



Evaluation of a Tier 3 soil organic carbon modelling framework for application on mineral grasslands at the field and farm scale

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Thesis submitted to the National University of Ireland Maynooth, in fulfilment of the requirements for the degree of

Doctor of Philosophy

Irish Climate Analysis and Research Units (*ICARUS*), Department of Geography, Maynooth University

Submitted: October 2025

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Summary

Soil organic carbon (SOC) is a vital component of the global carbon cycle, underpinning soil health, ecosystem resilience, and climate change mitigation. Grasslands dominate global agricultural land and are often managed, placing significant SOC stores within the domain of land managers. However, they remain underrepresented in international research and measurement, reporting and verification systems. Improving the accuracy and transparency of SOC estimates is increasingly critical as global national frameworks predominantly rely on a simple default Tier 1 methodology. Emerging policies and guidelines favour Tier 3 modelling approaches, which capture local variability and management impacts beyond the scope of Tier 1 methods. This thesis advances Tier 3 SOC modelling for mineral grasslands through the development and application of a transparent, flexible modelling framework. A review of SOC models highlighted three key knowledge gaps: (i) model formulation, (ii) model inputs, and (iii) model applicability at the farm scale. These were addressed across three research chapters, focusing on the RothC model.

Key findings include: (i) Model implementation - A generalised modelling framework was demonstrated to replicate RothC behaviour when appropriately amended and provides a common platform to focus future research efforts. (ii) Model input sensitivity - A multi-model ensemble analysis showed that simpler carbon input and evapotranspiration (ET) methods (e.g., Miami model, Thornthwaite ET) can perform as well as complex alternatives in data-limited contexts. (iii) Model development - A modular Mineral Grassland (MG) model was created, capable of operating at field and farm scales and accommodating future model extensions. (iv) Model evaluation - When tested on 28 Irish sites, the MG model showed good performance within the 73-105 Mg C ha⁻¹ range, suggesting internal biases linked to the constrained current input configuration. Overall, this research develops and demonstrates a modular spatial Tier 3 SOC modelling framework for mineral grasslands, offering a transparent, adaptable platform to support farm-scale SOC accounting and ongoing model refinement.

Acknowledgements

First and foremost, I would like to express my sincere gratitude to my supervisors, Donal O'Brien and Rowan Fealy, for their guidance, encouragement, and invaluable support throughout my PhD journey. Their expertise, constructive feedback, and patience have been instrumental in shaping this research and my development as a researcher.

I gratefully acknowledge the financial support of the Teagasc Walsh Scholarship Programme. I also consider myself fortunate to have undertaken my PhD through Teagasc and Maynooth University, both of which provided an excellent research environment, outstanding facilities, and valuable opportunities throughout my studies. I am grateful to my colleagues, collaborators, and everyone who contributed their time, knowledge, and encouragement during this work.

Completing a PhD is often described as a long, difficult, and at times solitary journey. However, after witnessing my mother face cancer with remarkable courage and resilience and seeing the unwavering support my father gave her throughout that time, my own challenges seemed small by comparison. Their strength, perseverance, and love gave me perspective every day and reminded me of what truly matters. I am deeply grateful for their unwavering encouragement and belief in me throughout this journey.

Data acknowledgements

We thank the Lawes Agricultural Trust and Rothamsted Research for information and data from the e-RA database. The Rothamsted Long-Term Experiments - National Bioscience Research Infrastructure (RLTE-NBRI) is funded by the UK Research and Innovation - Biotechnology and Biological Sciences Research Council (UKRI-BBSRC) under award BBS/E/RH/23NB0007 (2023-2028). The RLTE-NBRI is also supported by the Lawes Agricultural Trust.

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Chapter 1: Introduction

1.1 Soil organic carbon

Soil organic carbon (SOC) plays a central role in the global carbon (C) cycle, functioning as both a source and sink of atmospheric carbon dioxide (CO₂), one of the key greenhouse gases (GHGs) driving climate change (Ciais *et al.*, 2013; Smith *et al.*, 2020). Soil organic carbon constitutes the largest terrestrial C pool, storing more than twice the carbon contained in the atmosphere and terrestrial vegetation combined (Sanderman *et al.*, 2017; Scharlemann *et al.*, 2014). The terrestrial biosphere has emerged as a critical buffer against climate change, offsetting over one-quarter of anthropogenic CO₂ emissions (Piao *et al.*, 2019). Many of the stocks and flows within the global C cycle are well quantified and understood; however, there is considerable debate about the amount of C stored in, and emitted from, terrestrial ecosystems (Piao *et al.*, 2019; Scharlemann *et al.*, 2014; Tifafi *et al.*, 2018). The SOC pool contained within the soil is susceptible to anthropogenic pressures and land-use changes, making it a critical focus for climate mitigation and land management strategies (Stockmann *et al.*, 2013).

