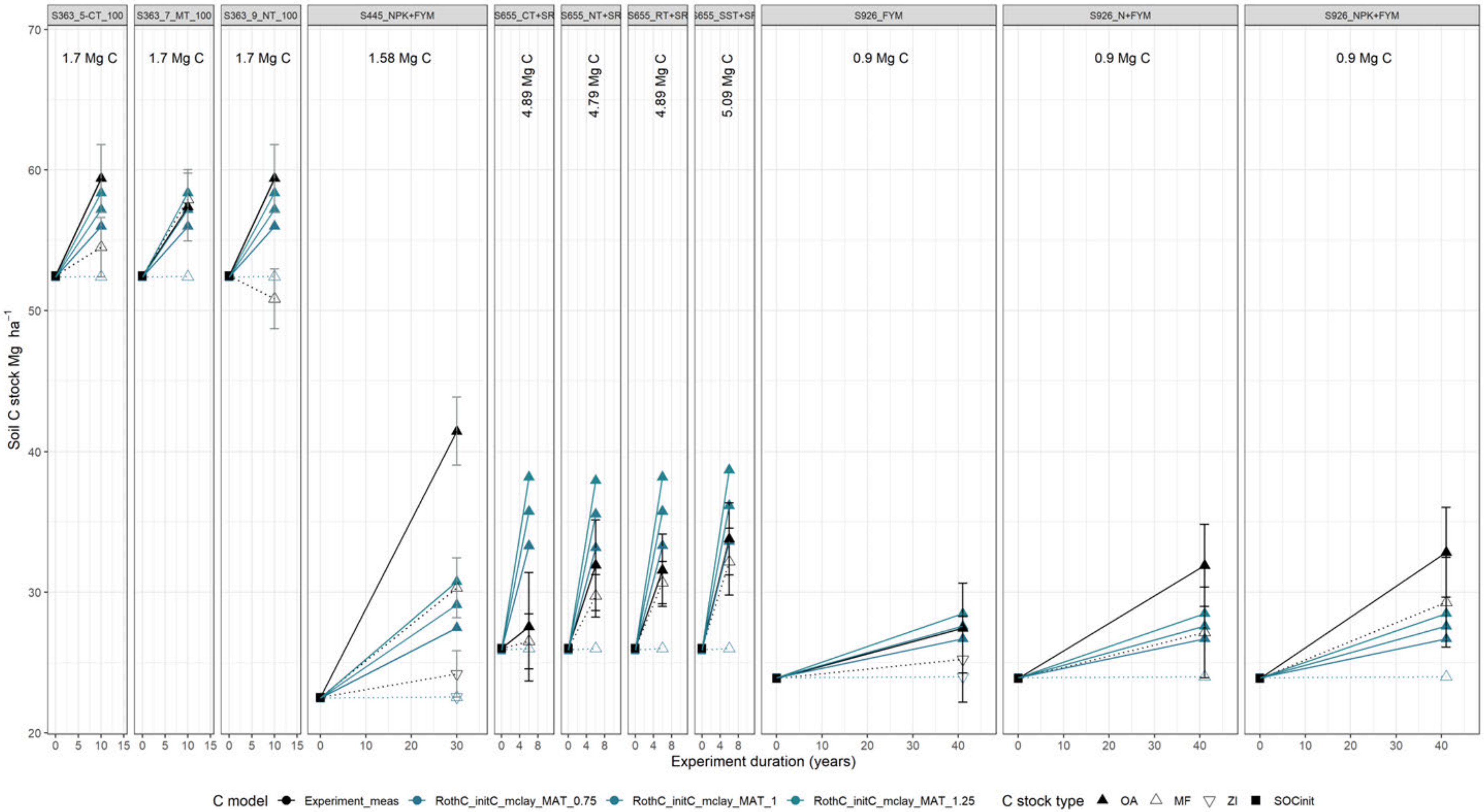

Figure 3.5: Measured and modelled SOC stocks from experiments that reported SOC$_{init}$, showing RothC model results where the only estimate was the amendment C quantity. Annual measured amount of organic amendment C added is shown. Colours refer to measurement (black) or different models. Point shapes indicate the soil C type (SOC$_{init}$, SOC$_{ref}$, OA, MF, ZI). Standard deviation (SD) ranges are shown for measured soil C values: black bars were reported in the study, grey bars are the dataset weighted mean (see Wiebe et al. 2006)

For many treatments, no model predicted ΔSC_{yr} to reasonable accuracy (Figures 3.4, 3.5). Figure 3.6 shows the measured ΔSC_{yr} compared to the closest modelled prediction. Across all managements and experiments with SOC$_{init}$ data (n = 23), eight different models predicted at least one of the measured ΔSC_{yr} rates best. There are patterns in which model performs best for a particular site, though rarely total consistency. In OA treatments, 8/11 ΔSC_{yr} rates were best calculated using RothC (Figure 3.6). In all eight of these treatments, there was no prediction skill lost (and possibly some improvement) by utilising SOC$_{ref}$ and at least one other secondary data point. In addition, seven of these eight cases were best modelled with a $\pm$25 % variation in organic amendment C input.

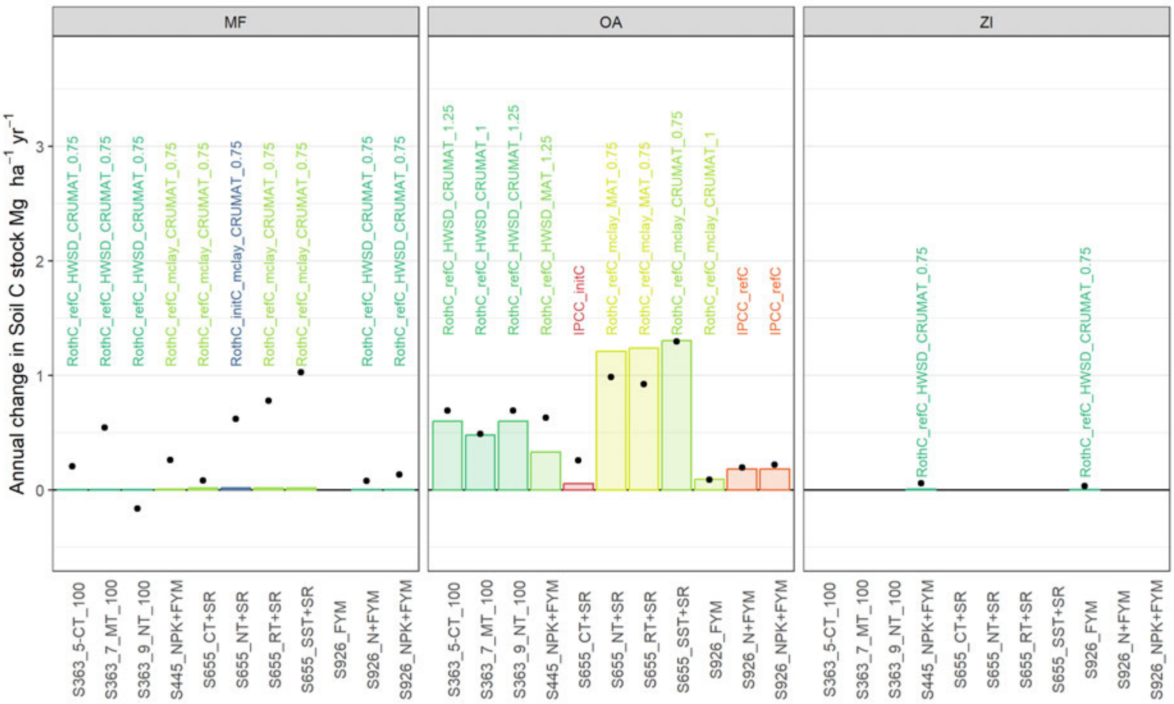

Figure 3.6: Measured rates of SOC stock change (black points) compared with the closest modelled rate of SOC stock change (coloured bars). Where multiple models had the same rate of change, the model with the lowest data cost (i.e. with the most estimated input values) was chosen. For non-OA treatments, there is no impact of the input C factor on model inputs or outputs.

3.3.3 Soil C stocks

For a given initial SOC value, predicted SOC stocks at the end of the experiment (SOC$_p$) for each MF or ZI treatment were similar to each other across models (maximum difference between models 0.40 Mg C ha^{-1}, Figures 3.8; 3.9; A.3.1), though they were not always similar to measured SOC at the end of the experiment (SOC$_t$). The spread of SOC$_p$ is larger for OA treatments (Figure 3.7), showing that input C values drive difference between predictions more than than MAT or clay data.

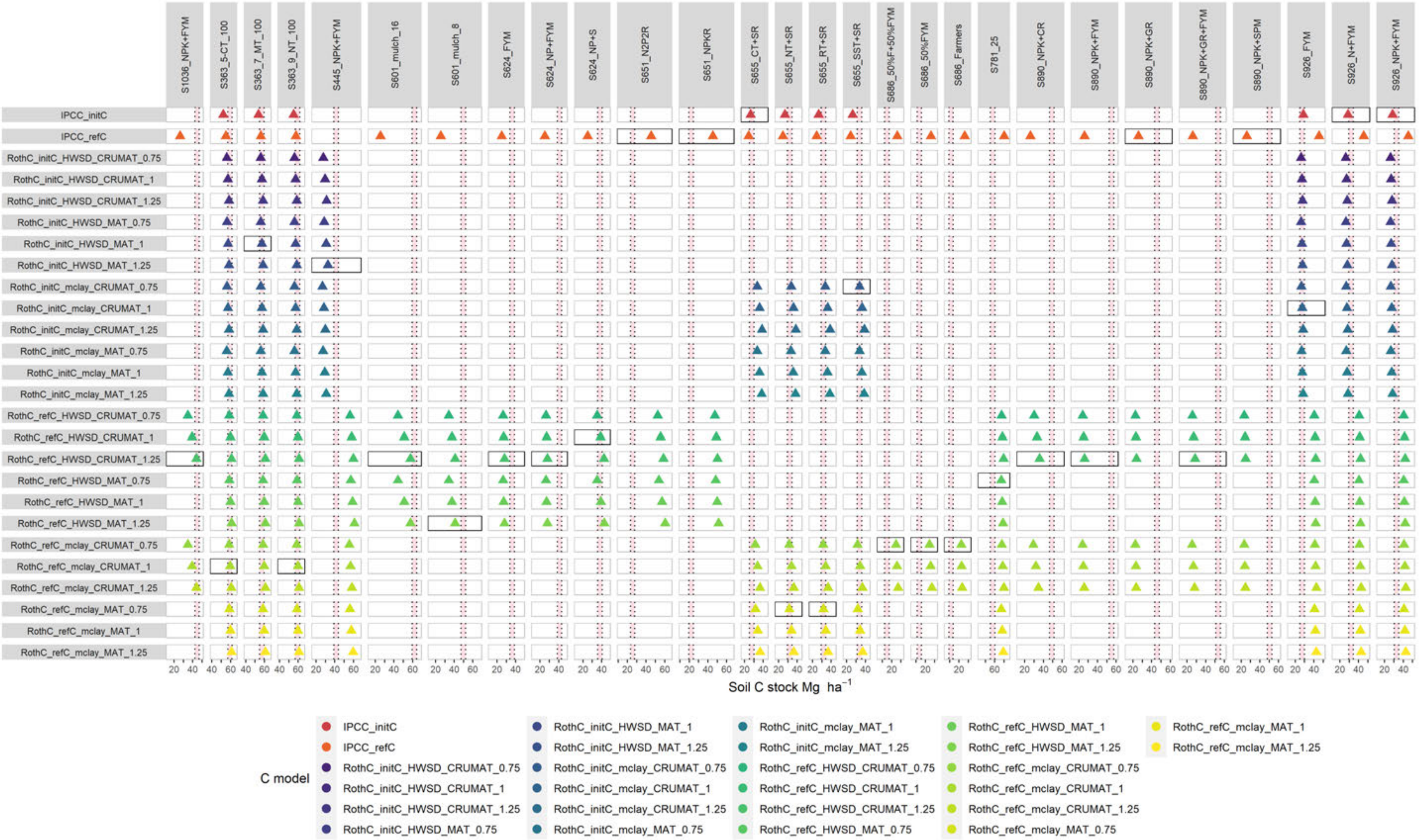

Figure 3.7: SOC$_p$ for OA treatments from each model. The red shading shows the range $\pm$ 1 SD from SOC$_t$. The closest model prediction of each treatment's SOC$_t$ is shown by the black box in each column.

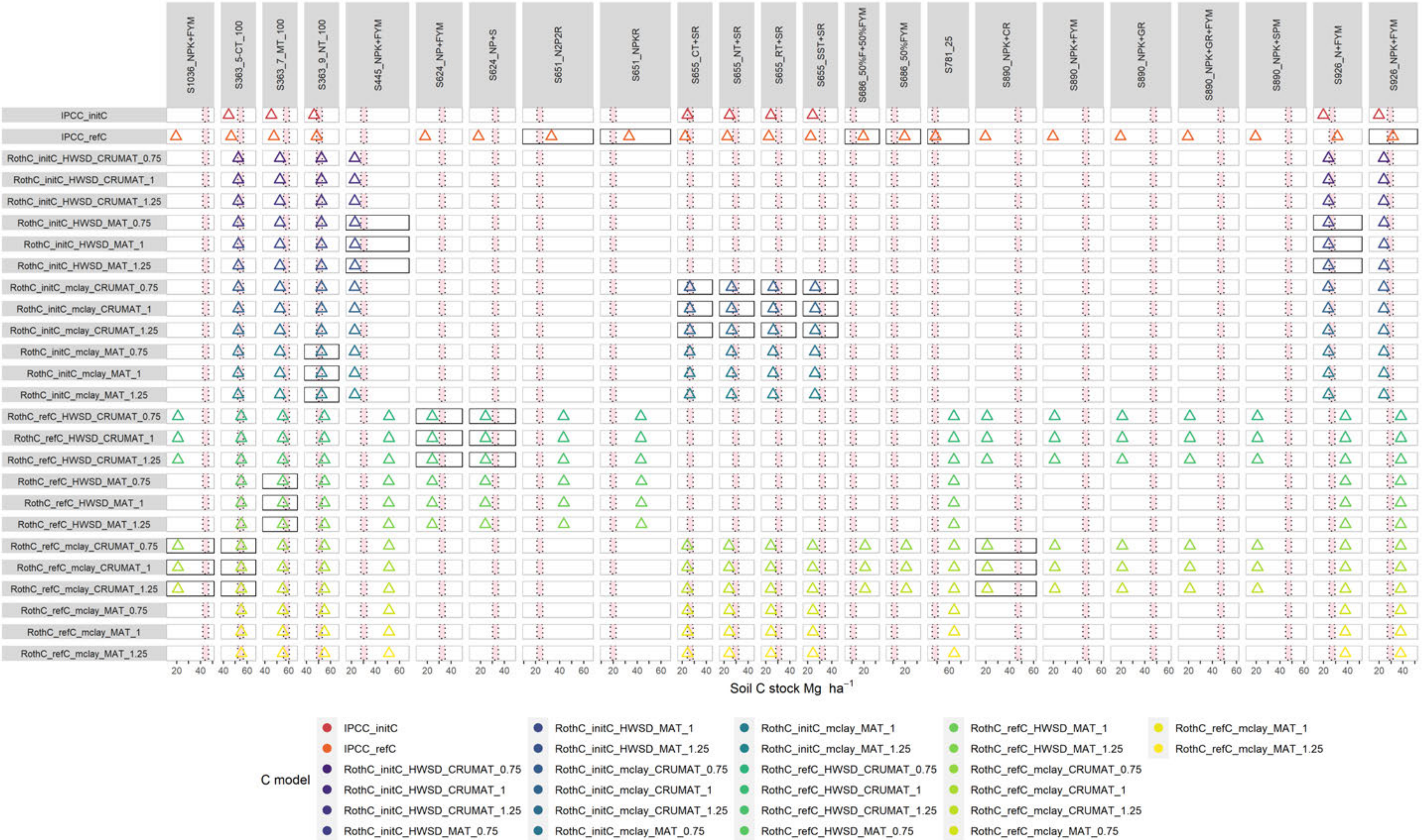

Figure 3.8: SOC$_p$ for MF treatments from each model. The red shading shows the range $\pm$ 1 SD from SOC$_t$. The closest model prediction of each treatment's SOC$_t$ is shown by the black box in each column.

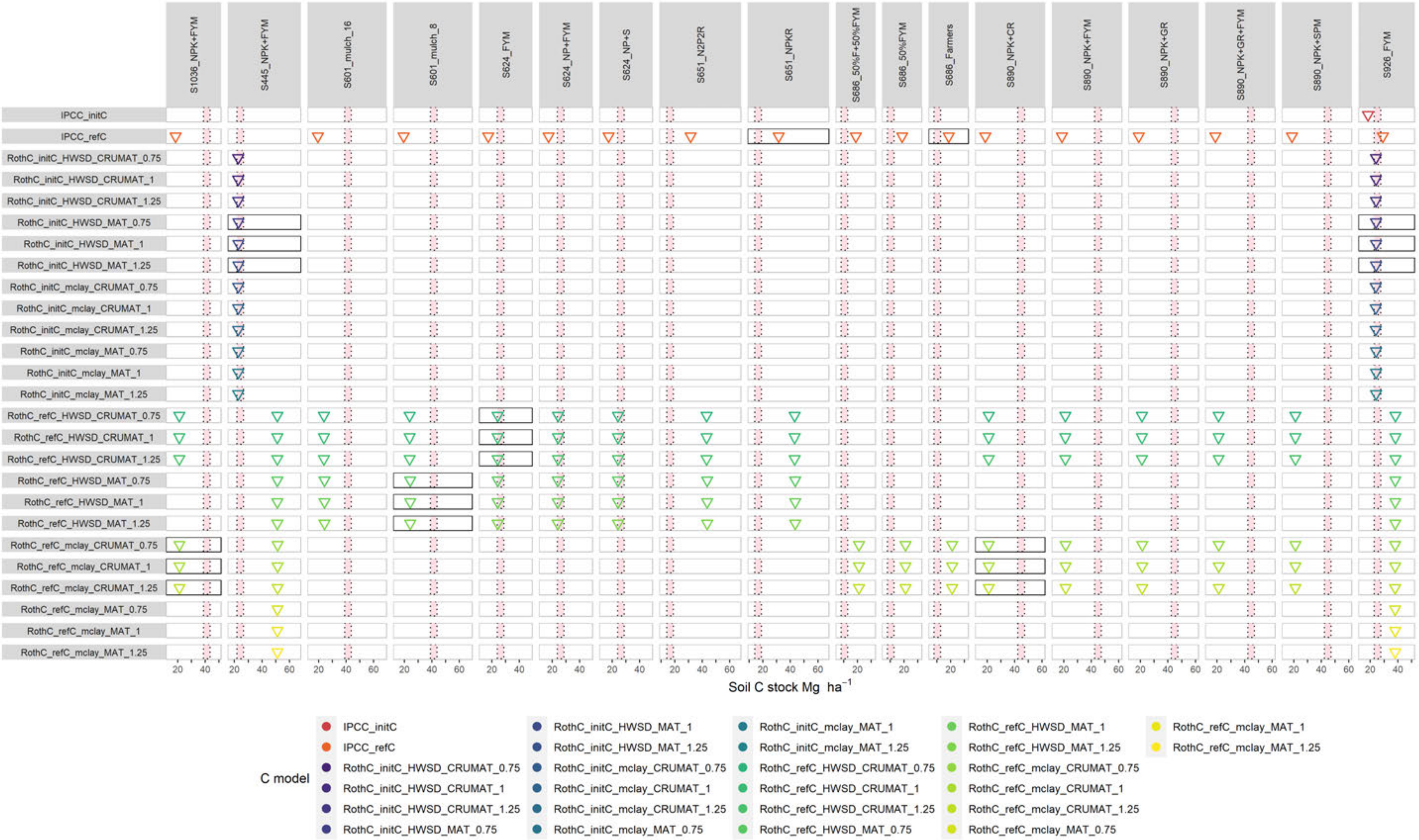

Figure 3.9: SOC$_p$ for ZI treatments from each model. The red shading shows the range $\pm$ 1 SD from SOC$_t$. The closest model prediction of each treatment's SOC$_t$ is shown by the black box in each column.

Comparing model predictions and measured values

SOC$_t$ ranged from 10 Mg C ha^{-1} to 62 Mg C ha^{-1}. SOC$_p$ ranged from 17 Mg C ha^{-1} to 70 Mg C ha^{-1}. The largest differences between measured and modelled values were associated with particular treatments, rather than particular models (Figures 3.7; A.3.1). Across all treatment types, SOC$_p$ was greater than SOC$_t$ in 44 % of simulations. IPCC calculations underestimated SOC$_t$ regardless of initial SOC stock ($p < 0.001$). RothC predictions utilising measured SOC$_{init}$ underestimated SOC$_t$ ($p < 0.001$), whilst those using SOC$_{ref}$ overestimated SOC$_t$ ($p < 0.005$). The proportion of model results within $\pm$ 1.96 SD of the measured mean varied significantly across models and treatments and estimating initial SOC had a negative impact on the model's ability to predict final SOC correctly (Figure 3.10). Overall, 60 % of models using SOC$_{init}$ were within $\pm$ 1.96 SD, compared to 25 % of models using SOC$_{ref}$.

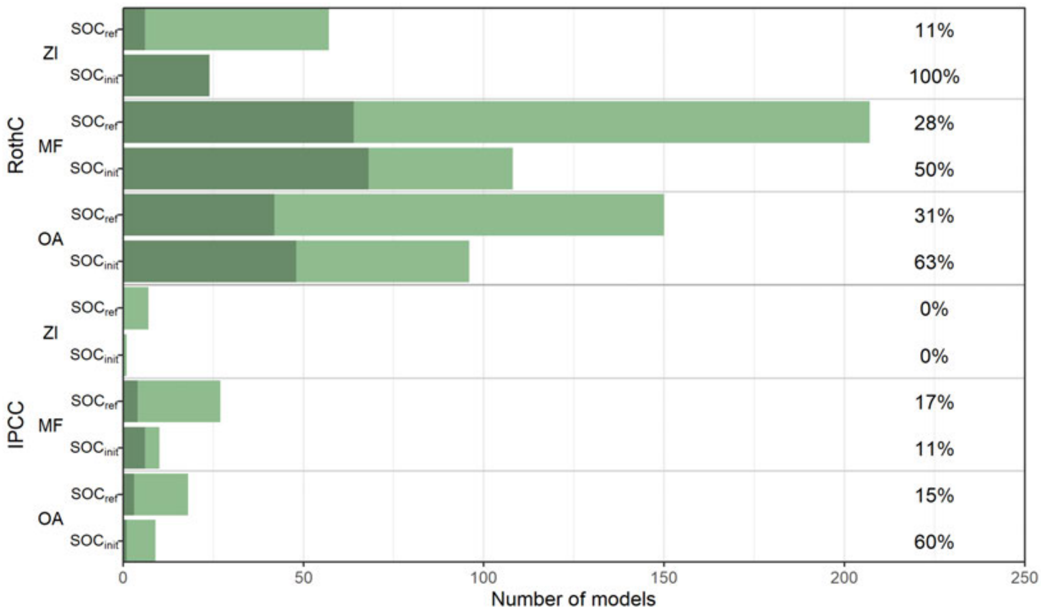

Figure 3.10: Total number of models (light green) and number of SOC$_p$ results within $\pm$ 1.96 SD of SOC$_t$ (dark green), by treatment type and initial SOC. SD values are as reported; if not reported, the dataset weighted mean is used (see Wiebe et al. 2006)

For OA treatments, annualised median SOC stock errors were usually negative when SOC$_{init}$ was used: SOC$_t$ was underestimated at more sites (Figure 3.11).

Some data were not available for some sites (Table 3.1), limiting the models that were run (see, for example, Figures 3.7, 3.8 and 3.9). Given that model errors were similar for a given treatment, but not across sites, aggregating results across sites must be done carefully. The range of errors shown for each model in Figure 3.11 is related to the specific subset of treatments modelled, not just the model used. The impact of this can be seen in comparing errors for the whole dataset with those for the subset of sites with both SOC_{ref} and SOC_{init} values reported: the median and inter-quartile range of errors are materially different.

For the subset of sites with both SOC_{ref} and SOC_{init} values reported, the IPCC median error did not change significantly when SOC_{ref} was used, though the range of errors widened (Figure 3.11).

When SOC_{ref} was used in RothC the median error normalised by time was positive (Figure 3.11). Over-estimating amendment C tended to increase the spread compared to the same model with measured amendment C. Notably, the spread of errors for RothC with primary data was larger than for some of the RothC models using secondary data (Figure 3.11).