Soil organic carbon is fundamental to many soil and ecosystem functions and is sensitive to both direct and indirect human impacts (Campbell and Paustian, 2015). Assessing SOC is vital for evaluating soil and ecosystem functions as SOC is considered a keystone indicator due to its pivotal role in soil systems, influencing nutrients for plant availability, improving soil fertility, acting as a plant hormone that can increase root growth and the release of organics by the roots, detoxifying harmful soil elements, and for binding toxic heavy metals making them unavailable to plants roots (Gerke, 2022).

Climate, soil, and land-use and management factors are the dominant factors that influence SOC stocks worldwide. Temperature and rainfall regulate the balance between C inputs from plants and impact climate-sensitive decomposition (Hartley *et al.*, 2021; Wiesmeier *et al.*, 2019). Soil properties such as soil texture and parent material impact the capacity of soils to stabilise SOC (FAO, 2005; McBratney *et al.*, 2014). Land use and management also play a decisive role, with management practices accelerating C losses through soil disturbance, while permanent vegetation can promote SOC accumulation (Guo and Gifford, 2002; Stockmann *et al.*, 2013). These combined effects drive the broad patterns of SOC stocks observed globally, as outlined in Figure 1.1.

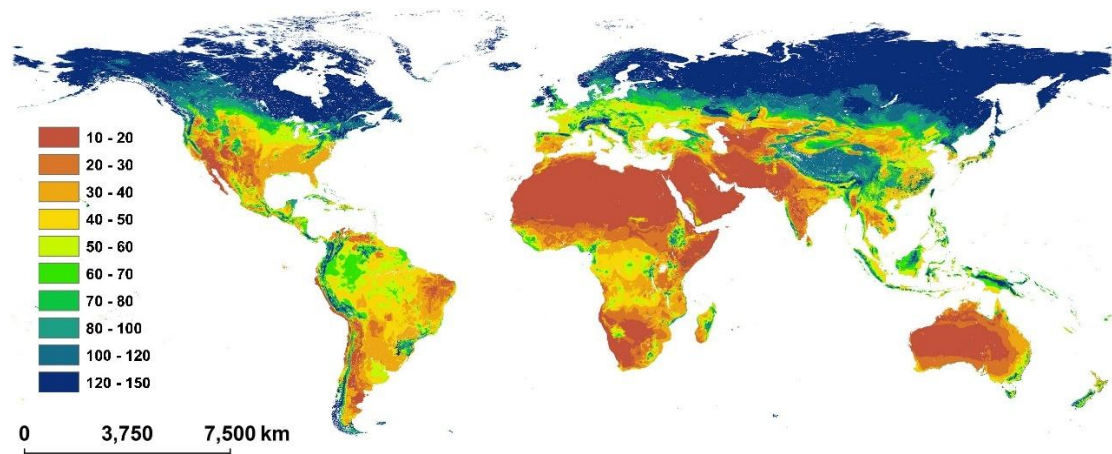


Figure 1.1 Soil C stock of the world's topsoil (0-0.3 m) in tonnes per C per hectare. The map was generated based on global datasets of C stocks from the study of Stockmann *et al.* (2015). (Source: Minasny *et al.*, 2017).

Most agricultural soils are depleted in carbon relative to the native ecosystems. Since the onset of widespread cultivation approximately 8,000 years ago, soils globally are estimated to have lost 140-150 Gt C (~510-550 Gt CO₂) through agricultural land-use (Sanderman *et al.*, 2017; Smith *et al.*, 2020). Degraded soils that store C below their natural capacity have been identified as an opportunity for soils to contribute to climate change mitigation through sequestration (Dynarski *et al.*, 2020). Soil carbon sequestration can be defined as the transfer of atmospheric CO₂ into the soil through plants, residues, and other organic solids, which are stored as SOC (Fuss *et al.*, 2018; Paustian *et al.*, 2019b).