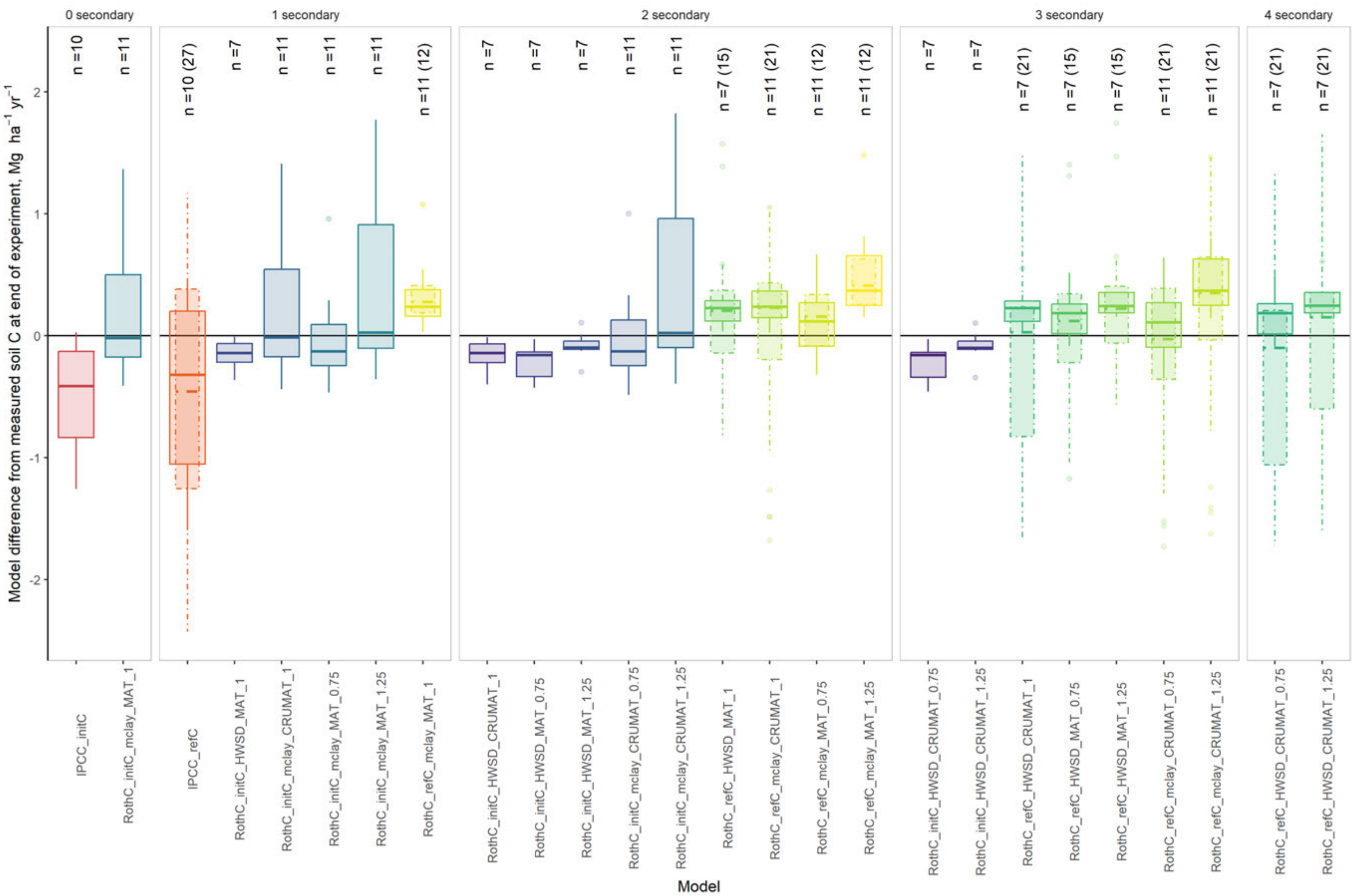

Figure 3.11: Model errors normalised by time ($\mathrm{SOC}_p - \mathrm{SOC}_t$ / duration) for OA treatments. Solid boxes are for the subset of sites with reported SOC_i, dotted boxes are for the full set of sites in Table 3.1. The number of treatments modelled is shown, with numbers for the full set (dotted boxes) in parentheses.

3.4 Discussion

There are several valuable pieces of information that a SOC model can predict to support agricultural decisions; ΔSC_{yr} in the event of a practice change, SOC stock at a given point in time for a given management and/or the difference in rates and/or stocks between potential management scenarios. This analysis compared the predictive ability of two models and different input data sources when predicting SOC stock at field sites using organic amendments and non-amended comparisons.

3.4.1 Model parameterisation

By reducing data collection burdens for farmers and agronomists, secondary data sources could broaden access to useful SOC information. This analysis found that, at site level, secondary data for SOC modelling differed to varying degrees from measured site data. Across the dataset, CRU MAT data was significantly different from measured site MAT ($p < 0.05$). The larger the difference between primary and secondary input data, the greater the expected difference between respective modelled SOC values might be, though impacts of combined differences may cancel out. In the case of S445, the influence of the overestimated MAT value (increased decomposition) was moderated by the overestimated clay value (increased humus formation). RothC sensitivity to different parameters is known to vary (Poeplau, 2016); in general, predictions will vary less when secondary data are used for less sensitive variables. A practical recommendation arising here is user review of secondary data. Though farmers may not be able to provide robustly sampled measured data for SOC modelling, they will often be able to sense check secondary data with their own information. If collated, sense check information could help clarify errors or bias in secondary datasets. Crucially, for online tools where secondary data can be automatically fetched (e.g. via an application programming interface (API)), it should still be made visible to the user, with an option to refine the data.

This study was not a systematic sensitivity analysis, and included experimental data with many different managements, durations and site characteristics. Whilst the number of model runs was significant (n= 798), the patchiness of input data (both primary and secondary) means that not all models were run for all sites. Results must be considered within this context and all conclusions drawn here would benefit from testing on a larger dataset and in different agricultural contexts. The shortcomings of soil data reporting are well discussed elsewhere (Poeplau & Don, 2015; Todd-Brown et al., 2022). In particular it is noted that Tautges et al. (2019) found different net impacts on soil C stocks at the depths modelled here (30 cm) compared to the whole profile.

Input biomass data for these modelling applications are another key consideration (Poeplau, 2016). A limitation of the RothC parameterisation presented here is the use of the fixed baseline PRI value in forward model runs, since the provision of nutrients through both organic and/or inorganic soil additions often increases crop productivity (Hijbeek et al., 2017). Given that the PRI value was used to optimise the RothC spin-up SOC to match initial SOC, altering it post-initialisation is not simple without time-series data on crop productivity. For OA treatments, the lack of such data is somewhat ameliorated by modelling the amendment C at $\pm$ 25 % of measured levels. Model runs for MF and ZI treatments do not reflect any changes in C input from the baseline PRI level, which results in minimal predicted change in SOC over time: a poor prediction for many of the MF treatments in the dataset (Figure 3.6).

3.4.2 Model results

Over modelled time horizons, predicted ΔSC_{yr} values from RothC models using SOC$_{ref}$ were similar to the equivalent model using SOC$_{init}$. Therefore, the use of SOC$_{ref}$ did not reduce the accuracy of RothC prediction of ΔSC_{yr} (Figure 3.6). In addition, Figure 3.6 suggests that the use of secondary clay or MAT data are, at worst, no less accurate for predicting ΔSC_{yr} than primary data. These findings suggest that farm decision makers could use secondary data for initial SOC, MAT and clay % without significantly affecting modelled ΔSC_{yr}. However, at some sites, no available model replicated the observed ΔSC_{yr} adequately and the predicted rate may still be far from the actual ΔSC_{yr} .

As parameterised here, the variation in organic amendment C quantities is the main driver of difference between RothC's predicted ΔSC_{yr} within a treatment: there is greater variation in SOC$_p$ values between models for experiments that have greater C inputs and any difference increases over time (i.e. more years of the same modelled management). Despite varying organic amendment C by $\pm$ 25 %, RothC consistently either overestimated (one site) or underestimated (three sites) ΔSC_{yr} compared to measured rates for all amendment C scenarios. The general underestimation of ΔSC_{yr} in longer experiments with low amendment C and/or inorganic fertiliser rates might be improved by including forecasted net primary productivity (NPP) increases driven by organic and inorganic fertilisers not otherwise represented within RothC (discussed above). However, the consistent site-level over- or under-estimation by RothC suggests that further calibration of decomposition rates is also needed.

For model users, it may be hard to predict changes in NPP without guidance, though organic and mineral soil amendments may be expected to affect productivity. If changes in NPP cannot be estimated, the RothC model should not be utilised for MF management, since there would be no representation of a potential impact on C inputs. RothC can be utilised for ZI management, where negligible change to

NPP is expected, and OA management where direct amendment C inputs are represented. Whilst this dataset is insufficient to derive new parameters, these findings suggest that, with this implementation, it is preferable to underestimate the amendment C input when supply to the soil is high and overestimate otherwise, particularly when inorganic inputs are applied.

Within a site, the initial SOC value drives clusters of RothC model predictions of SOC stock (Figure 3.7). SOC$_{init}$ yielded better predictions of SOC$_t$ than SOC$_{ref}$ across treatments and models (Figure 3.10). In addition, Figure 3.11 suggests that using SOC$_{init}$ is more likely to return a conservative value for SOC stock than using SOC$_{ref}$. This is affected by SOC$_{ref}$ being greater than SOC$_{init}$ in 3/4 sites modelled here. Whilst this is not a large sample, it is likely that IPCC SOC$_{ref}$ values designed for native vegetation (i.e. undisturbed land) will overestimate the initial SOC on land converted to, and/or with a long history of, cultivation since land conversion and cultivation tends to reduce SOC stock (Amelung et al., 2020; Jian et al., 2020, and references therein). The median model errors being consistently greater than zero for models using SOC$_{ref}$ supports this.

With the exception of overestimated C input, the replacement of primary data with secondary data did not systematically widen the inter-quartile range of RothC prediction errors. The impact of using secondary data for MAT and clay % instead of primary data was minor and generally did not change whether SOC$_p$ was within $\pm$ 1 SD of SOC$_t$ (Figure 3.7). This result challenges the assumption that primary data will systematically yield higher-quality information from SOC models than secondary data and is therefore worth the investment. This rather indicates that some secondary data can be applied to predict SOC stock over management time horizons without significant loss of model accuracy. This finding is partially a result of the spin-up approach used, which flexes PRI to match the desired initial SOC value. Using this approach limits the influence of the climate and soil data to the forward change in SOC; i.e. to the change in SOC from the given initial SOC value. The analysis here highlights how model implementation choices must support the needs of the relevant decision context, explored further below.

These results show clearly that the ability of the IPCC T1 method and RothC to replicate observed stocks and changes in SOC varies primarily by site, rather than by data sources and OA treatments. SOC$_p$ errors were generally more similar for models and treatments within a site than between sites (Figures 3.4, 3.7, A.3.1). The site specificity of model ability to predict SOC stock change can be seen in Figure 3.11 when comparing the subset of sites with SOC$_{init}$ and the full dataset: the inter-quartile range of model error (SOC$_p$ - SOC$_t$ / duration) extends for all models based on inclusion of more sites. This is a striking outcome, as it means that RothC- as parameterised here- is not successfully generic across the modelled contexts.

Though the modelled dataset includes field studies between 6 and 41 years in length, there was no clear pattern of model accuracy over time beyond that an error in predicted ΔSC_{yr} leads to a greater discrepancy between SOC$_p$ and SOC$_t$.

3.4.3 Implications for decision support applications

Across treatment types, it is more likely that the RothC model can predict within a useful range of measured values for SOC stock and ΔSC_{yr} than IPCC T1, even when secondary data are used. The IPCC T1 method was a worse predictor of both SOC stocks and ΔSC_{yr}, though it was consistently conservative and could be utilised where conservative estimates are a priority. Whilst it performed better overall, there is capacity for this implementation of RothC to provide significantly incorrect values regardless of the use of primary or secondary data. In aggregate, then, these findings suggest that utilising secondary data is a useful option for activities like project scoping and design, when data is often scarce, but that the accurate modelling of soil C for outcome-based projects requires more attention to model calibration.

Recommendations made above for using secondary data with RothC (assuming equilibrium SOC at the start of forward runs) are summarised here:

- Model users should review secondary data to reduce potentially large differences from field-level values.
- Secondary MAT and clay % can be utilised without loss of model skill for both ΔSC_{yr} and SOC stock prediction.
- Using RothC with inorganic fertilisers, whether or not organic amendments are also used, requires including the impact of inorganic fertilisers on crop productivity.
- Avoid overestimating C input to the soil when overall supply is high, and vice versa when supply is low.
- SOC$_{ref}$ can be used to predict rates of SOC change (Mg C ha^{-1} yr^{-1}, not %) , but is less reliable for SOC stocks.

3.4.4 Implications for modellers

Whilst this analysis yields some useful recommendations for farm decision makers seeking to understand SOC impacts of management, there are also important revelations for modellers and model builders. These revolve around site-specific model performance and representation of practices that have an observed impact on SOC.

Firstly, these results do not support the broad assumption by modellers that field-measured input data are the linchpin of strong model predictions. Rather, they indicate that sense-checked input data from secondary sources does not have universally negative impacts on model prediction. In many cases, secondary sources of RothC input data may be utilised with minimal loss of model skill for various predictions. In fact, given the quantified uncertainties and standardised methods in these datasets, they may have advantages over sparse primary data.

The primary patterns of difference in prediction accuracy here are the sites, not the input data; at some sites, RothC provides a poor prediction of SOC change and SOC stocks after a change in management. Aside from errors or bias in input data, sources of error in modelling include model parameters and model structure. Soil functioning is complex and there are remaining knowledge gaps, which are limitations for developing a 'correct' process-based model. For modellers assuming that the conceptual structure of RothC is correct, these results indicate that the model parameters are poorly calibrated for broad application.

To use models to distinguish between SOC impacts of management options, the accurate representation of management impacts on SOC is a priority. The IPCC T1 method explicitly captures more management choices that are seen to have an effect on SOC than RothC (e.g. tillage, use of inorganic fertilisers), though these do not often translate into more accurate predictions (Figures 3.6, 3.7). In theory, one benefit of a process-based model over an empirical one is the representation of interactions within the modelled system. RothC's greater input data requirements and dynamic representation of SOC processes should provide more information with which to accurately predict SOC stocks. However, these results show that RothC does not capture all relevant interactions affecting SOC under arable management. Without parameter representation of physical disturbance (i.e. tillage) or for inorganic fertilisers, RothC predictions are identical for site treatments with the same C input, regardless of differences in tillage or inorganic fertilisers. Sites S363 and S655 varied tillage in their treatments and measured differences in observed SOC_t and ΔSC_{yr}, which could not be represented in the RothC model.

Perhaps more powerfully than the broad observations of management impacts that are under-represented in RothC, the site-level patterns shown in these results indicate that RothC's default parameterisation is not sufficiently generic to model soil C change across all the sites in this study. Calibration methods applied through spin-up are not sufficient to enable effective prediction of C stock change across the sites in this study. A large number of published papers discuss calibrating RothC, including improving belowground biomass approximation, partition coefficients, decomposition rates and representing physical disturbance (e.g. Cagnarini et al., 2019; Dechow et al., 2019; Gottschalk et al., 2010; Poeplau, 2016). Organic C inputs from growing plant biomass will always be difficult to estimate, particularly when forecasting and when PRI is used as a calibrator during spin up. It is known that decomposition rates differ between types of organic inputs, see, for example, the RothC decomposition parameters derived by Peltre et al. (2012). Future work could consider such published RothC modifications and test them widely, with an aim of proposing a modification to the core RothC methodology. The published RothC user guide indicates a number of pathways for spin-up in the absence of measured pools of C analogous to those represented in the model (Coleman & Jenkinson, 1987): proposed calibrations must consider all of these user pathways.

3.5 Conclusions

Measuring SOC is a challenge for farmers and land managers, particularly due to spatial heterogeneity over small scales. SOC models can offer an alternative, but practical application of SOC models must be feasible for the target user and yield valuable information. Reducing the data burden of the RothC process-based model through secondary data sources for MAT and % clay did not detrimentally affect model predictions of SOC stocks or rates of change. However, depending on the site, RothC may or may not be able to accurately predict soil C evolution.

Using reference SOC values for native vegetation tended to lead to overestimation of SOC stocks on farmed land, but the projected ΔSC_{yr} was equally accurate with both SOC$_{ref}$ and SOC$_{init}$. Altering the quantity of C input had a significant effect on predicted ΔSC_{yr}; an increase in C input often drove rates that were closer to measured ΔSC_{yr}, partially because the model implementation omitted projections of crop productivity change over time.

The IPCC T1 methodology will likely only outperform RothC if a primary consideration is conservative prediction of ΔSC_{yr} or if differences in tillage practice are present.

For modellers, these results challenge a focus on accurate input data and instead indicate that further calibration steps are needed to ensure that RothC is generic enough for wide application.

Chapter 4

Model-data integration: options for employing user data to improve SOC predictions

4.1 Introduction

Whilst there exist various soil C models that can be applied to agricultural contexts at the field level, such global SOC models can be inaccurate at individual sites (Cagnarini et al., 2019; Chapter 3). For farmers and land managers, this reduces the value of model outputs and increases the risk associated with relying on them for decision support. This is particularly true where the model does not provide an explicit assessment of uncertainty.

Models are a key component in projections for carbon accounting. Increasingly, protocols for carbon credits require periodic SOC measurements to validate and/or calibrate projections of SOC stock change (Lavallee et al., 2024; Verra, 2023; Gold Standard, 2020), partially motivated by the aforementioned mixed predictive accuracy of models at site level. However, these protocols often do not provide methodologies for combining measurements with models (Oldfield, Lavallee, et al., 2022).

Measured data and models can interact in a number of ways. Campbell and Paustian (2015) mention using data to formulate, calibrate, drive or evaluate a model. Data assimilation is a further form of interaction, which has recently gained attention in environmental science (Carrassi et al., 2018). Data assimilation "*combines prior information from numerical model simulations with observed data to obtain the best possible description of a dynamical system and its uncertainty*" (Evensen et al., 2022). Because it seeks effective ways of integrating observed data to improve model predictions and uncertainty quantification, data assimilation is of increasing interest to those hoping to maximise the effectiveness of SOC management.

SOC measurements, as described in Chapter 1, are challenging for farmers, as they are costly, time-consuming and unreliable (Campbell & Paustian, 2015). Whilst some of these challenges are being reduced by new technologies such as soil probes and end-to-end sampling services, relying on comprehensive, regular sampling of soil organic C (SOC) on farms remains impractical in many contexts. However, it is possible that farmers and land managers may have - or be able to gather - a sparse time series of SOC data. Considering the strengths and weaknesses of both models and data, this chapter focuses on options for small datasets of SOC measurements to improve SOC model predictions at farm-level.

Taking together the diversity of patterns of SOC stock evolution observed during field studies and the innumerable differences between management across sites, it is a tall order to expect a single set of global model parameters to yield accurate predictions. Process-based models are based on the current understanding of soil functioning and typically parameterise fixed relationships between climate, environment and management. Process-based models such as RothC take a set of initial conditions and propagate the system state forward in time. Errors in model outputs imply missing processes and/or lack of process understanding.

Data assimilation into a model requires a decision on how to weight the importance of the site measured data against the prior knowledge contained within the model, particularly where the goal is prediction of future SOC stock change. Here, I used a range of approaches to assess how a farmer can best use time-series SOC data to improve model predictions. I investigated three model structures with varying levels of mechanistic influence, applied to the same dataset. The models are assessed for the following:

- Predictive capability
- Representation of uncertainty
- Volume of data required for reasonable outputs

The results are discussed in the context of on-farm decision support and implications for SOC modelling and measurement protocols.

4.2 Methods

I studied the structure and outputs of three models, listed below in order of increasing influence of measured data and decreasing influence of prior soil process understanding:

- **Model I: RothC**

  Process-based model, using one measured value of initial SOC to initialise the model.

- **Model II: Bayesian Hierarchical Modelling with RothC as the state-space model (BHM)**
  Bayesian structure containing the RothC model at its centre, using measured data and Markov Chain Monte Carlo methods to determine posterior distributions for RothC parameters.
- **Model III: Bayesian Regression (BRM)**
  Bayesian linear regression with SOC as the dependent variable, and independent variables similar to RothC input data.

This analysis is primarily focused on comparison of model prediction skill and representation of uncertainty. I therefore took care that the main differences between the models were as a result of their structure, with other aspects kept as consistent as possible across all models. Main examples of this included employing the same user data types to inform both empirical and mechanistic models, and consistent metrics for model skill. Models II and III were calibrated at the site level, and utilise the same split of training and testing data. This methods section first explains the calculation approaches for each of the three models, then metrics used for testing and comparing models, and finally summarises the dataset to which these methods were applied.

4.2.1 RothC

The RothC model was introduced in Chapter 3, and its structure is shown in Figure 3.1. In brief, it includes five conceptual soil C pools: resistant plant material (RPM), decomposable plant material (DPM), microbial biomass (BIO), humified organic matter (HUM) and inert organic matter (IOM). Decomposition rates are modified by temperature, moisture and soil cover.

Models I and II both utilised a modified version of the RothC functions found in the SoilR package. The changes from the published package allow values to be specified for various parameters usually held constant in RothC (Table 4.1). A further change to the code is to split out the derivation of the soil cover rate modifier, which is usually held inside the moisture rate modifier in SoilR. In the SoilR defaults, the soil cover status is only allowed to take a single TRUE or FALSE rather than a monthly vector (discussed in Chapter 3): the update for this analysis allows a monthly vector for soil cover to inform the rate modifier values over time.

In Models I and II, the measured data values for clay percentage and soil sampling depth were used as reported, climate data were gap-filled using CRU TS 4.06 (Climatic Research Unit et al., 2022). Irrigation in treatments was not included, since reporting of quantities was insufficient.

In Model I, the RothC default parameter values were used. Soil C pools were initialised in the same way as in Chapter 3; by optimising plant residue inputs to reach the measured initial SOC value (Jordon et al., 2022). The reported yield data was used to estimate plant residue inputs in forward runs using Equation 4.1.

$$C_{crop,\,i} = C_{plant} \bullet yield_i \bullet ((\frac{rs_i}{hi_i}) + res_i \bullet (\frac{1 - hi_i}{hi_i})) \tag{4.1}$$

Where $C_{crop,i}$ is the PRI from crop i (Mg C ha^{-1}), C_{plant} is the proportion of plant dry matter that is carbon, $yield_i$ is the measured dry matter yield of crop i (Mg DM ha^{-1}), hi_i is the harvest index of crop i, rs_i is the root:shoot of crop i, and res_i is a 0, 1 value for whether residues remained on the field or not.

Where plant material was applied as an amendment, the measured amendment dry matter value was multiplied by C_{plant} and added to the carbon inputs.

Where farmyard manure (FYM) was applied as an amendment, the measured FYM carbon was provided to the model without further modification, and modelled as set out in Coleman and Jenkinson (1987): 2 % to HUM and 49 % each to RPM and DPM.

4.2.2 Model II: Bayesian Hierarchical Model

The core approach for this model system was adapted from Davoudabadi et al. (2021, 2024). The aim was to improve soil C predictions by better calibrating RothC parameters to each site using measured data, whilst simultaneously recognising the uncertainty in measured data, in the modelled process and also in the model parameters. The approach is a multi-level "hierarchical" model using Bayesian methods. Some key terms and notation used in the following methods are summarised in Box A, below. In summary, a Bayesian Hierarchical Model (BHM) framework was constructed containing RothC as a state-space model for predicting soil carbon stocks. A Particle Marginal Metropolis Hastings (PMMH) method was utilised to estimate parameter values for the state-space model and sources of uncertainty. This section elaborates on these methods and is organised as follows: the central state-space model is explained, the BHM structure is introduced and then the Bayesian algorithms used to estimate the posterior distribution are summarised. The section concludes by summarising the specific application of these methods in this study. For further detail on the computational benefits of the selected algorithms compared to other options, the reader is directed to Davoudabadi et al. (2021).

State-space model

Auger-Méthé et al. (2021) define state-space models as '*a class of hierarchical models for time series that specifies the dynamic of the hidden states and their link to the observations*'. State-space models are valuable in ecology and environmental sciences as they can model natural processes and measurement error separately, yielding outputs that can differentiate between natural variation and imprecision in sampling (Auger-Méthé et al., 2021). Key to state-space models is the concept of hidden, or 'latent', variables. These latent variables are the true states of the environmental system, which are unknown because the (known) measured values contain errors. State-space models combine measured and latent variables to describe a system that evolves through time, while simultaneously assessing observation error. These hierarchical models contain multiple levels of stochasticity, i.e. multiple elements described well by a random probability distribution.