Grasslands are an integral component of the global C cycle (Lal, 2004; Stockmann *et al.*, 2013), but they have historically received less scientific and policy attention (Beillouin *et al.*, 2021; 2023), most likely due to the perception that grasslands are considered carbon-neutral (Poeplau, 2021). Grasslands occupy approximately 40% of the Earth's terrestrial surface area (Petermann and Buzhydan, 2021) and represent a major component of global agricultural land use. Grasslands can store large amounts of SOC per unit area (Poeplau, 2021), storing approximately 20% of global SOC estimates to a depth of 1 metre (Stockmann *et al.*, 2013). Therefore, relatively minor changes in grassland SOC can strongly impact atmospheric concentrations of CO₂ (Poeplau, 2021). Additionally, roughly 70% of global grasslands are managed (Conant *et al.*, 2017), which places significant control of global soil C stocks within the domain of land managers (Stoner *et al.*, 2021).

Well-managed grassland soils are capable of building up substantial amounts of SOC over time, thereby offering a means to help offset climate change through the sequestration of atmospheric CO₂ (Fornara *et al.*, 2020b; Stoner *et al.*, 2021). Gains in SOC not only contribute to lowering the carbon footprint of livestock production systems but also play a key role in improving soil health and strengthening the resilience of grassland ecosystems (Fornara *et al.*, 2020b).

Consequently, grasslands have also become a focus of international climate and soil policy. At the Conference of the Parties (COP) 23 in 2017, the Koronivia Joint Work on Agriculture (KJWA) was adopted, acknowledging agriculture as both highly vulnerable to climate change and a key sector for mitigation and adaptation (Rioux *et al.*, 2023). Within this framework, livestock and grazed grasslands were explicitly recognised as important and potential mitigation pathways, particularly through their ability to enhance soil carbon sequestration (Dondini *et al.*, 2023; Rioux *et al.*, 2023). These developments highlight that grasslands, once largely overlooked in climate strategies, are now increasingly regarded as critical ecosystems for carbon policies and global mitigation efforts. However, concerns around the permanency of the CO₂ store in soils remain, as soil carbon is vulnerable to climate change, particularly extreme heat and drought.

1.2 Measuring and estimating

Accurately quantifying SOC stocks and dynamics remains a central challenge in both global carbon accounting and national GHG inventories. The main difficulty lies in the spatial and temporal variability of SOC within soils. Soils are inherently heterogeneous, and even within a single plot, SOC concentrations often show significant variation (Luo *et al.*, 2016; Smith *et al.*, 1997). Moreover, SOC accumulates gradually over time. This slow rate of change, combined with small-scale variability, makes it difficult to detect meaningful changes in SOC stocks over typical monitoring or reporting periods (Smith *et al.*, 2020).

SOC is usually measured at numerous sampling points and then extrapolated across larger areas by multiplying average values by the land area of interest. This upscaling, however, introduces uncertainty, particularly when sampling fails to capture landscape-level variability (Hobley and Willgoose, 2010). The widespread variation in global SOC estimates reflects this problem. For example, Lin *et al.* (2024) compared five global SOC datasets and found estimates ranging from 577 to 2,678 Pg C to one metre depth, resulting in a nearly fivefold difference between estimates. These discrepancies arise from differences in assumptions, database coverage, and the way complex soil systems such as peatlands and permafrost are treated (Stockmann *et al.*, 2013; Tifafi *et al.*, 2018).

Direct field measurements of SOC remain the most reliable method, which involves soil coring followed by laboratory analysis of carbon concentrations (FAO, 2019; Kiely *et al.*, 2009; Smith *et al.*, 2020). However, undertaking field measurements at larger spatial scales is limited by logistical and financial constraints, including high costs, the need for destructive sampling, and challenges related to standardisation across sites (Scharlemann *et al.*, 2014; Smith *et al.*, 2020). Sampling depth is often restricted to the upper 30cm, despite considerable amounts of C being stored deeper in the soil profile. Bulk density is required to convert concentrations to stocks estimates but is highly variable and influenced by

management practices and mineralogy composition, which can introduce additional uncertainties (Stockmann *et al.*, 2013; Scharlemann *et al.*, 2014). Furthermore, coarse fragments are often ignored from calculations, even though they reduce the soil volume available for carbon storage (Fenton *et al.*, 2024; Poeplau, 2017).