In the case of soil carbon, the aim is to use measured data, which include some error, to understand the latent state of the soil carbon stock. Given latent states X and measurements Y, Davoudabadi et al. (2021) represent a generic state-space model with Gaussian noise as follows:

$$\begin{aligned} X_t &= f(X_{t-1}) + \mathbf{B}u_t + \varepsilon_t \\ Y_t &= g(X_t) + \nu_t \end{aligned} \tag{4.2}$$

Where ε_t and ν_t are vectors for state and measurement noise, respectively. Known (carbon) inputs, vector u_t, are multiplied by control-input matrix $\mathbf{B}$. The first equation is called the state model, and the second is the measurement (observation) model.

In this analysis, the state model is the process model RothC, introduced in the previous section. The model considers climate, environmental and management effects on the soil, but is fundamentally based on representing processes that are not directly observed.

SOC stock can be considered a latent variable that evolves with time as a Markov chain (Davoudabadi et al., 2021), which means that the next state depends only on the current state, and not the historical SOC stock. The state-space model can be utilised within a Bayesian Hierarchical Model structure, as described below.

Box A: Bayesian terms and notation summary

Some terms and notation used in this chapter are defined below. For a primer on Bayesian statistics, the reader is referred to van de Schoot et al. (2021).

Terms

$Prior$: existing knowledge about a given parameter: a probability distribution. These are chosen by the modeller and reflect how definitive (or vague) the existing knowledge is; priors are often described in terms of being informative or uninformative.

$Posterior$: updated knowledge about a given parameter, after combining the $Prior$ with new data: a probability distribution

$Conditional\ probability$: the probability of some event, given that an(other) event has already occurred

$Markov Chain Monte Carlo$ (*MCMC*): a type of algorithm for drawing samples from a distribution

$Metropolis Hastings$ (*MH*): an MCMC algorithm, useful when direct sampling from a probability distribution is difficult

$Burn-in$: initial samples of the MCMC, when the chain is unlikely to be at equilibrium, that are discarded

$Thinning$: reducing the large sample size of MCMC outputs by discarding samples in a regular manner (e.g. keeping every tenth sample)

Notation

$p(x)$: probability density function of random variable x

$p(x|E)$: conditional probability density function of random variable x given event E

X: state process, not observed

Y: observations (of SOC), noisy

θ: parameters, unknown

Bayesian Hierarchical Model structure

A Bayesian modelling approach combines *a priori* understanding of the system to be parameterised (the 'prior') with observed data to improve knowledge about model parameters, and therefore model results. The output is improved parameter estimates in the form of a posterior distribution and maximum likelihood estimation of parameter values.

In this application, the BHM framework allows separation of some complexities of soil carbon modelling. In process-based modelling of soil carbon, measurements (of soil carbon and other relevant quantities) are used alongside the current understanding of environmental processes and of parameter values. These three components each have uncertainties, which can be handled in the BHM structure.

In this study, the total BHM was the joint distribution (i.e. combination) of measured SOC data (Y), the process model (X) and the parameters (θ), shown in Equation 4.3 (see Box A for notation). These were three separate levels of the hierarchy. The first level is the observation model ($p\,(Y|X,\theta)$), containing noisy measured data that depend on the state variables, and the middle level ($p\,(X|\theta)$) models soil processes. These first two levels of the BHM were the two components of the state-space model in Equation 4.2. The final layer of the hierarchy ($p\,(\theta)$) contained the prior knowledge of the parameter values.

$$p\,(Y,\ X,\ \theta) = p\,(Y|X,\theta) \bullet p\,(X|\theta) \bullet p\,(\theta) \tag{4.3}$$

$$p\,(X,\theta|Y) = \frac{p(Y,\ X,\ \theta)}{p(Y)} \ = \ p\,(X|\theta,Y) \bullet p\,(\theta|Y) \tag{4.4}$$

The aim here was to better understand and estimate the RothC model process and parameters, given the observed data, therefore the posterior distribution of interest was the conditional probability of the process and parameters given the observations, shown in Equation 4.4. However, the probability density of the data ($p(Y)$) was difficult to calculate and sample directly and so the posterior distribution is challenging to evaluate. Instead, a Markov Chain Monte Carlo (see Box A) approach to estimating an expectation for the posterior distribution was used, detailed in the subsection *Bayesian methods to evaluate the posterior distribution.*

Process model structure and equations

The core of the process model used in this BHM was the RothC model, with its parameter values forming part of the final level of the BHM (see Table 4.1 and section on Priors, below).

Table 4.1: RothC model parameters allowed to vary in the BHM, and their defaults which are used in Model I (RothC) and as prior means in Model II (BHM). * Default for agricultural crops.

RothC process	RothC equation	Parameter	RothC default
Pool decomposition rates	If, at time i the pool p has SOC $SOC_{p,i} = Y$, then $SOC_{p,i+1} = Ye^{-abckt}$ t C ha^{-1} with k per pool	k_{DPM}	10
		k_{RPM}	0.3
		k_{BIO}	0.66
		k_{HUM}	0.02
		k_{IOM}	0
Temperature rate modifier	$a = \frac{a_1}{1+e^{(\frac{106.06}{T+18.27})}}$	a_1	47.9
Moisture rate modifier	$b = (1-b_1) + b_1 * \frac{(max.TSMD - acc.TSMD)}{(max.TSMD - 0.444 max.TSMD)}$	b_1	0.8
Soil cover rate modifier	$c = \begin{cases} c_1 & when\, soil\, vegetated \\ 1 & when\, soil\, bare \end{cases}$	c_1	0.6
Pool split for plant inputs	$PRI = (1 - \frac{1}{1+DR})DPM + (\frac{1}{1+DR})RPM$	DR	1.44 *
Pool split for FYM inputs	$FYM_C = (\frac{DR.FYM}{2})(DPM + RPM) + (1 - DR.FYM)HUM$	$DR.FYM$	0.98
Pool split from PM pools to CO_2, BIO + HUM	$\frac{CO_2}{BIO+HUM} = x_m e^{-x_e * clay\%} + x_c$	x_m	2.672
		x_e	0.0786
		x_c	3.0895
Proportion of BIO in BIO + HUM	$\pi_B + \pi_H = 1$	π_B	0.46

The remainder of this sub-section summarises the additional modelling steps taken to provide RothC with its required input data from the dataset.

Carbon inputs

Crop yields used in the model were observed yield values with random observation error. To calculate carbon inputs from crop yields, Equation 4.1 was used. Carbon input parameters included in the BHM parameter model were C_{plant}, h_i and rs_i.

SOC pool values

In order to run RothC forward, initial carbon stock values must be provided for each of the five pools (DPM, RPM, BIO, HUM, IOM). Often, the RothC model is run in inverse mode to yield equilibrium pool values. However, in this case, where the MCMC samples model parameters and state variables a huge number of times, this is prohibitively expensive to compute. Therefore, initial pool values were generated from the overall SOC value using simple proportions included in the parameter model of the BHM. The priors for these parameters were established by considering the pool proportions at the end of the spin-up when the 'out-of-the-box' RothC (Model I) was run in inverse mode. The means of these proportions were stable across sites and treatments in this dataset; their small variation is accounted for in the prior distribution (see Table 4.2). IOM was calculated using the equation from Falloon et al (1998) and never varied.

Site data

Soil sampling depth, clay percentage and climate data were not included in the parameter model of the BHM. Since the PMMH process was run for each site individually, adding these parameters would have risked overfitting. Uncertainty in these quantities is therefore not represented.

Observation model equations

Observations modelled by states are total organic carbon (TOC), used here to refer specifically to the sum of all SOC pools, and crop yields. The observation model equations for each state X_i, field j and time t are as shown in Equation 4.5.

$$Y_{i\ (j,\ t)} | X_{i\ (j,\ t)} \ = \ x_{i\ (j,\ t)} \ \sim \ \textit{log-normal}\left(ln(x_{i\ (j,\ t)}),\ \sigma_i^2\right) \tag{4.5}$$

Where $x_{i\ (j,\ t)}$ is the observation for state i in field j at time t and measurement error σ_i^2.

Priors for parameter model

Priors for parameters and state variables are shown in Table 4.2. Priors were generally somewhat informative (see Box A in Section 4.2.2). The priors for RothC parameters were the RothC default values. Crop parameter priors (h_i and rs_i) were from Spawn et al. (2020).

Bayesian methods to evaluate the posterior distribution

Since the posterior distribution is difficult to evaluate, Markov Chain Monte Carlo (MCMC) methods were employed to sample from the distribution. MCMC algorithms aim to approximate the target distribution by drawing samples from it. Here, they were used to sample the parameter values of interest. Referring back to the posterior in Equation 4.3, correlated random samples from $p(\theta|Y)$ were drawn by a variant of the MCMC Metropolis Hastings (MH) algorithm called the Correlated Pseudo-Marginal method (CPM). The Bootstrap Particle Filter (BPF) was used to draw samples from $p(X|\theta,Y)$.

At its core, the CPM algorithm (see Algorithm A.4.2) proposes a new sample of θ, tests the likelihood of the new sample and uses an acceptance condition to either keep the new sample as part of (i.e. evidence for) the developing distribution or reject it and return to the previous distribution. By repeating this many times, the large number of accepted samples can be expected to converge on describing the target posterior distribution. In this case, the CPM used fixed random numbers to produce highly correlated likelihood estimators (see Algorithm A.4.3, Davoudabadi et al., 2024), which helps reduce computation times.

Since the aim is prediction of SOC stocks (X), the number of SOC measurements (Y) is less than the number of latent states to estimate (Shumway & Stoffer, 2016). A filtering algorithm was used to estimate states (X) based on observed data, often in time-series systems like this one.

The posterior distribution for the SOC state was estimated by the Bootstrap Particle Filter (see Algorithm A.4.1). Particle filters such as the BPF are based on sequential importance resampling. They update empirical approximations to represent the new posterior distribution in light of each new observation by propagating a number of particles (potential SOC states) through the system (here, through time). In summary, particle values are proposed based on a user-specified proposal distribution. These values are assigned a weight based on the likelihood of the measured data given the particle estimate of SOC, and then resampled based on their weight, so that more likely SOC states are selected more often than less likely SOC states.

The combination of the CPM and BPF methods is called Particle Marginal Metropolis Hastings (PMMH). PMMH updates the parameters and maintains a set of particles that evolve over time in a structure that is computationally efficient for complex models such as this one (Davoudabadi et al., 2021).

Proposal distributions are shown in Table 4.2.

Application of PMMH to the BHM

In this study, the PMMH algorithms were applied to each site separately, using observation data for multiple treatments. A subset of the observation data was utilised in each case. This was to resemble the volumes of data available to most farmers, with the helpful side effect of reduced computation time.

Four MCMC chains of 10,000 samples were run for each site, discarding the first 1000 as burn-in and no thinning was performed (see Box in Methods section).

To assess whether the MCMC process has sampled sufficiently well and reached a stationary distribution, the Gelman-Rubin convergence diagnostic was used (Gelman & Rubin, 1992).

4.2.3 Model III: Bayesian Regression Model

The *brms* R package (Bürkner, 2017) was used for Bayesian regression modelling of SOC stocks. A linear regression based on the same variables as RothC (and therefore the BHM) was applied to each site, see Equation 4.6. Given that models were generated per site, there is no climate or soil type data used here, though a multi-site BRM would likely benefit from their inclusion. The same priors were used for all sites (Equation 4.6), with the mean for the intercept a being the mean of initial SOC stocks across the dataset, with a large standard deviation.

The BRM was generated using four chains of 10,000 samples, discarding the first 1000 as burn-in; the same as the BHM. The same subsets of observation data were also used (see Table 4.3) to investigate the impact of additional observation data on model predictions.

$$\begin{aligned}
TOC &\sim N(\mu, \sigma) \\
\mu &= a + b_1 X_{FYM} + b_2 X_{Org} + b_3 X_{Yield} + b_4 X_{Year} \\
a &\sim N(38, 10) \\
b_i &\sim N(0, 1) \\
\sigma &\sim U(0, 20)
\end{aligned} \tag{4.6}$$

where TOC is soil organic carbon (Mg C ha^{-1}), μ is the mean value for TOC, calculated using the second line of the equation and σ is variance. X_{FYM} is farmyard manure applied (Mg C ha^{-1}), X_{Org} is organic amendment applied (Mg DM ha^{-1}), X_{Yield} is crop yield (Mg DM ha^{-1}), X_{Year} is the calendar year (no adjustment), a is the intercept and b_i are coefficients.

4.2.4 Model testing: prediction

All models were trained on subsets of available observation data. At least one treatment per site was omitted from the Bayesian models' training, so that prediction of out of sample management could be tested. In cases where there were larger numbers of SOC measurements, the Bayesian models were trained on the initial set of measurements, leaving some amount of later measurements available to test prediction skill over time.

4.2.5 Field data

The dataset of SOC measurements used in this analysis is from published field experiments. The dataset was not collated systematically. Reviews repeatedly found a lack of long-term and time-series SOC stock data with sufficient meta-data (Bradford et al., 2023; McClelland et al., 2021; Poeplau & Don, 2015). Given the need for other RothC input data to also be reported, it was not feasible or sensible to attempt a new systematic review.

The experiment data used is summarised in Table 4.3. There were three sources of field data. Dimassi et al. (2014) varied tillage and crop rotations at Boigneville in France. Jha et al. (2021) included three sites in India, which each had three different amendment practices. Supplementary information was extracted from Jha et al. (2014). The third source of data was Rothamsted ERA (Rothamsted Research, 2012), from which the Hoosefield Barley long-term experiment is used; this varied the use of FYM. Aside from different climates and management, the different time horizons of these experiments are of interest in terms of predicting SOC stock change into the future. The RothC model was calibrated at the Rothamsted site, but Hoosfield Barley data was not used for this purpose. Data presented in figures were extracted using WebPlotDigitizer (Rohatgi, 2024).

Table 4.2: Parameter definitions, prior distributions and proposal distributions used in the Bayesian Hierarchical Model. N = normal distribution, $Tr.N$ = truncated normal distribution, U = uniform distribution. For where parameters are used in RothC, see Table 4.1

Param.	Definition	Prior distribution	Proposal distribution
a_1	Temperature rate modifier	$N(47.9, 10)$	$N(a_1, 2)$
b_1	Moisture rate modifier	$Tr.N(0.8, 0.4, u = 1)$	$N(b_1, 0.05)$
c_1	Soil cover rate modifier	$U(0, 1)$	$Tr.N(c_1, 0.1, l = 0, u = 1)$
k_{DPM}		$Tr.N(10, 5, l = 0.5)$	$Tr.N(k_{DPM}, 1, l = 0)$
k_{RPM}		$Tr.N(0.3, 0.2, l = 0.025)$	$Tr.N(k_{RPM}, 0.05, l = 0)$
k_{HUM}	Pool decomposition rates	$Tr.N(0.02, 0.01, l = 0)$	$Tr.N(k_{HUM}, 0.001, l = 0)$
k_{BIO}		$Tr.N(0.66, 0.4, l = 0.05)$	$Tr.N(k_{BIO}, 0.05, l = 0)$
k_{IOM}		Fixed: 0	
π_B	BIO part of BIO:HUM split	$Tr.N(0.46, 0.2, l = 0.1)$	$Tr.N(\pi_B, 0.02, l = 0)$
π_H	HUM part of BIO:HUM split	Fixed: $1 - \pi_B$	
DR	DPM:RPM for plant inputs	$N(1.44, 0.2)$	$Tr.N(DR, 0.05, l = 0)$
DR_{FYM}	DPM + RPM for FYM inputs	$U(0.7, 1)$	$Tr.N(DR_{FYM}, 0.02, l = 0.5, u = 1)$
x_m	CO_2 rate slope parameter	$N(2.672, 0.2)$	$N(x_m, 0.1)$
x_c	CO_2 rate constant	$N(3.0895, 0.4)$	$N(x_c, 0.1)$
x_e	CO_2 rate exponent	$N(0.0786, 0.05)$	$N(x_e, 0.01)$
C_{plant}	Plant C content	$N(0.5, 0.05)$	$Tr.N(0.01, l = 0.2)$
rs_{Wh}		$Tr.N(0.2, 0.05, l = 0.1)$	$Tr.N(rs_{Wh}, 0.02, l = 0)$
rs_{Ma}		$Tr.N(0.18, 0.05, l = 0.1)$	$Tr.N(rs_{Ma}, 0.02, l = 0)$
rs_{Sy}		$Tr.N(0.19, 0.05, l = 0.1)$	$Tr.N(rs_{Sy}, 0.02, l = 0)$
rs_{Ba}	Crop root-shoot ratios	$Tr.N(0.11, 0.025, l = 0.05)$	$Tr.N(rs_{Ba}, 0.001, l = 0)$
rs_{Pe}		$Tr.N(0.08, 0.025, l = 0.05)$	$Tr.N(rs_{Pe}, 0.001, l = 0)$
rs_{Sb}		$Tr.N(0.43, 0.1, l = 0.2)$	$Tr.N(rs_{Sb}, 0.02, l = 0)$
rs_{Sg}		$Tr.N(0.18, 0.05, l = 0.1)$	$Tr.N(rs_{Sg}, 0.02, l = 0)$
hi_{Wh}		$Tr.N(0.39, 0.1, 0.25)$	$Tr.N(hi_{Wh}, 0.01, l = 0.1, u = 1)$
hi_{Ma}		$Tr.N(0.53, 0.1, l = 0.25)$	$Tr.N(hi_{Ma}, 0.01, l = 0.1, u = 1)$
hi_{Sy}		$Tr.N(0.42, 0.1, l = 0.25)$	$Tr.N(hi_{Sy}, 0.01, l = 0.1, u = 1)$
hi_{Ba}	Crop harvest index	$Tr.N(0.46, 0.1, l = 0.25)$	$Tr.N(hi_{Ba}, 0.01, l = 0.1, u = 1)$
hi_{Pe}		$Tr.N(0.3, 0.1, l = 0.1)$	$Tr.N(hi_{Pe}, 0.01, l = 0.1, 1)$
hi_{Sb}		$Tr.N(0.4, 0.1, l = 0.1)$	$Tr.N(hi_{Sb}, 0.01, l = 0.1, u = 1)$
hi_{Sg}		$Tr.N(0.44, 0.1, l = 0.25)$	$Tr.N(hi_{Sg}, 0.01, l = 0.1, u = 1)$
p_{DPM}	SOC % DPM	$Tr.N(0.01, 0.005, l = 0)$	$Tr.N(p_{DPM}, 0.001, l = 0)$
p_{RPM}	SOC % RPM	$Tr.N(0.16, 0.02, l = 0)$	$Tr.N(p_{RPM}, 0.001, l = 0)$
p_{HUM}	SOC % HUM	$Tr.N(0.81, 0.05, l = 0)$	$Tr.N(p_{HUM}, 0.001, l = 0)$
p_{BIO}	SOC % BIO	Fixed: $1 - (p_{DPM} + p_{RPM} + p_{HUM})$	
σ^2_{TOC}	Variance TOC	$Tr.N(1, 0.2, l = 0)$	$Tr.N(\sigma^2_{TOC}, 0.1, l = 0)$
σ^2_{eWh}		Fixed: 0.25	
σ^2_{eMa}		Fixed: 0.25	
σ^2_{eSy}		Fixed: 0.1	
σ^2_{eBa}	Crop observation errors	Fixed: 0.25	
σ^2_{ePe}		Fixed: 0.25	
σ^2_{eSb}		Fixed: 0.5	
σ^2_{eSg}		Fixed: 0.25	
σ^2_{eIOM}	Observation error IOM	Fixed: 0.01	
σ^2_{eTOC}	Observation error TOC	Fixed: 0.5	
σ^2_{eFYM}	Observation error FYM	Fixed: 0.5	
Y_{TOC}	Initial SOC	$Tr.N(sitemean, 1, l = 0)$	$Tr.N(Y_{TOC}, 0.5, l = 0)$
Y_{IOM}	Initial IOM	Fixed: site mean using Y_{TOC} and Falloon et al. (1998)	

Table 4.3: Site and management information for experiments modelled. Refs: 1 Dimassi et al. (2014), 2 Jha et al. (2021), 3 (Rothamsted Research, 2012). Boigneville varies tillage: NT = no-till, ST = shallow till, FIT = full-inversion till. CC = Cover Crop, FYM = Farmyard Manure

Ref	Site location	Duration (years)	Clay (%)	SOC depth (cm)	Treatment name (**bold** = used to train models)	SOC_{init} (Mg ha^{-1})	Crops	Organic amendment	Mineral fertiliser	# obs.	Min. # training obs. (years of experiment)	# training treatments
1	Boigneville, France	41	24	28	**CM1_NT** **CM1_ST** **CM1_FIT**	41.9 - 42.5	wheat, maize	none	yes	11 11 11	24 (21 yrs)	6
					CM2_NT CM2_ST CM2_FIT	42.0 - 42.6	wheat, maize	CC (2002 - 2011)	yes	10 10 10		
					CM3_NT CM3_ST CM3_FIT	41.9 - 42.6	wheat, maize, barley, pea, sugarbeet	none	yes	10 10 10		
					CM4_NT CM4_ST CM4_FIT	41.8 - 42.4	wheat, maize, barley, pea, sugarbeet	none	yes	10 10 10		
					CM5_NT **CM5_ST** **CM5_FIT**	41.8 - 42.3	wheat, maize	CC (2002 - 2011)	yes	10 10 10		
					CM6_NT CM6_ST CM6_FIT	41.9 - 42.5	wheat, maize	none	yes	11 11 11		
2	Jabalpur, India	38	57	30	Nil_Jab **NPK_Jab** **NPK+FYM_Jab**	33.8	wheat, soybean	none none FYM	none yes yes	20 28 26	12 (9)	2
	Ludhiana, India	35	7.2	30	**Nil_Lud** **NPK_Lud** NPK+FYM_Lud	13.7	wheat, maize	none none FYM	none yes yes	33 35 21	12 (6)	2
	Palumpur, India	33	23.7	30	**Nil_Pal** NPK_Pal **NPK+FYM_Pal**	40.5	wheat, maize	none none FYM	none yes yes	20 21 22	12 (9)	2
3	Rothamsted, UK	146	20	23	**HB_Nil** **HB_FYM** HB_FYM5271	30.7	barley	none FYM FYM (1852 - 1971)	none	8 8 8	12 (113)	2

4.3 Results

The results of the two Bayesian approaches are presented first, then the three model approaches are compared within and between sites.

4.3.1 Bayesian Hierarchical Model

Computational resource use of this BHM was far less economical than was achieved by Davoudabadi et al. (2024). This is partly because the SoilR RothC functions are relatively slow and the RothC function rejects combinations of parameters that would yield negative respiration coefficients. Whilst this is correct behaviour, the workaround was to draw a totally new sample of parameters. It is likely that the computational efficiency of the BHM was also compromised by the inclusion of such a large number of RothC parameters.

Before using BHM outputs, it is necessary to check that the MCMC sampling has been effective and that the model is valid for prediction. Applying the convention that values of the Gelman-Rubin convergence diagnostic less than 1.2 indicate that parameter values from different chains are indistinguishable from one another (Brooks & Gelman, 1998), Figure 4.1 suggests that most parameters consistently converged across chains for each site and data subset. However, there are important exceptions in crop harvest indices and root:shoot values, as well as b_1 and π_B. With the exception of rs_{Ba} (which was only relevant at Rothamsted), each of these parameters has successfully converged in some cases but not in others. Interestingly, the RothC parameters that exceeded the threshold overlap across sites, suggesting that the BHM structure should perhaps be reviewed and weaker priors used. Since values do not exceed 1.2 by much, it is possible that a greater number of MCMC samples would result in more complete convergence. The following results utilise the BHM outputs, while acknowledging that some parameters did not converge as consistently across chains as would be ideal.

Figure 4.2 shows parameter posterior distributions for each site, alongside their prior distribution. The posterior distributions are from the BHMs using the largest training data subset, with all four chains combined. In Figure 4.2, the maximum likelihood estimates (MLEs) are the parameter values on the x axes that are associated with the maximum density value on the y axis. For most parameters, the MLEs are relatively consistent across sites, and many are similar to their prior MLE. A few parameters, including b_1, c_1, k_{RPM}, k_{HUM} and DR_{FYM} have MLEs that are (relatively) more different from their RothC defaults and show a common direction of change across sites (Figure 4.3), which could indicate a mechanistic error in RothC parameter values. Parameters c_1 and DR_{FYM} were given uniform priors (Table 4.2). Their RothC defaults are 0.6 and 0.98, respectively, whereas their posterior MLEs are around 0.43-0.55 and 0.83-0.86, respectively. A decrease in c_1 implies that soil cover is more influential for decomposition than RothC suggests. A decrease in DR_{FYM} implies that FYM has a greater input to the HUM soil C pool than RothC suggests: only 2 % of input FYM carbon goes to HUM in RothC, whereas the BHM result suggests this could be over 10 %. The posterior MLEs also suggest that temperature influence on decomposition (a_1) varies by site and that topsoil moisture deficit (through b_1) is less influential for decomposition, particularly at Boigneville. However, irrigation was present at the three Indian sites (Jha et al., 2021) and not included in the water provision modelled due to lack of quantitative data reported: the reduced influence of precipitation-induced topsoil moisture deficit at these sites is likely related to the provision of additional water through irrigation.