Due to these challenges, SOC models have a critical role to play in soil C research, providing a mathematical framework to enable soil C dynamics to be estimated across space and time (Campbell and Paustian, 2015). Soil organic carbon models represent the turnover or decomposition of SOC and its transformation in the soil-plant-atmosphere system (Senapati *et al.*, 2014). While models differ in complexity, they generally represent SOC as distinct pools with different turnover rates (Campbell and Paustian, 2015; Sierra *et al.*, 2012). Although a wide range of SOC models are available, most share a common mathematical framework and can be described as linear dynamical systems (Manzoni & Porporato, 2009; Sierra *et al.*, 2012).

There is now a pressing need to develop appropriate systems to evaluate emerging SOC measurement, reporting and verification (MRV) frameworks (Kuhnert *et al.*, 2022; Oldfield *et al.*, 2021), which place a heavy requirement on model-based approaches, in the absence of widely available data (Dondini *et al.*, 2023; Paustian *et al.*, 2019a; Peralta *et al.*, 2022; Smith *et al.*, 2020). Models contribute to MRV frameworks in different ways, such as providing baseline information, a means to interpolate measurements and projections, estimating SOC changes and providing information that can inform improved measurement planning (Kuhnert *et al.*, 2022). To date, there is still no globally accepted, standardised MRV framework.

1.3 International Policy Context

Countries that are Parties to the United Nations Framework Convention on Climate Change (UNFCCC) are required to submit annual National GHG Inventories. Within these inventories, Parties must report national SOC stocks and stock changes under the Land-Use, Land-Use Change and Forestry (LULUCF) sector. Reporting must follow the methodological framework outlined in the 2006 Intergovernmental Panel on Climate Change (IPCC) guidelines and their 2019 refinements. The IPCC employs a tiered system for SOC estimation, reflecting increasing levels of methodological detail and data requirements. Tier 1 is based on default emission factors and broad assumptions, Tier 2 uses country-specific activity data and emission factors, and Tier 3 requires data-intensive SOC models (IPCC, 2006; 2019). The transition from Tier 1 to Tier 2 and Tier 3 methodologies is emphasised in the 2019 Refinements as a necessary step to improve reporting accuracy (IPCC, 2006; 2019).

Soil organic carbon and soil C sequestration are also embedded within broader European Union (EU) policy frameworks. These include the EU Soil Strategy for 2030, the proposed EU Soil Health Law, the European Green Deal, the EU Biodiversity Strategy for 2030, and the European Mission: A soil deal for Europe. While not all these initiatives explicitly target SOC, they collectively acknowledge its importance in maintaining soil health, enhancing ecosystem services, and contributing to climate change mitigation.

In addition, more recent EU regulatory frameworks including the carbon removals and carbon farming framework (Regulation (EU) 2024/3012) and the revised LULUCF Regulation (Regulation (EU) 2023/839), both prioritise the adoption of Tier 3 methods for estimating emissions and removals in key land-use categories by 2030. This shift will compel EU Member States to adopt SOC models capable of supporting national reporting obligations and ensuring comparability across the EU.

1.4 Soil organic carbon models

Numerous SOC models, as well as broader soil biogeochemical models that incorporate SOC model components, are currently available. It is estimated that over 250 different models and sub-models exist (LeNoë *et al.*, 2023; Manzoni and Porporato, 2009; Sierra *et al.*, 2012). Despite this wide availability, only a relatively small subset are routinely employed in Tier 3 approaches at regional or national scales. For example, the RothC model is used in national inventories in Australia, Japan and Switzerland (Richards, 2001; Shiratio and Taniyama, 2003; Smith *et al.*, 2020). The United Kingdom employs a simplified version of the ECOSSE model, derived from RothC and adapted to organic soils (Smith *et al.*, 2010). Canada adopted the CENTURY model (Parton, 1987), while the United States uses the daily time-step version (Daycent) (Del Grosso *et al.*, 2005). Denmark uses the C-Tool in its national inventories (Taghizadeh-Toosi *et al.*, 2014).

Most of these models were developed and parameterised based on data from long-term field experiments, from which SOC decomposition dynamics were empirically derived. For example, the RothC model was parametrised using long-term experiments at Rothamsted, UK (Coleman and Jenkinson, 1996), while CENTURY and DayCent were initially based on long-term grassland and cropping experiments in Colorado, USA (Del Grosso *et al.*, 2005; Parton, 1987). ECOSSE was derived from RothC but specifically adapted to long-term datasets from Scottish organic soils (Smith *et al.*, 2010), while C-Tool was parameterised primarily using the Askov long-term experiments in Denmark, with subsequent refinements following evaluation at other European field sites (Taghizadeh-Toosi *et al.*, 2014).

It is important to emphasise that no SOC model is inherently superior; instead, the most appropriate model depends on the research objectives, data availability, and intended application. Models differ in their scope; some focus exclusively on SOC, while others also

simulate associated GHG emissions such as nitrous oxide (N₂O) and methane (CH₄) (Campbell and Paustian, 2015; Smith *et al.*, 1997).

1.5 Knowledge gaps

Soil organic carbon modelling inherently involves uncertainties, regardless of tool or context (Maas and Lal, 2023). These uncertainties complicate reliable SOC stock estimation and can arise from various sources, including model formulation, structure, parameterisation, input data, data sampling and the scaling of model results (Maas and Lal, 2023; Todd-Brown *et al.*, 2013; Qin *et al.*, 2016). Broadly, these knowledge gaps can be categorised into three key components: (1) Model formulation, (2) Model inputs, and (3) Scale of applicability.

1.5.1 Model formulation

Uncertainties in SOC modelling frequently stem from variations in models' structures and formulations (Todd-Brown *et al.*, 2013; Qin *et al.*, 2016). Generalised SOC decomposition frameworks such as SoilR (Seirra *et al.*, 2012), while widely utilised, may introduce additional uncertainties due to discrepancies between SoilR and its source models. SoilR is not a direct model emulation; instead, it functions as a generalised SOC modelling framework, potentially leading to variations in simulation outputs.

Several studies have implemented the same model (e.g., SoilR, Sierra *et al.*, 2012) but have documented different operational steps (Boone *et al.*, 2018; Geremew *et al.*, 2024; Hyun and Yoo, 2024; Lefebvre *et al.*, 2020; Moll-Mielewczik *et al.*, 2023; Riggers *et al.*, 2019; Spotorno *et al.*, 2024). For example, Lefebvre *et al.* (2020), Moll-Mielewczik *et al.* (2023), and Spotorno *et al.* (2024) reported code amendments to improve consistency with the source model, while Hyun and Yoo (2024), Geremew *et al.* (2024), and Riggers *et al.* (2019) did not document such amendments, highlighting potential inconsistencies in model implementations. These discrepancies, along with differences in model versions, may lead to variations that undermine the reliability of simulations. However, limited published research exists on the significance of these differences, preventing a more comprehensive understanding of their impacts.

1.5.2 Model inputs

Model inputs represent one of the largest sources of uncertainty in SOC stock estimation (Maas and Lal, 2023; Ortiz *et al.*, 2013; Riggers *et al.*, 2019; Wiesmeier *et al.*, 2016). Among these, estimates of C inputs have been found to exert a significant influence on model outcomes, and inconsistencies in estimation methods contribute substantially to model variability. For example, Wiesmeier *et al.* (2016) highlighted C input estimates as one of the most decisive parameters in SOC projections, while Ortiz *et al.* (2013), in their study modelling forest SOC, identified litter input as the dominant source of uncertainty.

The absence of standardised methods for estimating C inputs further compounds this problem. In a multi-model comparison study, Riggers *et al.* (2019) applied five different C inputs estimation methods and reported significant variability across outputs. Similarly, Keel *et al.* (2017) compared five allometric equations, with C input estimates ranging from 2.1 to 5.3 t C ha⁻¹ yr⁻¹. Maas and Lal (2023) also showed that three different remote sensing techniques produced divergent C input values, reinforcing the sensitivity of model outcomes to input choice.

Another critical input is potential evapotranspiration (ET). Many SOC models do not calculate ET internally and require the user to provide this parameter (Jenkinson, 1990; Parton *et al.*, 2001). The method chosen can strongly affect results. For instance, Maas and Lal (2023) demonstrated that RothC was sensitive to the selected ET estimation method, which directly influenced the behaviour of the model's moisture modifier and, consequently, estimated SOC stocks. This variability highlights the importance of systematically evaluating model inputs, where robust SOC estimates are needed to support national reporting.