It is particularly notable that central estimates of k decomposition parameters are higher in all posterior distributions than in RothC. Crop parameters sometimes did not converge across chains (Figure 4.1), but a common pattern seems to be an increase in both harvest index (hi) and root:shoot (rs) estimates compared to prior values. Referring back to Equation 4.1, this might suggest that residue inputs have a smaller contribution to SOC than anticipated.

Figure 4.3 shows the spread of parameter posterior MLEs across sites and training data subsets (chains combined), compared to prior means. Here, the spread of the boxplots indicates the magnitude of the impact of more data on the MLE of each parameter at each site. Due to the different uses and magnitudes of parameters (y-axis scales) it is not appropriate to compare MLE spread across parameters, only between sites for a particular parameter. Many parameters have greater between-site differences in value than changes between training datasets; examples include a_1, c_1, k_{RPM} and k_{HUM}. The addition of more training data did not affect the parameter MLE and the BHM at the site repeatedly converged on the same distribution. The difference in MLEs between sites demonstrates the value of local calibration. For several parameters, Boigneville demonstrates a different pattern from the other sites, whether in spread, MLE value or change from the prior.

In general, more training data did not have a significant impact on BHM predictions or prediction intervals (see Figure A.4.1).

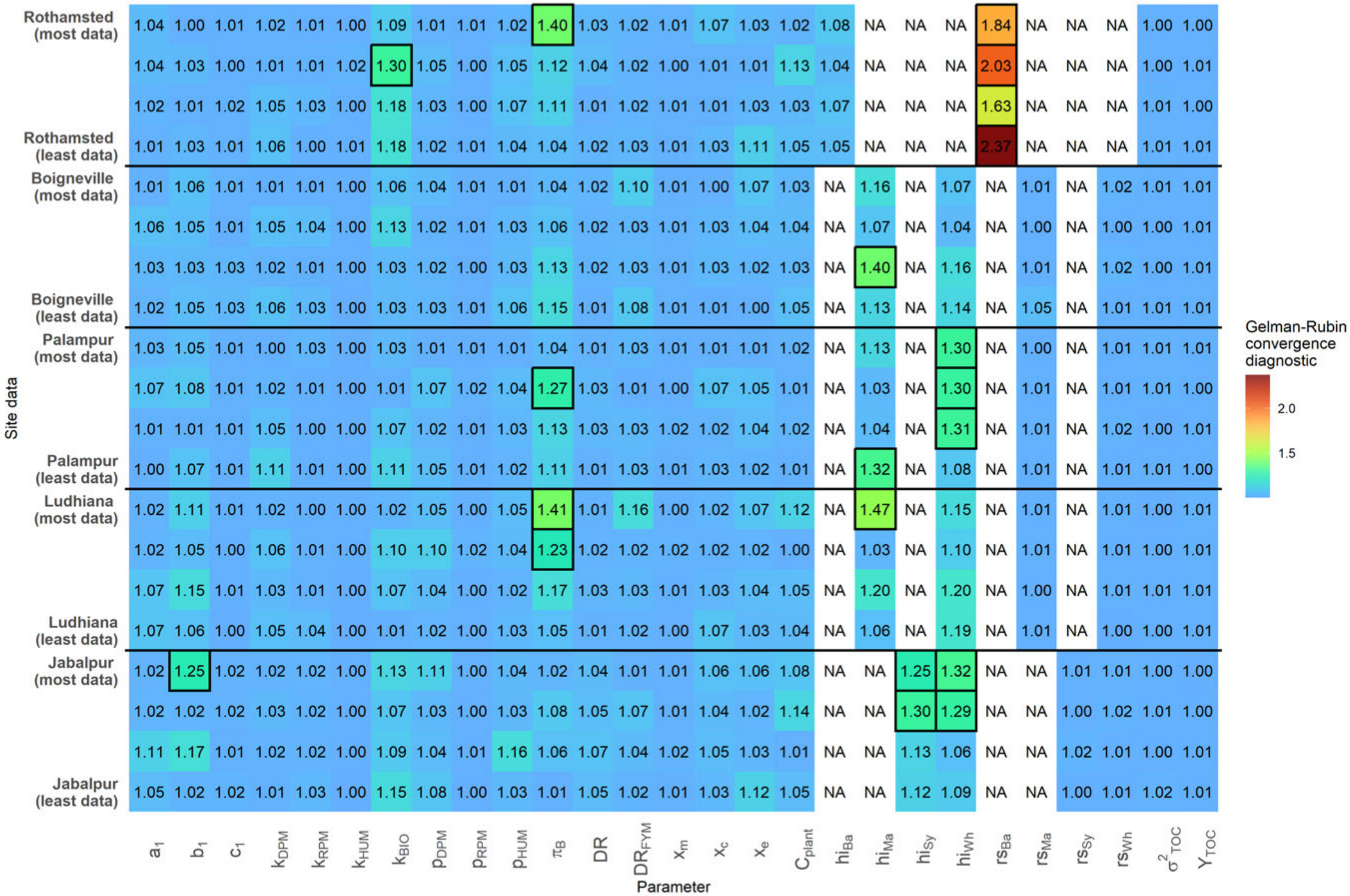

Figure 4.1: Gelman-Rubin convergence diagnostic values across four chains for each site and data subset. NA: parameter not modelled. Black boxes: values > 1.2. Parameters: a_1: temperature rate modifier, b_1: moisture rate modifier, c_1: soil cover rate modifier, k_i: pool *i* decomposition rate, π_B: BIO part of BIO:HUM split, π_H: HUM part of BIO:HUM split, DR: DPM:RPM for plant inputs, DR_{FYM}: DPM + RPM for FYM inputs, x_i: CO_2 rate coefficients, C_{plant}: plant C content, rs_i: crop root-shoot ratios, hi_i: crop harvest indexes, p_{DPM}: SOC % DPM, p_{RPM}: SOC % RPM, p_{HUM}: SOC % HUM, p_{BIO}: SOC % BIO, σ^2_{TOC}: variance TOC, σ^2_{eTOC}: observation error TOC, Y_{TOC}: initial SOC. Crops: *Wh*: wheat, *Ma*: maize, *Sy*: soybean, *Ba*: barley

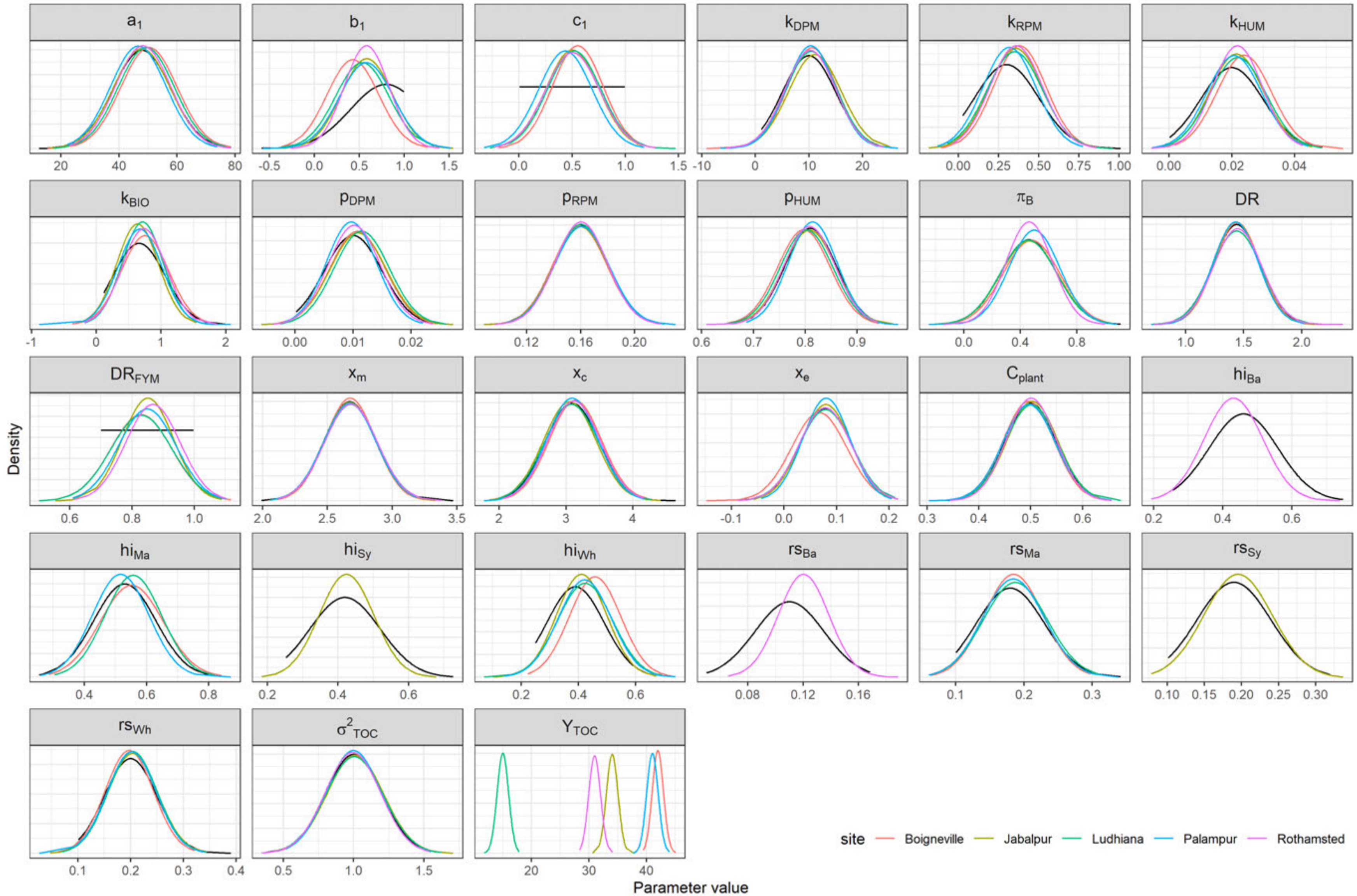

Figure 4.2: BHM parameter posterior distributions for the largest training data subset. Chains combined. Black lines show prior distributions (see Table 4.2). Parameters: a_1: temperature rate modifier, b_1: moisture rate modifier, c_1: soil cover rate modifier, k_i: pool *i* decomposition rate, π_B: BIO part of BIO:HUM split, π_H: HUM part of BIO:HUM split, DR: DPM:RPM for plant inputs, DR_{FYM}: DPM + RPM for FYM inputs, x_i: CO_2 rate coefficients, C_{plant}: plant C content, rs_i: crop root-shoot ratios, hi_i: crop harvest indexes, p_{DPM}: SOC % DPM, p_{RPM}: SOC % RPM, p_{HUM}: SOC % HUM, p_{BIO}: SOC % BIO, σ^2_{TOC}: variance TOC, σ^2_{eTOC}: observation error TOC, Y_{TOC}: initial SOC. Crops: *Wh*: wheat, *Ma*: maize, *Sy*: soybean, *Ba*: barley

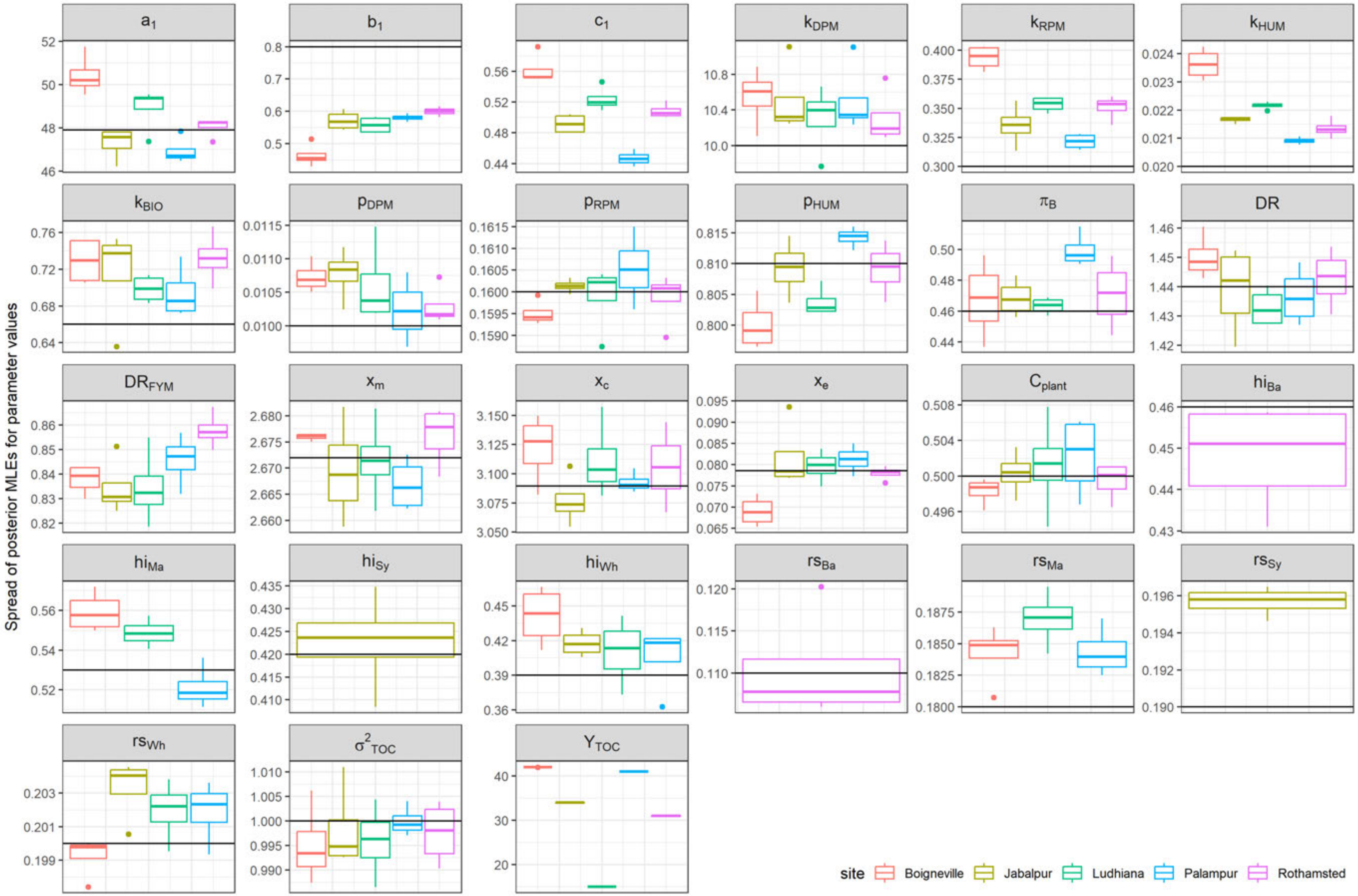

Figure 4.3: Site boxplots for BHM posterior maximum likelihood estimates across training data subsets. Parameter values are shown on the y-axis with black lines indicating prior means (see Table 4.2). Chains combined. Parameters: a_1: temperature rate modifier, b_1: moisture rate modifier, c_1: soil cover rate modifier, k_i: pool *i* decomposition rate, π_B: BIO part of BIO:HUM split, π_H: HUM part of BIO:HUM split, DR: DPM:RPM for plant inputs, DR_{FYM}: DPM + RPM for FYM inputs, x_i: CO_2 rate coefficients, C_{plant}: plant C content, rs_i: crop root-shoot ratios, hi_i: crop harvest indexes, p_{DPM}: SOC % DPM, p_{RPM}: SOC % RPM, p_{HUM}: SOC % HUM, p_{BIO}: SOC % BIO, σ^2_{TOC}: variance TOC, σ^2_{eTOC}: observation error TOC, Y_{TOC}: initial SOC. Crops: *Wh*: wheat, *Ma*: maize, *Sy*: soybean, *Ba*: barley

4.3.2 Bayesian Regression Model

Figure 4.4 shows the model coefficient values for each site and data subset using Equation 4.6. Whilst included in the regression model (Equation 4.6), none of the training data included organic amendments, so these terms are omitted from model outputs. Coefficients have clear between-site differences, and also vary as more training data are used. More data at Rothamsted increased the positive impact of C inputs (FYM and $Crop\ yield$) on SOC, and decreased the impact of time. At Boigneville, the impact of $Crop\ yield$ on SOC has a negative MLE, increasing with additional data, whilst the $Year$ coefficient gets increasingly positive. Overall, coefficients for Ludhiana and Boigneville are significantly more constrained than for other sites. This may be because these two sites did not have FYM in their treatments, reducing the number of modelled parameters.

Figures 4.5-4.9 show BRM predictions for each site through time, with one plot for each treatment/training data subset combination. The measured data are also plotted, with standard deviation from the mean (SD) shown where this data was available. In most cases, the trajectory of the BRM predictions is similar for all training data subsets. Across sites, it seems that more training data are beneficial for short term future predictions, but not necessarily for long-term predictions or those for unseen treatments. In some cases, the smaller training data subsets yield prediction intervals that successfully include future measured data, but additional training data drives a narrowing of the model prediction interval that leaves some data outside of its range. This is true for NPK_Jab, NPK+FYM_Jab (Figure 4.6) and NPK_Lud (Figure 4.7).

As might be expected, the BRMs sometimes perform worse on unseen treatments compared to those they were trained on. The Ludhiana BRMs (Figure 4.7) were not trained on the treatment including FYM, resulting in no useful coefficient to predict the FYM treatment. Predictions from these linear BRMs typically diverge from observed SOC data over time: they are more reliable for short term prediction than long term prediction.

The BRM was trained on the most treatments (and data) at Boigneville, and in most cases the linear prediction is reasonable. However, one main difference between treatments in Boigneville is tillage, and this is not reflected in the BRM structure. Given the absence of FYM, this means that, for a given year, the predictions between treatments at Boigneville can only vary due to crop yield. Nevertheless, the most constrained prediction intervals are associated with the Boigneville site (Figure 4.5). Conversely, the long timescales over which the sparse Rothamsted SOC training data was gathered leaves greater model uncertainty over the trajectory of SOC (wide prediction intervals) and a generally poor prediction.

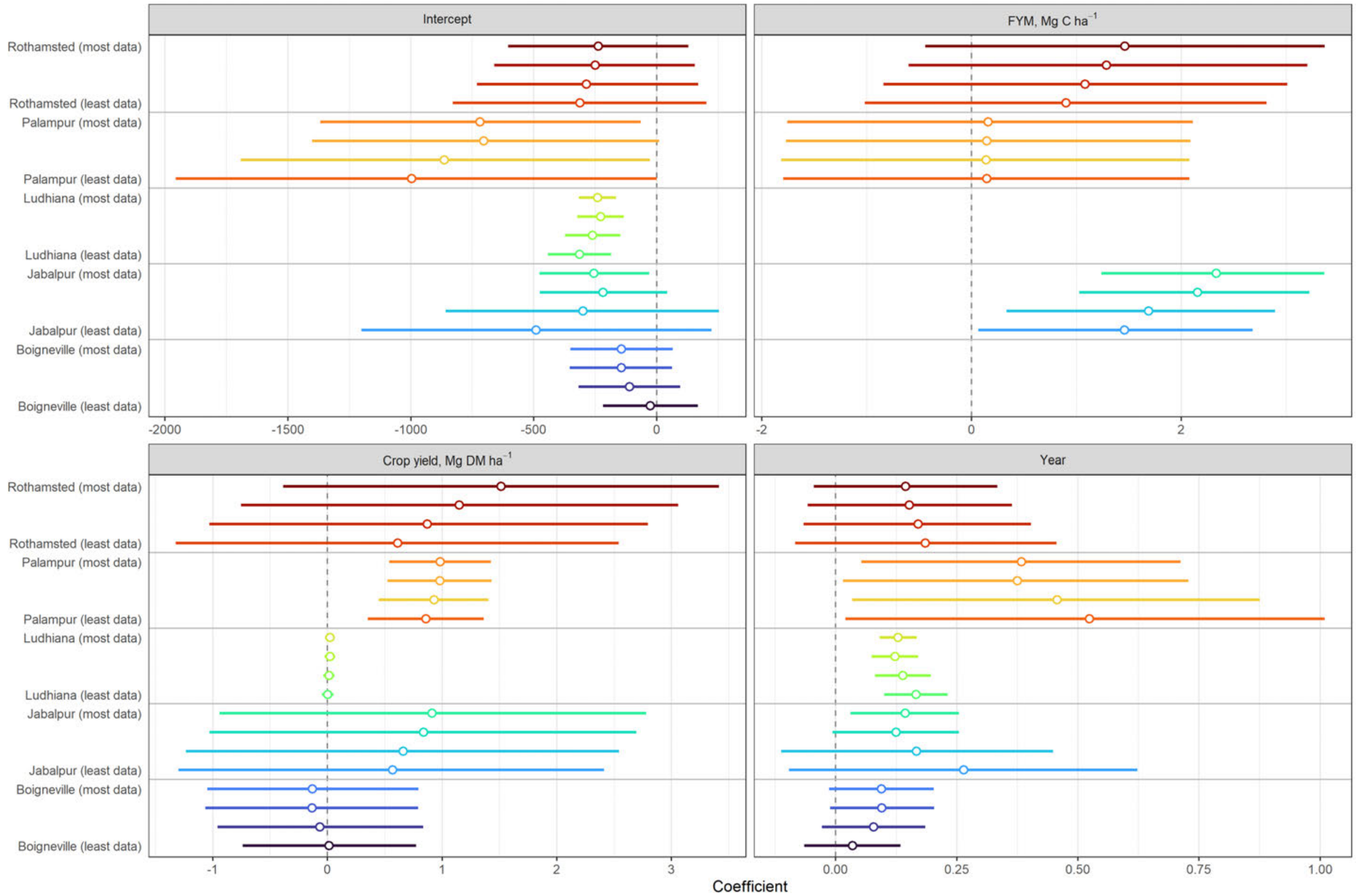

Figure 4.4: Coefficient values for each BRM, 95% credible interval. Coefficients are not shown where the training data did not include any values for that variable- specifically FYM for both Boigneville and Ludhiana (which was trained on Nil and NPK treatments).

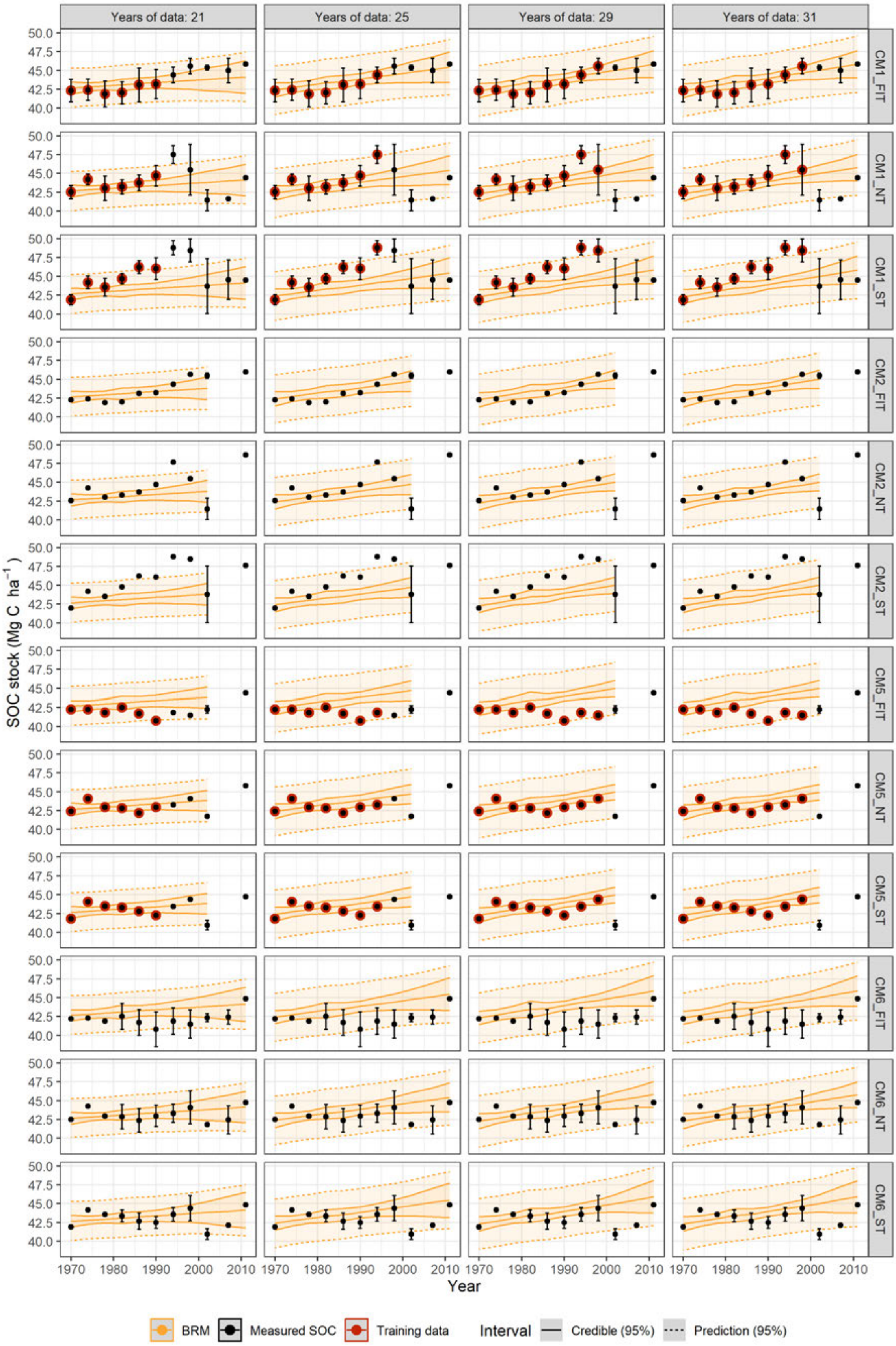

Figure 4.5: Predictions from BRMs given different training data subsets for Boigneville. Prediction and credible intervals of the model are shown. The standard deviation of measured data is shown where this was available.

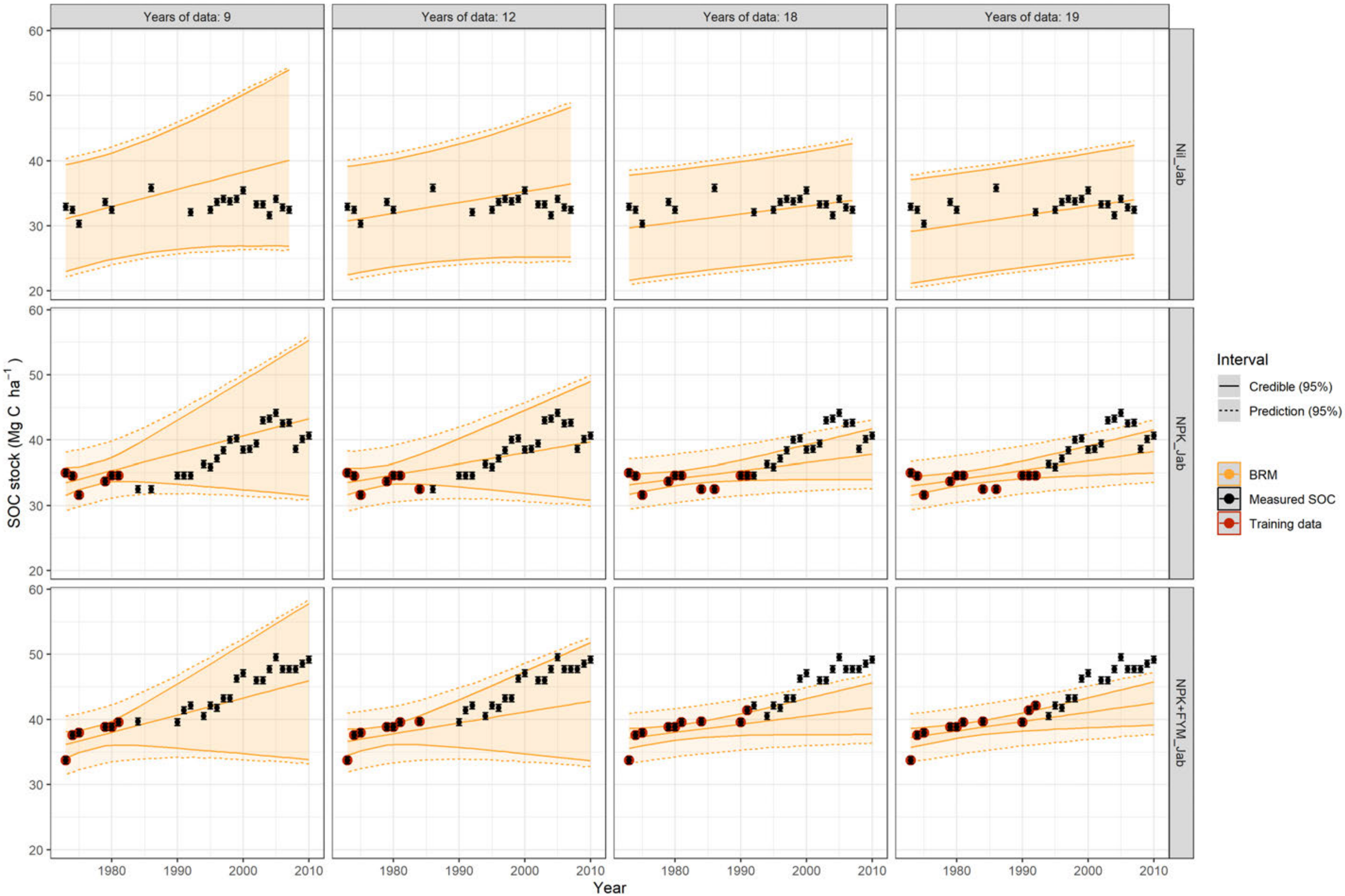

Figure 4.6: Predictions from BRMs given different training data subsets for Jabalpur. Prediction and credible intervals of the model are shown, $\pm$ 1 standard deviation of measured data is shown where this was available.

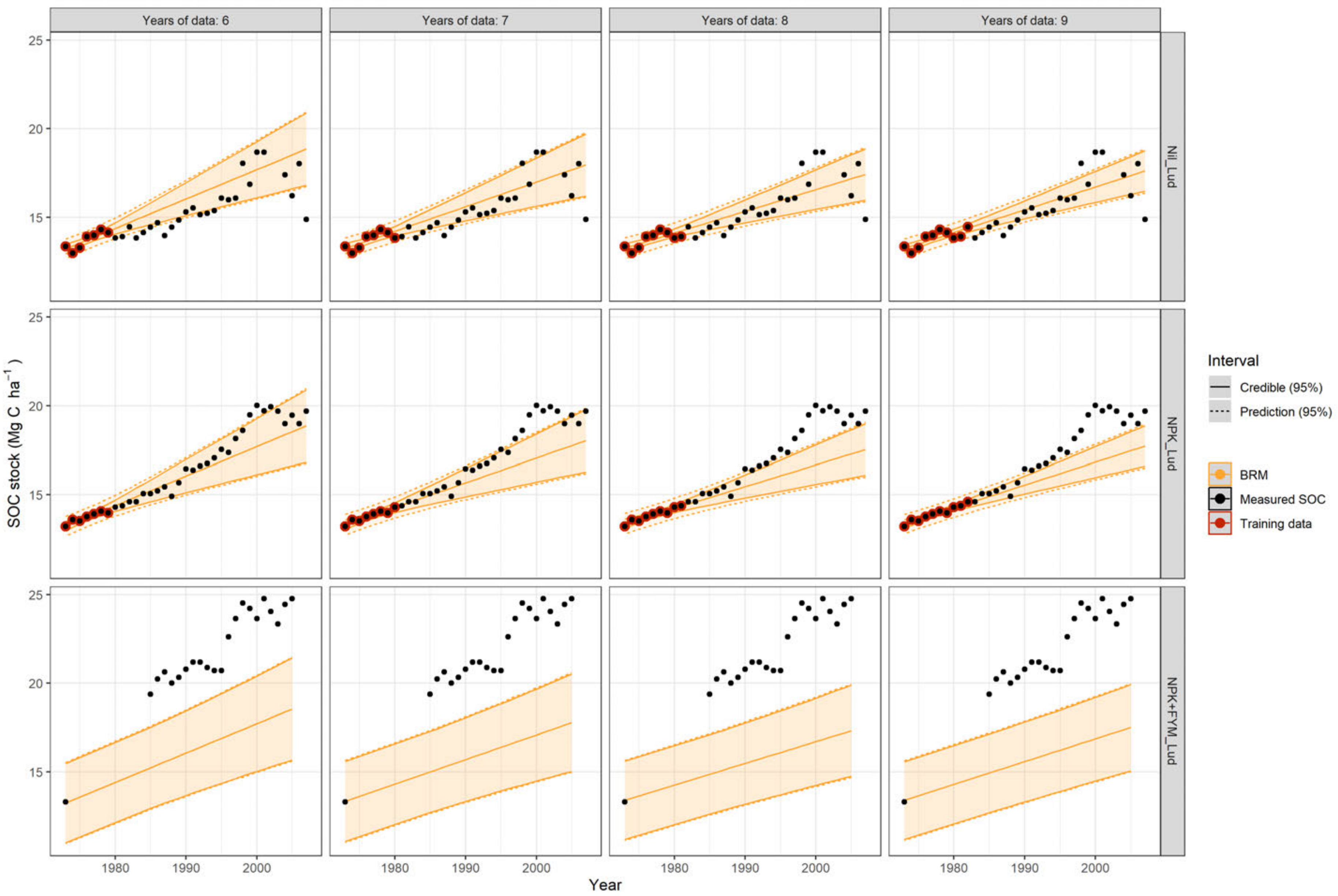

Figure 4.7: Predictions from BRMs given different training data subsets for Ludhiana. Prediction and credible intervals of the model are shown. Note: the standard deviation of measured data was not available for this site.

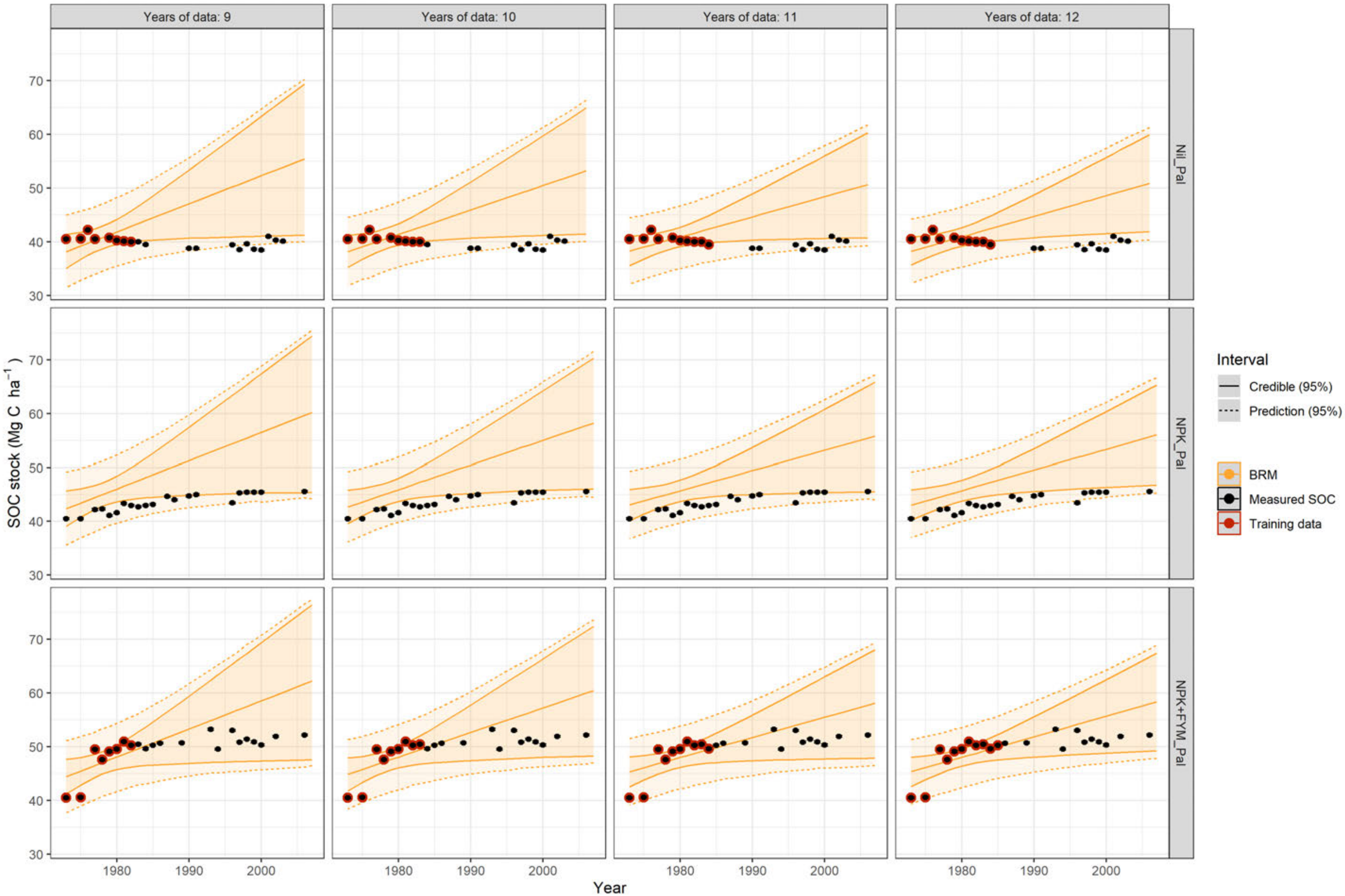

Figure 4.8: Predictions from BRMs given different training data subsets for Palampur. Prediction and credible intervals of the model are shown, $\pm$ 1 standard deviation of measured data is shown where this was available.

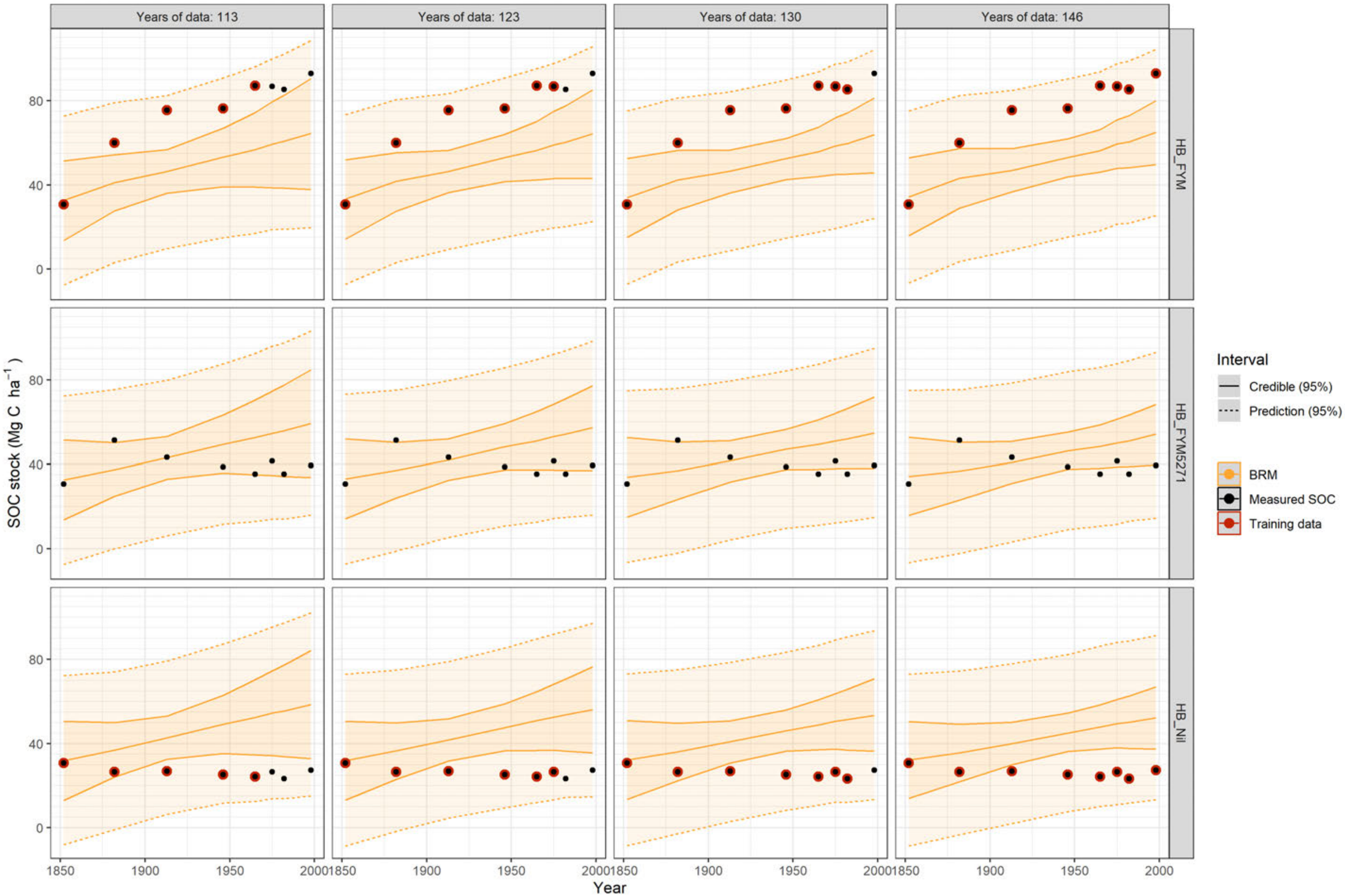

Figure 4.9: Predictions from BRMs given different training data subsets for Rothamsted. Prediction and credible intervals of the model are shown. Note: the standard deviation of measured data was not available for this site.

4.3.3 Model comparison

The three models used here have significantly different approaches, but are all intended to help predict SOC change over time. The RothC model uses only one SOC value to initialise, whereas the BHM and BRM are trained on sparse observed datasets. Figures 4.10-4.14 compare all three models for each site in turn. Note that y-axes are different for each treatment.

As seen in Chapter 3, the ability of the RothC model to predict SOC stock changes over time varies significantly between sites. For some treatments at Boigneville, RothC's prediction at the end of a 42 year run is a 75 % increase in SOC stock, where observed values show a roughly 10-20 % increase. RothC seems to have greatest capability for predicting SOC change when there are fewer sources of extra C, i.e. the Nil treatments. These results, combined with the higher posterior estimates for decomposition parameters, suggest that RothC overestimates C retention from inputs.

For Rothamsted, Jabalpur, Ludhiana and Palampur, the BHM prediction does not diverge significantly from the RothC prediction. At Boigneville, the BHM prediction is much more different from RothC and a better prediction for the measured data. Further, the BHM prediction interval is narrower. Due to having more treatments, the Boigneville training datasets were larger than those for other sites. This is likely to contribute to the stronger predictive capability of the trained models. In addition, the Boigneville site had measured data at 3-5 year intervals, where Ludhiana and the other Indian sites had some stretches of annually measured SOC data and Rothamsted measurements were decadal. The modelling outputs are affected by the frequency of SOC measurements used as training data.

Except for Rothamsted, the 95% prediction intervals for the BHM approach are consistently wider than those for the BRM and all observed SOC values are within the 95% PI for the BHM predictions. On the other hand, of the three models, the BRM often provides the closest central prediction to measured SOC values.

The results for Rothamsted are different from the other sites as the RothC model predicts the change in soil C most accurately (Figure 4.14). This is likely driven by an accurate description of the added FYM carbon in RothC in terms of allocating its composition to RothC pools. However, the lack of improvement by BHM or BRM is worth examination. The relatively poor BRM performance suggests that a linear model is not useful over the much longer time horizon of the Rothamsted data. The BHM for Rothamsted shows the greatest lack of convergence (Figure 4.1) and took longest to complete, which indicates that the RothC prior was difficult to improve upon using this dataset.

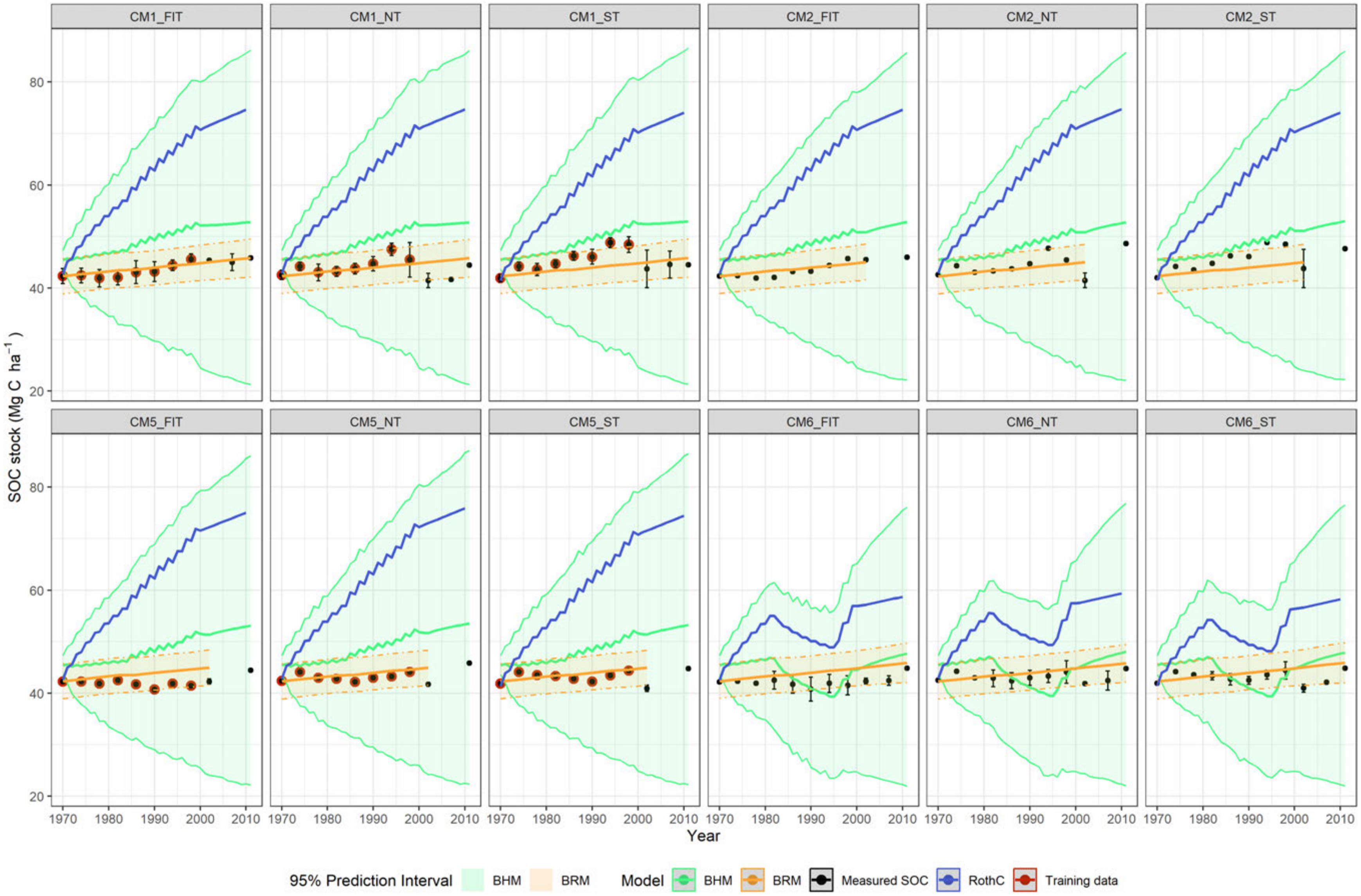

Figure 4.10: Model predictions from RothC, BHM and BRM compared to measured data at Boigneville, split by treatment. The subset of observations used to train the BHM and BRM are circled in red: this plot shows the models with the largest amount of training data. The standard deviation of measured data is shown where this was available.