1.5.3 Model applicability at farm scale

Uncertainty in SOC modelling also arises when applying models at the farm scale. Many large-scale approaches, such as the IPCC Tier 1 method or global products like the GSOCseq model, operate at coarse spatial resolutions (≥ 1 km²) that are inadequate for capturing variability within farms. In contrast, models that are applied at the point scale require large amounts of data, typically not available for many locations. The mismatch between the resolution of available models and the scale at which landowners and policymakers seek information represents a critical knowledge gap. Developing a framework that is both data-efficient and capable of producing reliable SOC estimates at the farm scale is essential for advancing inventory reporting and supporting site-specific land management decisions.

1.6 National case study: Ireland

The Republic of Ireland (hereafter Ireland) provides a relevant case study for examining the knowledge gaps identified above. Agriculture accounts for 36.2% of Ireland's GHG emissions (EPA Ireland, 2025). Under the Climate Action and Low Carbon Development (Amendment) Act 2021, Ireland is committed to reducing agricultural emissions by 10% by 2025, and 25% by 2030 relative to 2018 levels. Achieving these targets will require improved soil carbon accounting at the farm scale to capture mitigation efforts arising from sustainable land management practices that favour soil C sequestration. The combination of a grassland-dominated landscape, ambitious climate policy commitments, and the need for farm-scale assessment makes Ireland an ideal case study to explore the challenges of Tier 3 SOC modelling for grasslands.

Ireland has a total land area of 6.9 million hectares. In 2023, land cover comprised of grasslands (59.4%), wetlands (17.2%; including peatlands, marshes and bogs), woodlands (11%), croplands (10.5%; arable and temporary grasslands), and settlements (1.8%) (EPA Ireland, 2025). The dominant soil type is mineral, covering ~71% of the land area, while organic soils account for ~17%, and organo-mineral soils account for ~10% (EPA Ireland, 2025).

National SOC stock estimates vary depending on the methodology and soil depth considered. Tomlinson (2005) estimated total SOC stocks at 2,048 Mt in 1990 and 2,021 Mt in 2000, while Khalil *et al.* (2013) reported 2.824 Gt C to depths greater than one metre using empirical and GIS-based approaches. Organic soils contribute disproportionately to these totals. Haughey (2021) emphasised that organic soils only cover ~17% of the land area but contain a significant fraction of national stocks. As organic soils are recognised as significant C sinks, recent studies including Jovani-Sancho *et al.* (2021) (development of forest peat soil emission factors), Aitova *et al.* (2023) (development of Irish peatland emission factors) and Tuohy *et al.* (2023) (drainage status of grassland peats) have aided the transition from Tier 1 to Tier 2 reporting under organic soils (EPA Ireland, 2025). As a result, organic soils are comparatively well studied relative to mineral soils.

Grasslands are central to Ireland's agricultural emissions profile and mitigation potential. Permanent grasslands occupy ~76% of the utilised agricultural area (Haughey, 2021) and underpin livestock systems, making soil-based mitigation critical. Grassland SOC stocks are substantial, with Khalil *et al.* (2013) estimating 246.9, 608.1, 829.5, and 1079.3 Tg at depths of 0-10cm, 0-30cm, 0-50cm and 0-100cm, respectively. Irish soils also exhibit high SOC concentrations (32-63 g kg⁻¹), and well-managed swards can sequester between 1.1 and 1.4 t C ha⁻¹ yr⁻¹ (Minasny *et al.*, 2017; Watson *et al.*, 2007). These figures highlight that grasslands here are important C sinks and have the potential to offset emissions from livestock systems while improving food security and ecosystem resilience. To realise this potential, however, accurate quantification of SOC stock baselines and changes is essential.