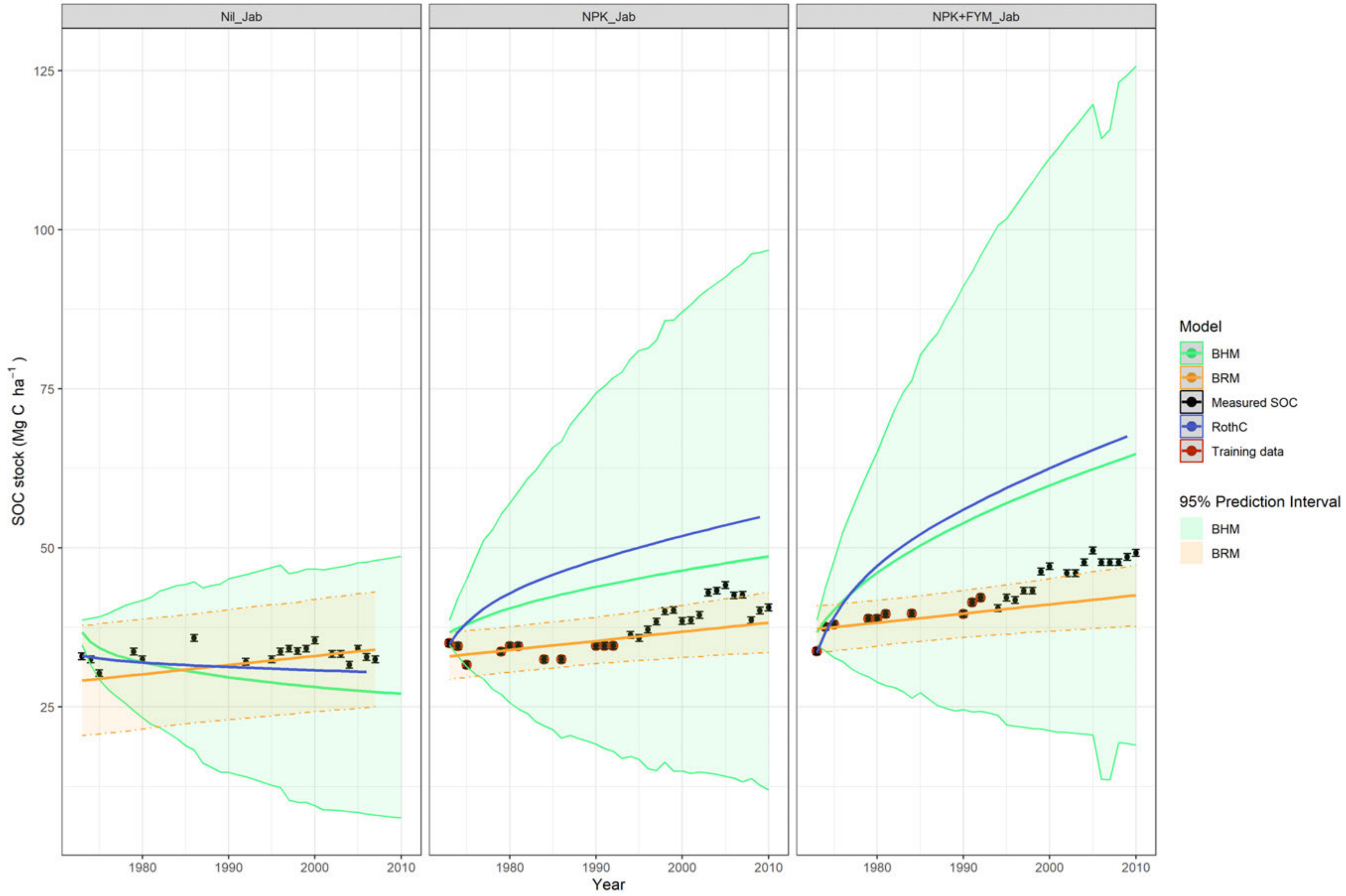

Figure 4.11: Model predictions from RothC, BHM and BRM compared to measured data at Jabalpur, split by treatment: this plot shows the models with the largest amount of training data. The subset of observations used to train the BHM and BRM are circled in red. The standard deviation of measured data is shown where this was available.

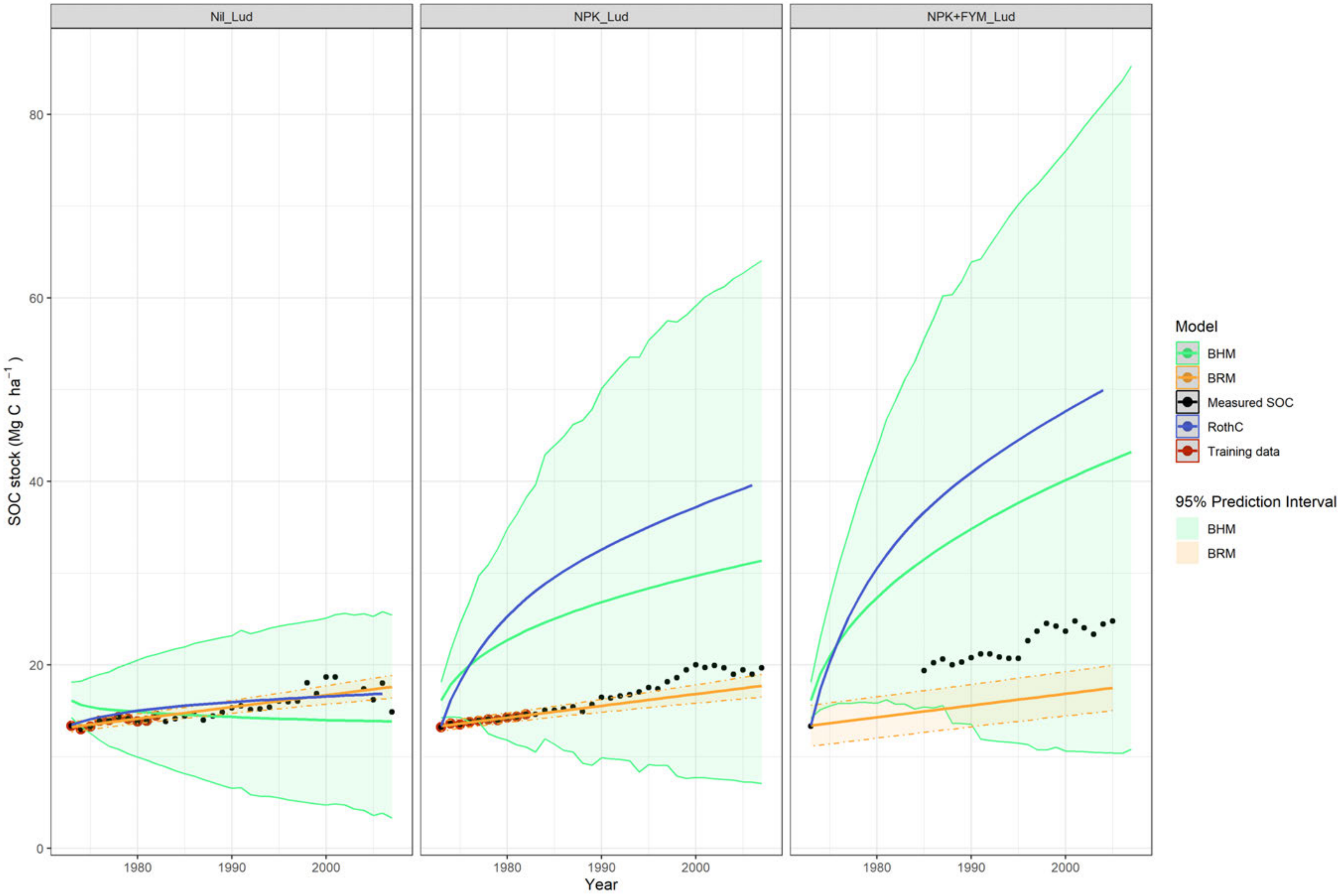

Figure 4.12: Model predictions from RothC, BHM and BRM compared to measured data at Ludhiana, split by treatment: this plot shows the models with the largest amount of training data. The subset of observations used to train the BHM and BRM are circled in red. Note: the standard deviation of measured data was not available for this site.

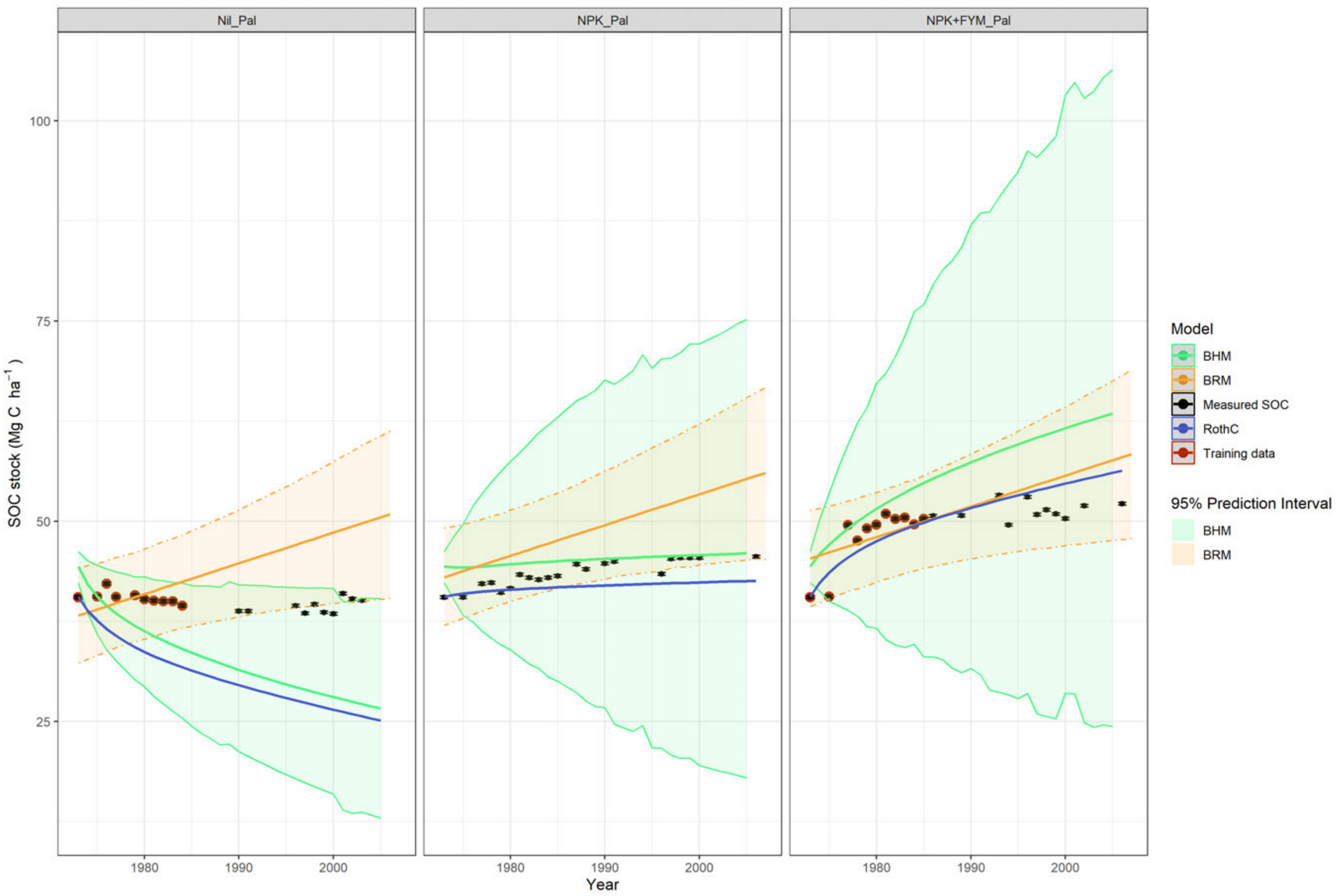

Figure 4.13: Model predictions from RothC, BHM and BRM compared to measured data at Palampur, split by treatment: this plot shows the models with the largest amount of training data. The subset of observations used to train the BHM and BRM are circled in red. The standard deviation of measured data is shown where this was available.

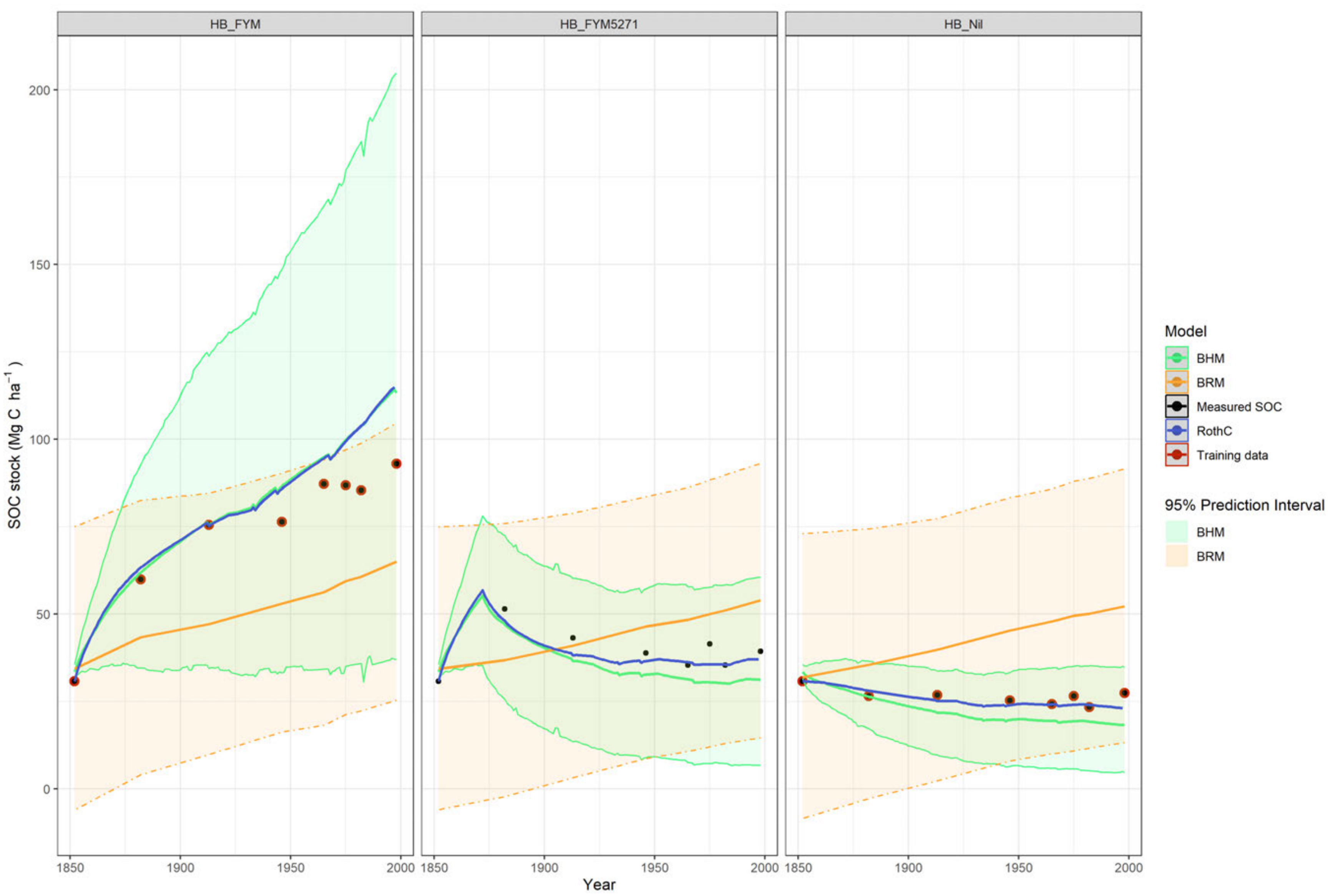

Figure 4.14: Model predictions from RothC, BHM and BRM compared to measured data at Rothamsted, split by treatment: this plot shows the models with the largest amount of training data. The subset of observations used to train the BHM and BRM are circled in red. Note: the standard deviation of measured data was not available for this site.

4.4 Discussion

Prediction of soil C change over time in managed landscapes is challenging because drivers span microscopic to global scales (Wiesmeier et al., 2019). Capturing all these drivers in a single model that is generic enough to be applied to a broad range of settings is unlikely. Whilst it is also infeasible to rely solely on direct measurement as a means of understanding soil C (Bradford et al., 2023), small datasets could be useful to calibrate soil C models to more local conditions. Given the uncertainty in both model parameters and measured training data, Bayesian methods are a sensible choice for combining soil C models and data (Davoudabadi et al., 2021).

I used time series soil C data from five sites to train two Bayesian models. The sites varied in environment, climate and management, as well as the patterns of soil C data collected. Minimal subsets of the data were used to train the models, with the aim of identifying minimum data requirements to undertake the model training process. This analysis cannot make global conclusions from the small sample of site-level results, but can further the discourse on the value of process-based models, model-data assimilation and soil C measurement protocols.

4.4.1 Model predictions

The RothC process-based model overestimated soil C accumulation across most treatments, with the majority of exceptions being treatments with no non-crop inputs (mineral or organic). Thiagarajan et al. (2022) also observed this at Canadian sites. The RothC defaults were the BHM priors, and this remains evident in the BHM posterior distributions and prediction: the BHM typically shows a similar prediction to RothC, whilst calibrated to be somewhat closer to the observed soil C levels. The BHM results suggest that the priors specified were too informative; preventing the data from affecting the parameter values strongly enough to significantly affect the models' predictions. In addition, there were a small number of instances where parameters did not meet the accepted threshold of the Gelman-Rubin diagnostic for convergence across chains. Given that the diagnostic values are proximal to the threshold, it is likely that a smaller set of parameters and/or longer chains of MCMC samples would have been beneficial for clearer convergence.

The posterior BHM distributions suggest that climate-induced topsoil moisture deficit is less influential than RothC suggests across the modelled sites, though some un-modelled irrigation in modelled treatments may have contributed to that conclusion. Evidence that temperature's influence on decomposition rates varies by site might suggest a missing representation of the adaptation of soil microorganisms to hotter temperatures in warmer climates. A more sophisticated function of the temperature response could consider difference in temperature from a locally determined optimum.

Posterior BHM distributions for all sites suggest that RothC underestimates the role of soil cover in slowing decomposition, and underestimates decomposition rates (k) in general. However, this analysis allowed Bayesian calibration of both initial SOC pool proportions (p) and the pool decomposition rates (k). The only methodological step taken to control covariance between these quantities was the use of fairly informative priors. These relationships between parameters should be considered further in future work.

The posterior distributions of RothC parameters have each been informed by one site and directly represent a set of model parameters that best fit the site's data, given the methods applied; including the information in the prior and soil process mechanisms in RothC. Conclusions about the generic RothC parameters and the representation of processes can be tentatively drawn where there are similar posterior distributions across sites. Where parameters have a similar posterior MLE across sites that is different from the RothC default, this could indicate a mechanistic difference and re-calibration suitable for the generic model. Given the variety of climates, soils and management practices covered in this dataset, cases where there is a pattern in direction of change in the MLE from the prior value across sites can also be tentatively identified as mechanistic differences. However, care should be taken in making adjustments to any parameter in isolation. Expanding this analysis to include a wider array of management, environment (including soil type) and climate combinations would benefit any review of RothC defaults.

The BRM linear model is data-led and, of the three models, tended to fit the data best over short predictive periods. This model has no equilibrium or saturation dynamic included and as such would predict soil C accrual forever given a favourable C input level. As for the linear models from Chapter 2, this makes the BRM suitable for use over management timescales for the majority of arable soils that are at a soil C deficit (Six et al., 2024), but not suitable for long-term prediction. BRM predictive capability in untrained treatments was variable and the coefficients in the were somewhat uncertain (Figure 4.4), with some credible intervals crossing zero. Whilst increasing the amount of training data was rarely detrimental to the uncertainty of a given coefficient, it is notable that in many cases the credible interval did not get narrower with additional information. Across all coefficients, the Ludhiana BRM had the narrowest credible intervals, though this was not reflective of better predictive capability (Figure 4.7). In particular, the Ludhiana BRM could not model the impact of FYM, an additional organic C input, since it was not trained on this treatment. For decision support, this is a critical limitation of the BRM approach: the model has no scope to represent treatments for which it has not been trained.

Applications of the BRM approach are limited to short and medium term predictions of soil C stocks for treatment types and sites for which a model has been trained. Through coefficients, BRMs can give insights on the relative importance of different factors for managing soil C at the site, as well as the uncertainty associated with that conclusion (Figure 4.4). Therefore, it is best suited to considering changes associated with new combinations of practices the model has been trained on.

Comparing the models shows that central BHM predictions were often better than RothC but not as good as the BRM. None of the models were reliable over multi-decadal time horizons. The BHM's wide prediction intervals consistently include all the data in a way not matched by other models; better representation of uncertainty is a strength of this method.

4.4.2 Soil C data collection

Where data was available, SDs of measured SOC data indicate the uncertainty in measured data. At Boigneville, the uncertainty of some measured data was of a similar magnitude to the prediction uncertainty of the BRM, and the BRM prediction interval always overlapped with $\pm$ 1 SD of measured data. This observation uncertainty is a key consideration for the measurement and use of SOC data, as the variation between measured values can be greater than the change in mean SOC stock. For example, the data at Ludhiana was collected roughly annually in the training data subsets. Despite being relatively small, some of the implied year-on-year changes in SOC stock would be hard for a model to explain and predict, showing abrupt, sporadic changes in direction despite no significant changes in management (see Figures 4.7 and 4.12). On the other hand, the less than decadal measurement frequency at Rothamsted (see Figures 4.9 and 4.14) is too rare to capture the level of SOC stock change that is of interest to land managers, though it is well predicted by RothC. The poor predictive capability of the BRM at this site suggests that other factors are influencing the SOC stock at this temporal resolution.

Overall, annual measurement of SOC stock change focuses on short term fluctuations which are likely dominated by drivers such as weather, whilst decadal measurement of SOC stocks highlights the impact of long term drivers such as the climate. Both of these are hard (or impossible) for a land manager to affect, and challenging for a SOC model to predict if the modelled scope does not explicitly include these drivers. Measuring SOC stock every 3-5 years, as was done at Boigneville, is recommended for capturing the impact of management on soil. The empirical modelling benefit of this is exemplified by the relatively strong predictive capability of both Bayesian approaches at the Boigneville site.

Modellers would usually expect that a larger training dataset would improve a model's predictive capability (Fer et al., 2018). However, in both BHM and BRM, more data did not always help predictions and sometimes worsened long-term predictions and prediction intervals (e.g. Jabalpur, Figure 4.6). The BRM coefficients were rarely better constrained (Figure 4.4) and the BHM convergence actually sometimes got worse with more data (Figure 4.1). However, both BRM and BHM perform best at Boigneville, where they were trained on most data because of a greater number of treatments. Relative to the other sites, the Boigneville dataset has more treatments - therefore more data - and a preferable frequency of SOC measurement data. It is difficult to identify how each of these dataset characteristics contribute to the better model predictions. Overall, it is clear that predictions are closer to observed SOC stocks where the model has been trained on the treatment; particularly the combination of C inputs present. Taken together, these results suggest that training the model on a variety of treatments is more beneficial for predictive capability than additional time-series data on a small number of treatments.

4.4.3 Summary of implications for decision support and carbon accounting

- Models
  - Across sites, default RothC parameters underestimate overall decomposition rates and the importance of soil cover for moderating decomposition. The known omission of irrigation data and the broad approach used to describe FYM is a factor in this conclusion, but underestimation of decomposition is reflected across sites and treatments, demonstrated by the BHM posterior distributions.
  - There is potential for Bayesian methods to combine existing soil C models and measured data for field scale predictions, but more attention is needed to develop a globally robust approach with reasonable computation resource requirements.
  - A data-led empirical model can outperform process-based methods. However, the between-site differences in BRM coefficients show no scope for a global baseline regression model of this structure. Therefore the BRM cannot exist without training data: it is not suitable for soil C predictions in the absence of historic site data.
- Measurements
  - Whilst there is variation in model predictive ability, no model reliably predicts soil C over decadal timescales and across sites. However, for these sites, results do align with existing guidance that annual soil C time-series can be too noisy and that measurements every 3-5 years are best for monitoring and modelling (Farm Net Zero, 2021; Spencer et al., 2011; Verra, 2023)

- 12 soil C measurements is sufficient for training models, and greater benefit is found when there are more treatments included than longer time series.

4.5 Conclusion

Default SOC models often fail to reproduce observed patterns of SOC stock change over time at specific sites. This reduces the reliability of model outputs for farmers and land managers, and has been acknowledged by MRV protocols through new mandates to validate models with measured data. Assimilating data into model predictions offers an opportunity to calibrate models for a particular site and can better represent combined measurement and model uncertainty.

Using 12 or more soil C measurements to calibrate RothC for a site using a BHM PMMH approach improved predictions of soil C change. However, the improvements in this analysis were limited and the computational efficiency of the implementation was poor. These could potentially be remedied by less informative priors and longer MCMC chains, and code improvements, respectively.

A BRM based on a minimal amount of existing knowledge and giving more weight to the measured data typically provided a further prediction improvement on both RothC and the BHM. This model was rapidly generated in R, but requires training data for a given site and management to generate the model (unlike the other two methods that included process-based state-space models).

Overall, the results shown here indicate that the use of measured data in SOC modelling improves predictive capability over the short term, but none of the implemented methods reliably predicted longer term evolution of SOC stock. To best enable model-data assimilation methods to represent the impact of management on SOC, measurements should be taken at intervals of several years and include as many management combinations as possible.

Uncertainties in SOC prediction remain high. Future work should hone model-data assimilation methods for soil C prediction at field scale and develop practical protocols for both soil C measurement and for revision of existing predictions given new data.

Chapter 5

Discussion: what next for cropland soil C management?

Given challenges in measuring soil C including cost, inaccuracy and variability, soil C models offer an opportunity for quantitative decision support at farm level. They can also help us to test and develop hypotheses about the processes governing changes in soil C over time (Le Noë et al., 2023).

5.1 Revisiting objectives

The first three objectives of this thesis were met by Chapters 2, 3 and 4, as summarised below.

1. **Establish useful empirical models for soil C prediction with cover crops as a focus practice**
   Chapter 2 showed that parsimonious empirical models can be established for a single practice choice that both minimise data requirements (including avoiding baseline soil C) and meet key decision support needs such as direction of soil C stock change. The combination of statistical and practical model selection criteria allowed optimisation for explanatory power and user feasibility.
2. **Understand the impact of using public datasets instead of measured data as model inputs**
   Chapter 3 showed that the use of public datasets for non-carbon model input data did not, on average, affect model performance at a site level. The rate of change in soil C is more likely to be adequately predicted than is absolute soil C stock. The ability of RothC to predict soil C over time varied far more by site than by input data source, which means that the model's parameterised processes lack the ability to represent a broad range of agro-environmental conditions.
3. **Explore methods to combine models with site data**
   Chapter 4 indicated that combining data with models is an important priority for research, though none of the tested approaches successfully predicts soil C over decadal timescales. Data relating to a variety of treatments is more effective for calibrating models to predict soil C stocks over management timescales than long time series of data.

This final chapter addresses the final objective to reflect on the implications of the thesis for soil science, land managers and protocols. It draws the work in earlier chapters together and includes next steps for the diverse community interested in soil C modelling at field scale. These include immediate and longer term priorities for farmers, for academics and for policymakers and protocols.

5.2 Improving soil C models

5.2.1 Process-based models need site-level calibration

Process-based soil C models are designed to reflect the latest available understanding of soil functioning and interactions with environment, climate and management. One theoretical benefit of constructing such a model is broad applicability: unlike statistical models, mechanistic models parameterise universal relationships. Chapters 3 and 4 used (process-based model) RothC and showed that more attention to local calibration of the core model is needed to improve site-level predictions (see Figures 3.11, 4.2).

Recent research has drawn attention to the challenges of initialising conceptual soil C pools (Herbst et al., 2018; Klumpp et al., 2017), and in particular the influence of the assumption that the soil C pool is in equilibrium at the start of an experiment (Herbst et al., 2018; Yeluripati et al., 2009), discussed further in Section 5.3.2. Work in this thesis certainly suggests that initialising RothC using an explicit equilibrium assumption (Chapters 3 and 4) does not, on its own, provide reliable calibration to a particular site, particularly in the absence of precise representation of other factors including the impact of fertilisers on NPP, the varied composition of manures and the impact of irrigation on soil water balance and decomposition. The Bayesian Hierarchical Model (BHM) in Chapter 4 used proportions to split initial measured soil C into the RothC pools. However, the inclusion of both pool proportions (p) and decomposition rates (k) in model calibration means that it is not possible to draw conclusions about the validity of this initialisation method. Future work should apply the BHM methods to smaller sets of RothC parameters to address specific questions like this. For example, fixing decomposition rates and allowing pool proportions to vary would be a useful investigation of the common assumption that soil C stock is at equilibrium at the end of spin-up.

The need for extensive site-level calibration suggests that RothC is lacking or misrepresents important processes affecting soil C dynamics. Given persisting unknowns and debates about soil functioning and drivers of soil C change (Baveye, 2023; Derrien et al., 2023), it is perhaps unavoidable that process-based soil C models are limited in reflecting soil C dynamics, and are therefore, regardless of the input data quality, unable to achieve the desired accuracy for all use cases. Attention has been drawn to the shortcomings of soil models based only on either soil physics or soil biology (Baveye, 2023; Blagodatsky

& Smith, 2012), and new evidence supports the importance of microbial dynamics as a driver of soil C change (Dynarski et al., 2020; Lehmann, Hansel, et al., 2020). To improve soil C predictions from process-based models, new processes could be included. However, whilst this could improve central prediction, prediction uncertainty could increase alongside costs of providing the extra data for new parameters (Derrien et al., 2023; Lehmann, Hansel, et al., 2020).

Any changes to models must balance improved accuracy with increased complexity (Blagodatsky & Smith, 2012). Developing the next generation of models is worthwhile for science, but perhaps not for farm decisions. To progress, then, "*model[ling] with intent*" (Lehmann, Bossio, et al., 2020) has two priorities: new approaches to modelling on agricultural management timescales, and calibration of new and existing models to a wider array of agricultural contexts (Baveye, 2023; Garsia et al., 2023; Le Noë et al., 2023).

5.2.2 Calibration needs better soil data

Progress to calibrate and evaluate models requires good time-series data for a broader array of climate, environment, soil and management combinations (Chenu et al., 2018; Le Noë et al., 2023). This means that soil C data collection in managed landscapes is critical, even if it is not sufficient for soil C management. The work in this thesis encountered various widely identified issues with soil C data, including a lack of bulk density measurements and difficulty identifying and accessing time-series data from a diverse range of environments. In Chapter 2, depth of soil C measurement was shown to be explanatory in initial statistical models, despite the application of a recognised standardisation method. This would not have been the case had the standardisation been effective in minimising the effect of soil depth as was intended. As discussed in Section 1.2.2, rigorous sampling of the whole soil profile is needed to clarify the impacts of soil disturbance on soil C stocks. Standardisation of datasets containing mixed sampling approaches may be necessary for analysis, but risks obscuring relationships such as this.

Todd-Brown et al. (2022) highlight the large volume of existing soil data that remains underutilised due to difficulties with access, interpretation and collation of multi-source data, and propose tools including community data practices and vocabulary to break down some of these barriers. In order to tackle prevailing challenges in soil science and modelling, all data producers and managers should recognise the potential of their soil data as a contribution to larger syntheses, whether they are involved in utilising existing data or collecting new data. Important efforts are underway to consolidate soil data (Todd-Brown et al., 2022), but more data from agricultural and managed systems is needed (Malhotra et al., 2019). To this end, data sharing, which has gained traction in scientific communities in recent years (Lawrence et al., 2023), is a priority. The FAIR principles (Findable, Accessible, Interoperable and Reusable) for data management and stewardship were developed collaboratively to lend clarity to this process and ultimately benefit progress towards key goals (Wilkinson et al., 2016). Responsible collation, labelling and sharing of soil C data broadens the range of agro-environmental scenarios available for model calibration, and simultaneously distributes the costs of this endeavour between different stakeholders (Lawrence et al., 2023). For broadest impact, farm data should be included, with due consideration for farmer privacy (Paustian et al., 2019).

5.3 Implications for decision support

5.3.1 More accessible and accurate field scale modelling is possible, for some applications

Farmers must balance multiple factors in making management decisions, and soil C has to take its place amongst them. Requirements for carbon crediting schemes must be stringent, but, as Phelan et al. (2024) highlight, meeting them may not currently be a key motivator for decisions on farms. Therefore, for many land managers, accurate projections of soil C stocks through time are not necessarily required. Likely direction of soil C change is critical information for soil C management, more so than accurate soil C stock values. In Chapter 2, in order to select a model that was able to capture the potential for negative soil C stock change, we had to combine statistical and practical selection processes. The selected empirical model, based on cover crop above-ground biomass, reflected known drivers of soil C change and highlights the importance of successful cover crop establishment as a precursor for soil C accrual. Combining statistical and practical model selection methods yields methods that are scientifically credible and useful to data-restricted land managers.

Chapters 2 and 3 demonstrated that prediction of rate of change in soil C stocks is less elusive than prediction of absolute stocks. Simple empirical models can predict rates of soil C change with sufficient accuracy, avoid the need for baseline soil C and use estimated input data. While use of reference soil C stock values in RothC meant that absolute stocks through time did not match measured values, it did not have a deleterious impact on predicted rates of soil C change, and could be used to compare different management options. However, use of a rate of change omits equilibrium and saturation dynamics and can therefore be misleading over longer timescales (Jensen et al., 2022).

Decision support tools based on models and data like this may be sufficient for farmers who do not need to accurately quantify stocks of soil C for outcome-based schemes. Indeed, work in this thesis suggests that it is possible to get relevant information to support some decisions using simple methods with low data cost. Applications for these simpler methods include policy level scenario planning and target identification, where measured field-level data is not accessible. However, in cases where the end goal is to set up outcome-based projects, conclusions from such high level estimation would need to be confirmed at local level and with well-calibrated models. Choosing soil C prediction methods and how to apply them to support decisions must include confirming that the outputs can safely be used as evidence in the given decision context.

5.3.2 Predictions are materially affected by model implementation choices, potentially more than input data

Prioritisation of accurate input data is understandable in work aiming to improve and validate soil C models. However, Chapter 3 indicates that focusing on improving the accuracy of input data to the exclusion of other choices associated with model implementation is misguided for applying existing models for soil C prediction at field scale.

In every application that stretches the use of data or a model, for example using measured data for model input values that were defined in the abstract, additional assumptions and approximations are made. Further, in the case of soils, a heterogeneous landscape is represented as homogeneous. As in Chapter 2, in Chapter 3 the reported soil C data from Foster et al. (2020) were converted to soil C stocks and standardised to a specific depth. The plant residue inputs were optimised for the resulting initial soil C value using RothC, with the assumption that the initial soil C was at some equilibrium.

On the other hand, in Chapter 4, the data were not standardised and the plant residue inputs were determined using yield data (i.e. changes in NPP were included). The initial RothC pool values were determined using proportions. Broad conclusions about RothC are that it is not always accurate at a particular site. However, at first glance, further findings in Chapter 3 and Chapter 4 diverge. Chapter 3 suggests that RothC (given measured initial soil C) tends to underestimate rates of change. Chapter 4, meanwhile, suggests that RothC tends to overestimate rates of change. These conclusions are linked to the representation of C inputs in the model implementation. Since Chapter 3 does not include changes in NPP, whilst Chapter 4 does, the results of Chapters 3 and 4 together suggest that RothC is prone to overestimating the soil C accrual associated with increased C input. The posteriors of the Bayesian Hierarchical Model in Chapter 4 reflect this in the striking consensus across sites that default RothC decomposition parameters are too low.

Every paper that uses an existing model has had to take decisions about model implementation considering available data. For process-based soil C modelling, decisions on how to model the climate (e.g. Smith et al., 2005; Tao et al., 2023), input C changes (e.g. Gollany et al., 2021; Gottschalk et al., 2010) and initial values of soil C pools (e.g. Klumpp et al., 2017; Wiltshire et al., 2023; Xu et al., 2011) are all necessary and led by the objectives of the study. Chapter 3 highlights that potential productivity changes must be estimated for RothC to be able to represent the impact of mineral fertilisers; this is a particular precursor for studies aiming to compare the relative impact of organic and mineral nitrogen. The widespread equilibrium assumption that is used in initialisation is more often practically convenient rather than scientifically supported, as there is consensus that few managed soils are in equilibrium (Klumpp et al., 2017; Wutzler & Reichstein, 2007).

Given the findings in this thesis that model implementation choices have greater impact than reasonable input data choices, further work should be done by measuring, reporting and verification (MRV) protocols, in collaboration with modellers, to provide guidance on best practice for initialisation and implementation assumptions in soil C modelling for a given objective.

5.3.3 The need to (re)set expectations around uncertainty

The uncertainty in quantifying and modelling soil C stocks is an issue of risk for management decisions and outcome-based incentives such as carbon credits. Better representation of uncertainty levels is important and has three main components: uncertainty in data, in model structure and in model parameter values. Rationalising, quantifying and representing the different sources of uncertainty remains a challenge and is insufficiently represented in MRV protocol guidance (Lavallee et al., 2024). This thesis contributes to these considerations in several indirect ways. Firstly, Chapter 2 is an example of minimising data uncertainty through parsimony and choosing measurable quantities. Secondly, Chapters 2 and 3 suggest that field level predictions of rates of soil C change can be better constrained than predictions of soil C stock over management timelines, and may not need baseline soil C data. Third, Chapter 3 shows secondary data can be reasonable substitutes for primary input data. These secondary datasets have some advantages compared to sparse field data, as overall biases and errors can be identified and quantified. Finally, results in Chapter 4 highlight that annual measurement of soil C is counterproductive for model calibration, since the pertinent drivers of change at this scale are not generally management related and measurement uncertainty is larger than the implied stock change.

The Bayesian methods in Chapter 4 address uncertainty more directly. Approaches such as the Bayesian Hierarchical Model (BHM) in Chapter 4 can estimate all three sources of uncertainty and should, therefore, be investigated further. The BHM outputs in Section 4.3 show widening uncertainty over time (heteroskedasticity), with very large prediction intervals after 10-20 years. Many readers would be dissatisfied with such wide prediction intervals. However, whilst reducing uncertainty in field-scale soil C prediction is important, fair representation of and guidance on uncertainty is more so. Wide prediction intervals do not directly imply lack of understanding; the functional complexity of soils is not fully represented in simpler process-based models (Lehmann, Hansel, et al., 2020) and quantified uncertainty helps to capture this as part of any assessment. Meanwhile, continuing discussion to unpick drivers of wide prediction intervals helps to highlight priorities for data collection and model improvement.

5.4 Data vs theory

As discussed in Chapter 1, the impacts of cropland management on soil C stocks are driven by complex interactions of soil, environment, climate and land use. Whilst soil science has been able to clarify many of the relevant processes and interactions, others remain unclear. Indeed, the recent focus on soil biology as an influence on soil C change patterns could perhaps lend weight to the view that the complexity of soil C change cannot be accurately described by mechanics alone, much like the prevailing view of ecology (Lehmann, Hansel, et al., 2020).

However, the need to improve soil health and particularly soil C stocks is great and so understanding and estimating potential impacts remains an important endeavour.

Prediction of future soil C change requires some modelling, but should the models be based on soil science concepts, or rather give weight to available measured data? Chapter 4 begins to ask this question, finding that data-led models perform best for management combinations they have been trained on. By including predictor variables, most models include some assumed knowledge about soil dynamics, but this can be minimised using weak Bayesian priors. The disadvantage of data-led models remains the inability to predict the impact of new management action (without further invoking soil science).

From another angle, since existing process-based models are not sufficiently generic to be widely applicable at site level and have not been validated across the diversity of farming contexts (Garsia et al., 2023), the power of a small amount of high-quality soil C data to locally calibrate a model and improve predictions could be significant, given the right statistical methods. Davoudabadi et al. (2021) outlined Bayesian methods to combine models and data and explained how features of these methods tackled challenges in field-scale soil C modelling. Recently, applying Bayesian methods to combine models and data has gained significant interest in environmental sciences (Carrassi et al., 2018), though many efforts have been at broader spatial scales (e.g. Bloom et al., 2016; Luo et al., 2016; Xiao et al., 2014). The family of approaches are variously referred to as model-data synthesis, fusion, integration or assimilation; here, the latter is used, as defined in Chapter 4.

Chapter 4 applied model-data assimilation methods similar to Davoudabadi et al. (2024) to the RothC model. Bayesian calibration resulted in some improvement in prediction, with indications that a weaker set of parameter priors and longer MCMC chains could lead to further improvement. Model-data assimilation does not improve the conceptual representation of the underlying model, but hopefully improves predictions by providing a model calibrated on site-specific information and clearer representation of uncertainty, given appropriate error data (Malhotra et al., 2019). As tentatively indicated by some results in Chapter 4, with enough site-level implementations, model-data assimilation could contribute evidence for altering parameters in default models. Future work should explore the merits of model-data assimilation to unlock the combined potential of data and science for accurate site-level soil C predictions.

5.5 The role of policies and protocols to enable soil C management

Field experiments have shown that additional C input and reduced soil disturbance are generally beneficial for soil C stocks, and rarely detrimental. There is consensus that both soil C and net environmental benefits are not uniform across agro-environmental gradients: soil C storage has limits, it is infeasible to provide exogenous organic C for all agricultural land and some soil C benefits are offset by detrimental environmental impacts such as increased N_2O emissions (Rubin et al., 2023). How can soil C models be utilised to support decisions and action towards a more resilient global agricultural system that works for all life on Earth?

Soil C modelling is relevant in a number of applications, each with their own tolerances and foci. Soil scientists seek to understand more about functioning and dynamics from micro- to macro-scale. Soil carbon credits need to carefully consider additionality, uncertainty and permanence in their quantification. On farm, however, the decision context that models may be part of is broader. The first consideration for any management must be cost: cost to implement, potential changes in yield, changing risk and any financial incentive for which conditions can be met.

Chapter 3 suggested that RothC and the IPCC Tier 1 method were not consistently sensitive to practice change. They both reflected the prevailing broad understanding of soil C change, rather than helping the user to discern between practices in their context. If soil C models draw the same broad conclusions about suggested practices as are already accepted by the community at large and cannot discern untested scenarios then soil C models can add value for those devising practice-based policy recommendations, but do not help at a farm level. At farm level, then, the lower risk is to focus on meeting financial incentive requirements linked with choice of practices (which can be controlled) rather than achievement of outcomes (which can not).

In theory, carbon credits offer an incentive for farmers to choose practices that are expected to accrue soil C by rewarding that outcome. In practice, the complexity around quantification (i.e. cost and risk) and the varied requirements of the programmes are limiting their uptake and efficacy (Black et al., 2022; Davidson, 2022; Phelan et al., 2024). If carbon credits for soil C are to be an effective tool for enabling carbon sequestration, the route to accurate soil C predictions needs to be clear and widely applicable. The signals from farmers are that complexity and uncertainty need to be minimised, and standardised methods established.

In addition, Phelan et al. (2024) found that important considerations about additionality and permanence in carbon credit programmes do not align with farmer expectations in the UK. In particular, they found that almost all farmers who responded to their survey were already undertaking practices that might be expected to sequester soil C, which rules them out of many carbon credit programmes on the basis of additionality. To encourage and enable participation, Phelan et al. (2024) propose a transition period during which farmers already undertaking desired practices are able to engage in carbon credit schemes. Whilst this would challenge the use of equilibrium assumptions in model intitialisation, there are other initialisation approaches which could be used, as discussed previously.

Complexity and uncertainty in soil C modelling have so far hampered use in MRV protocols and outcome-based sustainable agriculture policy (Garsia et al., 2023; Smith, Soussana, et al., 2020). Soil science continues to develop new understanding of soil functioning and C dynamics, and has made important breakthroughs in recent times. This has led to discussion of a "*new generation*" of soil C models (e.g. Abramoff et al., 2018; Baveye, 2023; Berthelin et al., 2022; Caruso et al., 2018; Wieder et al., 2013) to try and better capture the diverse multi-scale drivers of soil C change. However, whilst beneficial for broader goals in environmental science and society, developing a new generation of more complex soil C models does not tackle the urgent barriers to accessibility of useful soil C information for land managers (Kanari et al., 2022). The higher costs of greater data collection are combined with the increased uncertainty associated with more complex models in un-calibrated contexts (Shi et al., 2018). Indeed, with the latter, the task of representing agro-environmental diversity intensifies, adding further pressure to data collection. As Baveye (2023) put it, *"after significant effort and a tremendous amount of luck, modellers could stumble on a model whose mathematical structure enables them to fit any set of experimental data on soil carbon dynamics anywhere in the world, but the odds of that happening in time to contribute to the solution of some of the environmental threats facing us at the moment do not seem great"*.

To enable broader access, a better priority is to explore methods to combine existing soil C models with evidence through model-data assimilation, as in Chapter 4. This is a pragmatic route as these methods are an urgent gap in MRV protocols and carbon credit programmes. MDA methods do not themselves expand the data required for carbon credit verification processes, as soil C measurement is already a stated requirement (Lavallee et al., 2024). Bayesian methods that account for the different sources of uncertainty could be used. Development of these methods now, combined with new focus on collating and sharing new and existing soil data, could result in a step change in the availability of calibrated models for accurate soil C prediction at field level. Once established, model-data assimilation methods could also be utilised on the next generation of carbon models.

To achieve the maximum impact of these activities, work needs to be undertaken collaboratively to generate methods that are mathematically valid, usable and useful (Bradford et al., 2023). Data should be shared utilising FAIR principles (Todd-Brown et al., 2022; Wilkinson et al., 2016). Researcher priorities should be led by needs of land managers and policymakers and overall requirements for openness, clarity, consistency, credibility and value for users should be maintained.

5.6 Conclusions

Soil carbon plays an important role in functioning ecosystems and so supports biodiversity and food security on Earth. For resilience against a changing climate, agricultural land managers should seek to protect and increase their soil C stocks. Some of these actions sequester carbon in soils and so can also be said to mitigate climate change.

How farmers and land managers can best manage their soil C remains context specific, meanwhile rigorous measurement of stocks remains prohibitively costly. Models that can predict change in soil C have an important role to play. Whether to give simple indications of direction of change or precise predictions of soil C stock evolution, accuracy of and quantified uncertainty in predictions is a key consideration.

This thesis examined how models can be used to support decisions about soil C at field scale. Simple empirical methods can be effective for indicating drivers of soil C storage and direction of change, but are not suitable for predicting absolute soil C stocks. Existing process-based models do not provide accurate predictions of soil C stocks unless calibrated to the context.

Soil scientists are discussing a new generation of models that will further improve understanding of soil dynamics and hopefully improve accuracy, but these will not tackle access issues for land managers. A worthwhile focus is statistical methods that combine theory with data to improve model usefulness at temporal and spatial scales relevant to management.

Appendix A.1

Appendix: Supplementary information for Chapter 1

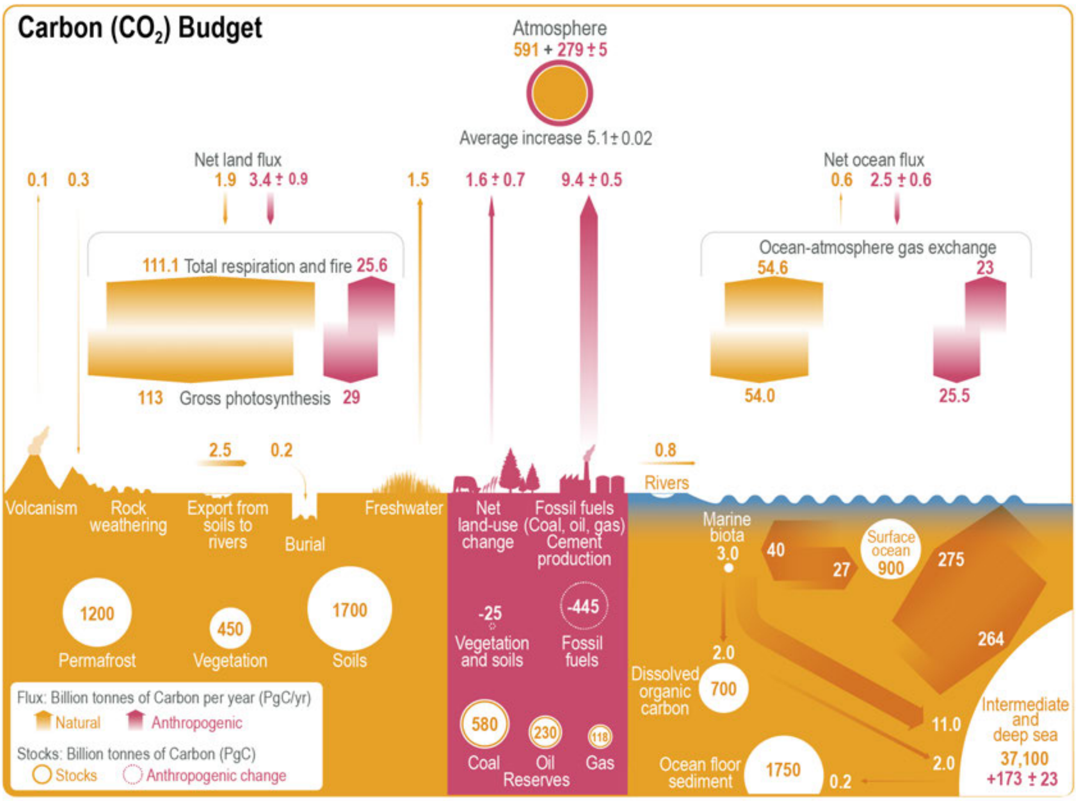

Figure A.1.1: Global Carbon budget (2010–2019), from Canadell et al. (2021)

Appendix A.2

Appendix: Published supplementary information for Chapter 2

Supplementary Table 1: Summary of coefficients for models shortlisted using nested comparison. Values given to two decimal places, or more where needed (indicated with *italics*). Pr(>|t|) given to three decimal places.