Despite this potential, SOC stock estimates for mineral grasslands in Ireland continue to rely on Tier 1 methodologies (EPA Ireland, 2025). Tier 3 modelling studies have been largely limited to single sites (e.g., Dondini *et al.*, 2009; Khalil, 2014; Necpálová *et al.*, 2014; van Groenigen *et al.*, 2011), restricting their broader application. Saunders *et al.* (2022) applied the ECOSSE model across multiple grassland sites; however, it was hindered by data limitations in relation to generating model inputs and reliable SOC stock observations. These experiences highlight the operational challenges of implementing Tier 3 SOC models, which often require extensive model inputs and SOC measurements (e.g., Necpálová *et al.*, 2014; Saunders *et al.*, 2022) as well as limitations associated with the programming

environments in which the SOC models are developed (Flattery *et al.*, 2018; Sierra *et al.*, 2012). To date, Ireland, like many EU countries, lacks an appropriate, standardised approach for estimating SOC stocks in mineral grasslands at the farm scale, where mitigation opportunities are most effectively implemented. Ireland provides an interesting case study for advancing data-efficient Tier 3 SOC modelling frameworks that can support standardised, farm-scale carbon accounting.

1.7 Research aims and objectives

Given the scarcity and limited availability of SOC measurements, models are indispensable tools for providing consistent estimates in data-limited environments (Campbell and Paustian, 2015; Moll-Mielewczik *et al.*, 2023; Smith *et al.*, 2020). The overarching aim of this research is therefore to develop and evaluate a Tier 3 modelling approach for estimating SOC stocks at the field to farm scale. To achieve this aim, the following research objectives have been identified:

1. Assess and validate generalised SOC modelling frameworks to increase usability and ensure faithfulness to the source model.
2. Quantify the sensitivity of major model drivers to improve understanding of the key processes influencing SOC stock estimation.
3. Evaluate model sensitivity to different model inputs, namely C and ET to identify an efficient and reliable model configuration recognising data availability.
4. Develop a multi-point SOC modelling framework to enable standardised comparison across diverse grassland sites at the farm scale.
5. Investigate environmental drivers of measured SOC stocks to inform model calibration and guide potential improvements.

1.8 Thesis structure

This thesis is divided into seven chapters. **Chapter 1** introduces an overview of the research context, highlighting the urgent need for Tier 3 SOC modelling approaches to estimate carbon stocks in an underrepresented mineral grassland, and sets out the research aim and objectives. **Chapter 2** reviews the role of grasslands in the global C cycle, focusing on climatic, edaphic, and management factors that govern SOC dynamics. It examines traditional and emerging approaches for SOC quantification, their role in MRV systems, and evaluates SOC models as core components of these frameworks. **Chapter 3** provides a conceptual and structural analysis of SOC models. It outlines the architecture of single-, two-, and multi-pool models, describing how decomposition C inputs and environmental modifiers are computationally represented. The chapter also discusses how the generalised SOC modelling framework can be used to compare model behaviour and structure in a fair, standardised approach.

Chapters 4 to 6 comprise the core research chapters, each addressing a specific knowledge gap. **Chapter 4** examines the implementation of models within a general modelling framework. It evaluates the SoilR package (Sierra *et al.*, 2012) against the RothC source model and replicates a long-term experiment to provide a benchmark baseline. This chapter addresses Objectives 1. **Chapter 5** analyses the sensitivity of the RothC to major model drivers and variations in externally derived inputs. Using a one-at-a-time sensitivity analysis, climate scenario testing, and a model input ensemble to evaluate how input uncertainty propagates under temperate mineral grassland conditions. This chapter addresses Objectives 2 and 3. **Chapter 6** develops a generalised SOC modelling framework for estimating SOC stocks in Irish mineral grasslands at field and farm scales. The model integrates a climate module, a C input model, and the RothC model in R. It also examines local environmental drivers of SOC to inform site-specific calibration. This chapter addresses Objectives 4 and 5.

Chapter 7 synthesises and critically discusses the findings, highlighting their significance for Tier 3 SOC modelling and MRV frameworks. The chapter highlights the key findings in relation to the research objectives and outlines the main contributions to knowledge. The chapter concludes by synthesizing the study's limitations, proposed refinements, policy implications, and overall conclusions.

Chapter 2: Research Context

2.1 Carbon cycle

Carbon (C) is a fundamental element in all known life forms on Earth, comprising approximately half of the dry biomass of living organisms (Chapin *et al.*, 2006; Ussiri and Lal, 2017). The global C cycle describes the exchange of C among four principal Earth system reservoirs: the atmosphere, hydrosphere, terrestrial biosphere, and lithosphere (Ussiri and Lal, 2017). These reservoirs differ significantly in their C storage capacity and turnover time, with C transferred among them via numerous physical, chemical, and biological processes (Ciais *et al.*, 2013; Ussiri and Lal, 2017).