	Estimate	Std. Error	df	t value	Pr(>|t|)
M2ri: AEZ & CC C:N ratio					
(Intercept)	1.62	0.45	30.44	3.62	0.001
AEZ: subtropical warm	-1.26	0.49	30.21	-2.56	0.016
CC C:N ratio	0.01	0.01	38.72	1.68	0.101
(AEZ subtropical warm):(CC C:N ratio)	-0.01	0.01	38.89	-1.33	0.192
M2ri: CC season & CC biomass					
(Intercept)	2.7	0.74	57.73	3.64	0.001
CC season: overwinter	-2.47	0.75	53.45	-3.3	0.002
CC season: summer	-1.66	0.93	42.2	-1.78	0.082
CC biomass	0.01	0.09	51.76	0.07	0.948
(CC season: overwinter):(CC biomass)	0.07	0.1	54.25	0.75	0.458
M2r: CC C:N ratio & % clay in soil					
(Intercept)	-1.78	0.55	50.77	-3.22	0.002
CC C:N ratio	*0.002*	*0.004*	36.03	0.57	0.573
% clay in soil	21.29	4.82	52.53	4.42	*4.96×10^{-5}*
M2r: CC C:N ratio & % silt in soil					
(Intercept)	2.73	0.84	25.45	3.25	0.003
CC C:N ratio	*0.003*	*0.004*	36.66	0.81	0.421
% silt in soil	-7.94	3.05	26.03	-2.6	0.015
M2r: Bulk density & CC biomass					
(Intercept)	-3.36	1.52	38.22	-2.21	0.034
Bulk density	2.39	1.06	38.19	2.25	0.03
CC biomass	0.14	0.04	69.93	3.84	0
M2r: CC C:N ratio & MAT					
(Intercept)	3.71	1.62	15.95	2.29	0.036
CC C:N ratio	*0.003*	*0.004*	37.39	0.71	0.481
MAT	-0.19	0.1	15.66	-1.97	0.067
M2r: CC C:N ratio & Experiment duration					
(Intercept)	1.24	0.41	18.96	3.05	0.007
CC C:N ratio	*0.004*	*0.005*	37.08	0.85	0.4
Experiment duration	-0.12	0.06	16.98	-1.87	0.078
M2r: CC C:N ratio & MAP					
(Intercept)	2.05	0.86	17.22	2.37	0.03
CC C:N ratio	*0.003*	*0.004*	37.48	0.74	0.462
MAP	*-0.001*	*0.0008*	16.6	-1.75	0.099
M2ri: CC C:N ratio & Tillage					
(Intercept)	0.74	0.34	25.35	2.22	0.036
CC C:N ratio	0.01	0.01	39.07	1.09	0.284
Tillage: no tillage	-0.05	0.54	25.32	-0.08	0.933
Tillage: reduced tillage	-0.69	0.57	23.28	-1.22	0.235
(CC C:N ratio):(Tillage: no tillage)	-0.01	0.01	38.79	-0.55	0.586
(CC C:N ratio):(Tillage: reduced tillage)	*0.0002*	0.01	38.65	0.02	0.985
M2r: MAP & Soil pH					
(Intercept)	4.83	2.02	47.66	2.39	0.021
MAP	*-0.001*	*0.0005*	36.83	-2.25	0.03
Soil pH	-0.47	0.25	48.29	-1.86	0.069

Appendix A.3

Appendix: Supplementary information for Chapter 3

Table A.3.1: Copy of Table 5.5 from Ogle, Kurz, et al. (2019): Relative Carbon Stock Change Factors (over 20 years) for Management Activities on Cropland. These factors were used for IPCC T1 estimates of SOC stock in Chapter 3.

Type	Level	Temperature Regime	Moisture Regime	IPCC Defaults	Error	Description
Land Use	Long term cultivated	Boreal	Dry	0.77	0.14	Represents area that has been converted from native conditions and continuously managed for predominantly annual crops over 50 yrs. Land-use factor has been estimated under a baseline condition of full tillage and nominal ('medium") carbon input levels. Input and tillage factors are also applied to estimate carbon stock changes, which includes changes from full tillage and medium input.
		Boreal	Moist	0.7	0.12	
		Boreal	Wet	0.7	0.12	
		Cool Temperate	Dry	0.77	0.14	
		Cool Temperate	Moist	0.7	0.12	
		Cool Temperate	Wet	0.7	0.12	
		Tropical	Dry	0.92	0.13	
		Tropical	Moist	0.83	0.11	
		Tropical	Wet	0.83	0.11	
		Tropical Montane	NA	NA	NA	
		Warm Temperate	Dry	0.76	0.12	
		Warm Temperate	Moist	0.69	0.16	
		Warm Temperate	Wet	0.69	0.16	
	Paddy rice	Boreal	Dry	1.35	0.04	Long-term (> 20 year) annual cropping of wetlands (paddy rice). Can include double-cropping with non-flooded crops. For paddy rice, tillage and input factors are not used.
		Boreal	Moist	1.35	0.04	
		Boreal	Wet	1.35	0.04	
		Cool Temperate	Dry	1.35	0.04	
		Cool Temperate	Moist	1.35	0.04	
		Cool Temperate	Wet	1.35	0.04	
		Tropical	Dry	1.35	0.04	
		Tropical	Moist	1.35	0.04	
		Tropical	Wet	1.35	0.04	
		Tropical Montane	NA	1.35	0.04	
		Warm Temperate	Dry	1.35	0.04	
		Warm Temperate	Moist	1.35	0.04	
		Warm Temperate	Wet	1.35	0.04	
	Perennial/ tree crop	Boreal	Dry	0.72	0.22	Long-term perennial tree crops such as fruit and nut trees, coffee and cacao.
		Boreal	Moist	0.72	0.22	
		Boreal	Wet	0.72	0.22	
		Cool Temperate	Dry	0.72	0.22	
		Cool Temperate	Moist	0.72	0.22	
		Cool Temperate	Wet	0.72	0.22	
		Tropical	Dry	1.01	0.25	
		Tropical	Moist	1.01	0.25	
		Tropical	Wet	1.01	0.25	
		Tropical Montane	NA	1.01	0.25	
		Warm Temperate	Dry	0.72	0.22	
		Warm Temperate	Moist	0.72	0.22	
		Warm Temperate	Wet	0.72	0.22	
	Set aside	Boreal	Dry	0.93	0.11	Represents temporary set aside of annually cropland (e.g., conservation reserves) or other idle cropland that has been revegetated with perennial grasses.
		Boreal	Moist	0.82	0.17	
		Boreal	Wet	0.82	0.17	
		Cool Temperate	Dry	0.93	0.11	
		Cool Temperate	Moist	0.82	0.17	
		Cool Temperate	Wet	0.82	0.17	
		Tropical	Dry	0.93	0.11	
		Tropical	Moist	0.82	0.17	
		Tropical	Wet	0.82	0.17	
		Tropical Montane	NA	0.88	0.5	
		Warm Temperate	Dry	0.93	0.11	
		Warm Temperate	Moist	0.82	0.17	
		Warm Temperate	Wet	0.82	0.17	

Table A.3.1 continued:

Type	Level	Temperature Regime	Moisture Regime	IPCC Defaults	Error	Description
Management	Full till	Boreal	Dry	1	NA	Substantial soil disturbance with full inversion and/or frequent (within year) tillage operations. At planting time, little (e.g., <30%) of the surface is covered by residues.
		Boreal	Moist	1	NA	
		Boreal	Wet	1	NA	
		Cool Temperate	Dry	1	NA	
		Cool Temperate	Moist	1	NA	
		Cool Temperate	Wet	1	NA	
		Tropical	Dry	1	NA	
		Tropical	Moist	1	NA	
		Tropical	Wet	1	NA	
		Tropical Montane	NA	1	NA	
		Warm Temperate	Dry	1	NA	
		Warm Temperate	Moist	1	NA	
		Warm Temperate	Wet	1	NA	
	Reduced till	Boreal	Dry	0.98	0.05	Primary and/or secondary tillage but with reduced soil disturbance (usually shallow and without full soil inversion). Normally leaves surface with >30% coverage by residues at planting.
		Boreal	Moist	1.04	0.04	
		Boreal	Wet	1.04	0.04	
		Cool Temperate	Dry	0.98	0.05	
		Cool Temperate	Moist	1.04	0.04	
		Cool Temperate	Wet	1.04	0.04	
		Tropical	Dry	0.99	0.07	
		Tropical	Moist	1.04	0.07	
		Tropical	Wet	1.04	0.07	
		Tropical Montane	NA	NA	NA	
		Warm Temperate	Dry	0.99	0.03	
		Warm Temperate	Moist	1.05	0.04	
		Warm Temperate	Wet	1.05	0.04	
	No till	Boreal	Dry	1.03	0.04	Direct seeding without primary tillage, with only minimal soil disturbance in the seeding zone. Herbicides are typically used for weed control.
		Boreal	Moist	1.09	0.04	
		Boreal	Wet	1.09	0.04	
		Cool Temperate	Dry	1.03	0.04	
		Cool Temperate	Moist	1.09	0.04	
		Cool Temperate	Wet	1.09	0.04	
		Tropical	Dry	1.04	0.07	
		Tropical	Moist	1.1	0.05	
		Tropical	Wet	1.1	0.05	
		Tropical Montane	NA	NA	NA	
		Warm Temperate	Dry	1.04	0.03	
		Warm Temperate	Moist	1.1	0.04	
		Warm Temperate	Wet	1.1	0.04	

Table A.3.1 continued:

Type	Level	Temperature Regime	Moisture Regime	IPCC Defaults	Error	Description
Input	Low	Boreal	Dry	0.95	0.13	Low residue return occurs when there is removal of residues (via collection or burning), frequent bare-fallowing, production of crops yielding low residues (e.g., vegetables, tobacco, cotton), no mineral fertilization or N-fixing crops.
		Boreal	Moist	0.92	0.14	
		Boreal	Wet	0.92	0.14	
		Cool Temperate	Dry	0.95	0.13	
		Cool Temperate	Moist	0.92	0.14	
		Cool Temperate	Wet	0.92	0.14	
		Tropical	Dry	0.95	0.13	
		Tropical	Moist	0.92	0.14	
		Tropical	Wet	0.92	0.14	
		Tropical Montane	NA	0.94	0.5	
		Warm Temperate	Dry	0.95	0.13	
		Warm Temperate	Moist	0.92	0.14	
		Warm Temperate	Wet	0.92	0.14	
	Medium	Boreal	Dry	1	NA	Representative for annual cropping with cereals where all crop residues are returned to the field. If residues are removed then supplemental organic matter (e.g., manure) is added. Also requires mineral fertilization or N-fixing crop in rotation.
		Boreal	Moist	1	NA	
		Boreal	Wet	1	NA	
		Cool Temperate	Dry	1	NA	
		Cool Temperate	Moist	1	NA	
		Cool Temperate	Wet	1	NA	
		Tropical	Dry	1	NA	
		Tropical	Moist	1	NA	
		Tropical	Wet	1	NA	
		Tropical Montane	NA	1	NA	
		Warm Temperate	Dry	1	NA	
		Warm Temperate	Moist	1	NA	
		Warm Temperate	Wet	1	NA	
	High no manure	Boreal	Dry	1.04	0.13	Represents significantly greater crop residue inputs over medium C input cropping systems due to additional practices, such as production of high residue yielding crops, use of green manures, cover crops, improved vegetated fallows, irrigation, frequent use of perennial grasses in annual crop rotations, but without manure applied (see row below).
		Boreal	Moist	1.11	0.1	
		Boreal	Wet	1.11	0.1	
		Cool Temperate	Dry	1.04	0.13	
		Cool Temperate	Moist	1.11	0.1	
		Cool Temperate	Wet	1.11	0.1	
		Tropical	Dry	1.04	0.13	
		Tropical	Moist	1.11	0.1	
		Tropical	Wet	1.11	0.1	
		Tropical Montane	NA	1.08	0.5	
		Warm Temperate	Dry	1.04	0.13	
		Warm Temperate	Moist	1.11	0.1	
		Warm Temperate	Wet	1.11	0.1	
	High with manure	Boreal	Dry	1.37	0.12	Represents significantly higher C input over medium C input cropping systems due to an additional practice of regular addition of animal manure.
		Boreal	Moist	1.44	0.13	
		Boreal	Wet	1.44	0.13	
		Cool Temperate	Dry	1.37	0.12	
		Cool Temperate	Moist	1.44	0.13	
		Cool Temperate	Wet	1.44	0.13	
		Tropical	Dry	1.37	0.12	
		Tropical	Moist	1.44	0.13	
		Tropical	Wet	1.44	0.13	
		Tropical Montane	NA	1.41	0.5	
		Warm Temperate	Dry	1.37	0.12	
		Warm Temperate	Moist	1.44	0.13	
		Warm Temperate	Wet	1.44	0.13	

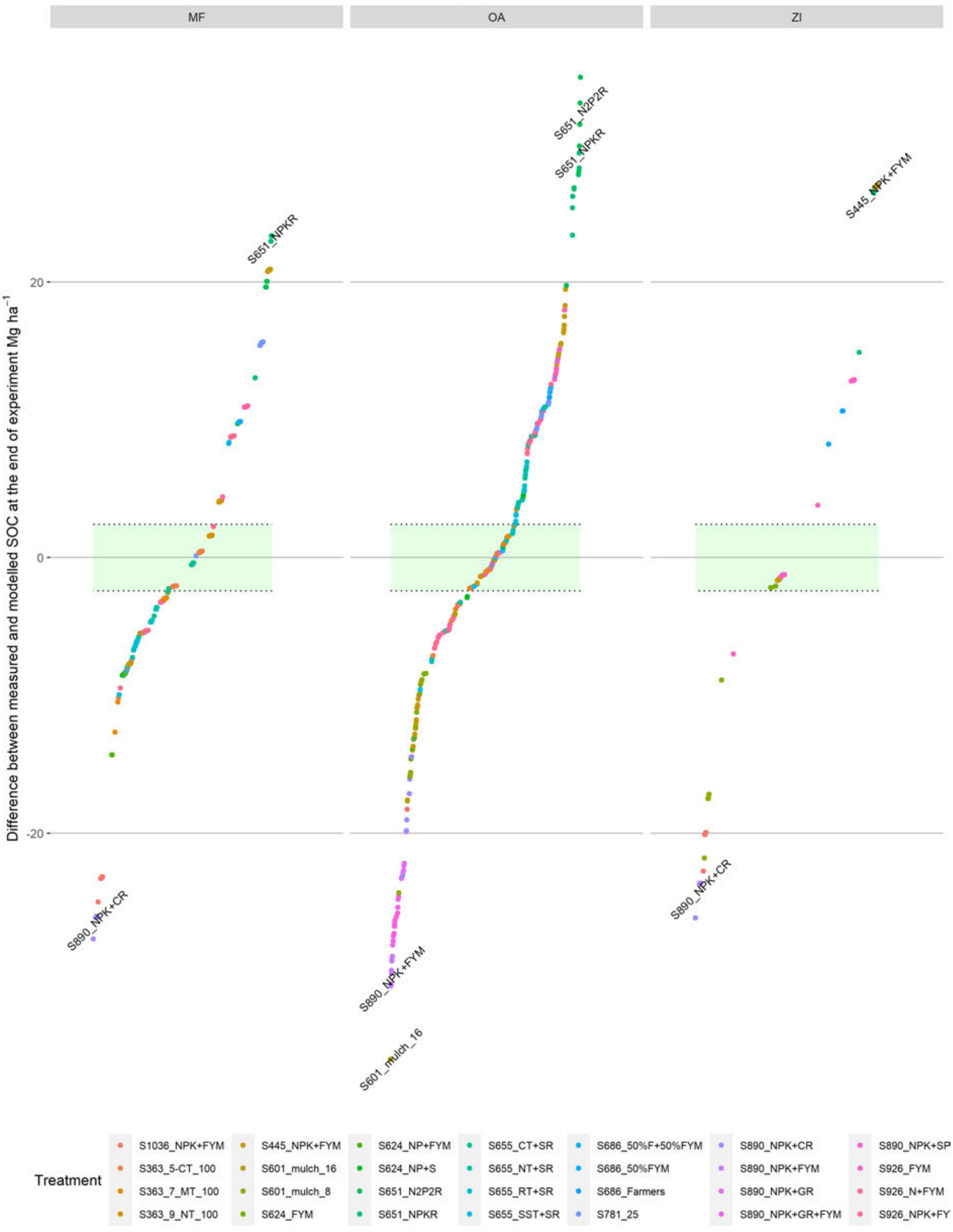

Figure A.3.1: Difference between measured and modelled SOC at the end of experiments: colours denote different treatments, one point for each model. Split by management type.

Appendix A.4

Appendix: Supplementary information for Chapter 4

Algorithm A.4.1 Algorithm: Bootstrap Particle Filter, from Davoudabadi et al. (2024)

```
for k = 1,...,N do
    t = 1, draw sample X^k_(1) ~ p(X_(1))
for t = 2,...,T do
    for k = 1,...,N do
        Draw sample X^k_(t) ~ p(X_(t) | X^{*k}_(t-1))
        Calculate weights w^k_(t) = p(Y_(t) | X^k_(t))
    Estimate the log-likelihood component for the t^th observation, l̂_(t) = log( Σ_j w^j_(t) / N )
    Normalise weights W^k_(t) = w^k_(t) / Σ_j w^j_(t) for k ∈ {1,2,...,N}
    Resample with replacement N particles X^k_(t) based on the normalised importance weights
    Estimate the overall log-likelihood L* = Σ_t l̂_(t)
```

Where (as printed in mathematical form):

- for $k = 1,...,N$ **do**
  - $t = 1$, draw sample $X^k_{(1)} \sim p(X_{(1)})$
- for $t = 2,...,T$ **do**
  - **for** $k = 1,...,N$ **do**
    - Draw sample $X^k_{(t)} \sim p(X_{(t)}|X^{*k}_{(t-1)})$
    - Calculate weights $w^k_{(t)} = p(Y_{(t)}|X^k_{(t)})$
  - Estimate the log-likelihood component for the t^{th} observation, $\hat{l}_{(t)} = log\left(\frac{\Sigma_j w^j_{(t)}}{N}\right)$
  - Normalise weights $W^k_{(t)} = \frac{w^k_{(t)}}{\Sigma_j w^j_{(t)}}$ for $k \in \{1,2,...,N\}$
  - Resample with replacement N particles $X^k_{(t)}$ based on the normalised importance weights
  - Estimate the overall log-likelihood $L^* = \Sigma_t \hat{l}_{(t)}$

Algorithm A.4.2 Algorithm: Correlated pseudo-marginal algorithm, from Davoudabadi et al. (2024)

- Initialise θ_0
- **for** $m = 1,...,M^*$ **do**
  - Sample $\theta^* \sim Q(.|\theta_{m-1})$
  - Sample $\xi \sim N(0,I)$ and set $U^* = \tau U_{m-1} + \sqrt{1-\tau^2}\xi$
  - Compute the estimator $\hat{p}(Y|\theta^*,U^*)$ using Algorithm A.4.3
  - Compute the acceptance ratio:

$$r = \frac{\hat{p}(Y|\theta^*,U^*)p(\theta^*)Q(\theta_{m-1}|\theta^*)}{\hat{p}(Y|\theta_{m-1},U_{m-1})p(\theta_{m-1})Q(\theta^*|\theta_{m-1})}$$

  - Accept (θ^*,U^*) with probability $min(r,1)$ otherwise, output (θ_{m-1},U_{m-1})

Algorithm A.4.3 Algorithm: Particle filter with fixed random numbers, from Davoudabadi et al. (2024)

Sample $U_{(j^*)} \sim N(0,1)$ and $V_{(i^*)} \sim N(0,1)$ for all $j \in \{1,...,TN\}$ and $i^* \in \{1,...,T\}$
Sample $X^k_{(1)} \sim p(.|U_{1:N},\theta)$ for all $k \in 1,...,N$
for $t = 1,...,T-1$ **do**
    Sort the collection $X^1_{(t)},...,X^N_{(t)}$
    Compute importance weights $w^k_{(t)}$ and log-likelihoods $\hat{l}_{(t)} = log\left(\frac{\Sigma_k w^k_{(t)}}{N}\right)$ for $k \in \{1,...,N\}$
    Sample $X^k_{(t)}$ based on systematic resampling using random values $V_{1:T}$ and normalised weights $W^k_{(t)}$ for $k \in \{1,...,N\}$
    Set $X^k_{(t+1)}$ as a sample from $p(.|X^k_{(t)},U_{Nt+1:N(t+1)},\theta)$ for $k \in \{1,...,N\}$
Estimate the overall log-likelihood $L^* = \Sigma_t \hat{l}_{(t)}$

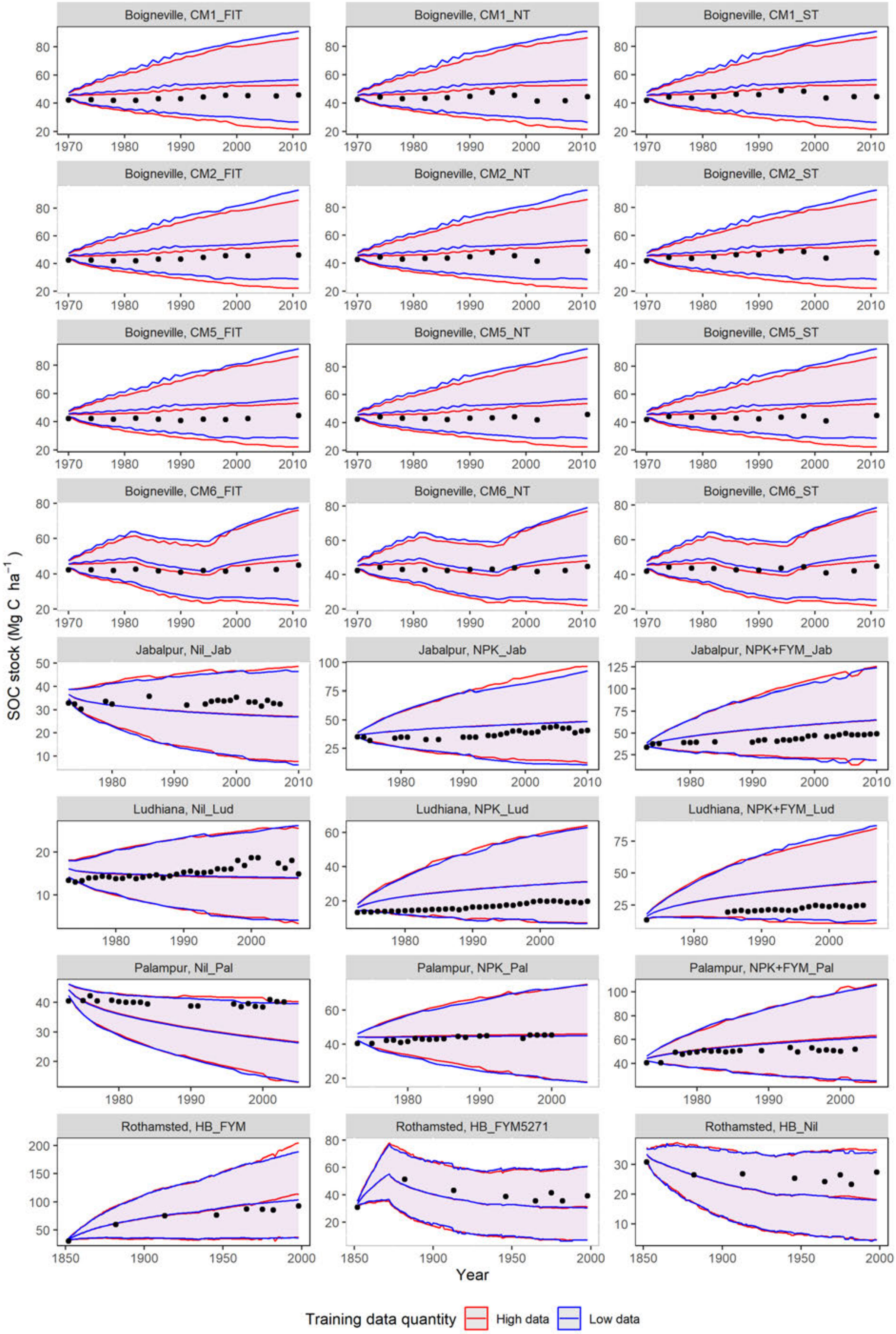

Figure A.4.1: BHM predictions using the low and high training data subsets.

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