The atmosphere contains the smallest and most rapidly cycling C pool, estimated at 828 to 885 Gt C (Ciais *et al.*, 2013; Friedlingstein *et al.*, 2023). It serves as a critical intermediary for C exchange with the biosphere and oceans. The oceans represent the most extensive and active C reservoir, storing approximately 39,000 gigatons of C (Gt C). Ocean-atmosphere exchanges are modulated by ocean circulation, solubility dynamics, seasonal temperature changes, and the biological pump (Crisp *et al.*, 2022). The terrestrial biosphere contains between 450 and 650 Gt C in vegetation (Ciais *et al.*, 2013) and an estimated 1500-3400 Gt C in soils, to a depth of one metre (Batjes, 1996; Sanderman *et al.*, 2017; Smith *et al.*, 2020; Tifafi *et al.*, 2018). Additional stores include 300 to 700 Pg C in wetlands and substantial C reserves in permafrost (Ciais *et al.*, 2013; Tifafi *et al.*, 2018). The lithosphere, encompassing sedimentary rocks and fossil C, constitutes the largest C store by orders of magnitude, with C exchanges driven by weathering and volcanic activity on timescales exceeding 10,000 years (Ciais *et al.*, 2013; Ussiri and Lal, 2017; Malhi, 2002).

Carbon fluxes between these reservoirs are interconnected via both natural and anthropogenic pathways, characterised as complex and varying over space and time (Falkowski *et al.*, 2000; Tifafi *et al.*, 2018). The flux cycle is divided into two domains: fast and slow. The fast C cycle includes rapid fluxes among the atmosphere, biosphere, ocean surface, and shallow sediments, with turnover times ranging from years to millennia (Ciais *et al.*, 2013; Falkowski *et al.*, 2000; Grace, 2004). Fast fluxes from the oceanic domain include ocean circulation, seasonal heating and cooling, and biological processes. From the terrestrial domain, these include the uptake of CO₂ via photosynthesis and the release of CO₂ from autotrophic and heterotrophic respiration (soil respiration) (Crisp *et al.*, 2022). Other relatively minor contributions to the terrestrial C dynamics include fires, other land disturbances, and emissions from crop production and grazing (Crisp *et al.*, 2022). The natural C cycle involves approximately 210 Gt of atmospheric CO₂ being cycled yearly between the atmosphere, land, and oceans (Malhi, 2002).

In contrast, the slow C cycle involves relatively small fluxes over long residence times, primarily associated with geological C storage. Atmospheric CO₂ is altered over geological timescales through chemical weathering of silicate and carbonate rocks, which form bicarbonate ions that are transported to the ocean and ultimately buried as marine carbonates (Ciais *et al.*, 2013; Ussiri and Lal, 2017). Subduction and volcanic outgassing return this C to the atmosphere, completing the geological loop (Ciais *et al.*, 2013; Ussiri and Lal, 2017). Atmospheric CO₂ also varies naturally over glacial to interglacial periods, as shown in the Vostok Ice Core, with background atmospheric CO₂ levels ranging between 180 and 280 parts per million (ppm) during glacial and interglacial periods, respectively. The slow domain is irrelevant on time scales of human history and is often assumed to be a constant; however, it remains the most crucial cycle on geological time scales (Ciais *et al.*, 2013; Ussiri and Lal, 2017; Malhi, 2002).

Many of the stocks and flows within the global C cycle are well quantified and understood; however, there is considerable debate about the amount of C stored in and emitted from terrestrial ecosystems (Piao *et al.*, 2019; Scharlemann *et al.*, 2014; Tifafi *et al.*, 2018). Scharlemann *et al.* (2014) reviewed 27 global SOC estimate studies and found considerable variation. The median across all estimates was 1460.5 Gt C. However, the range was from 504 to 3000 Gt C, as demonstrated in Figure 2.1. This variation reflects inconsistencies in databases, sampling depths, geography coverage, and methodological scope. While more recent studies have refined SOC estimates using higher-resolution global datasets (e.g., Georgiou *et al.*, 2022; Lin *et al.*, 2024; Padarian *et al.*, 2022), Scharlemann *et al.* (2014) remains the most comprehensive temporal synthesis of historical variability in global SOC stock estimates.

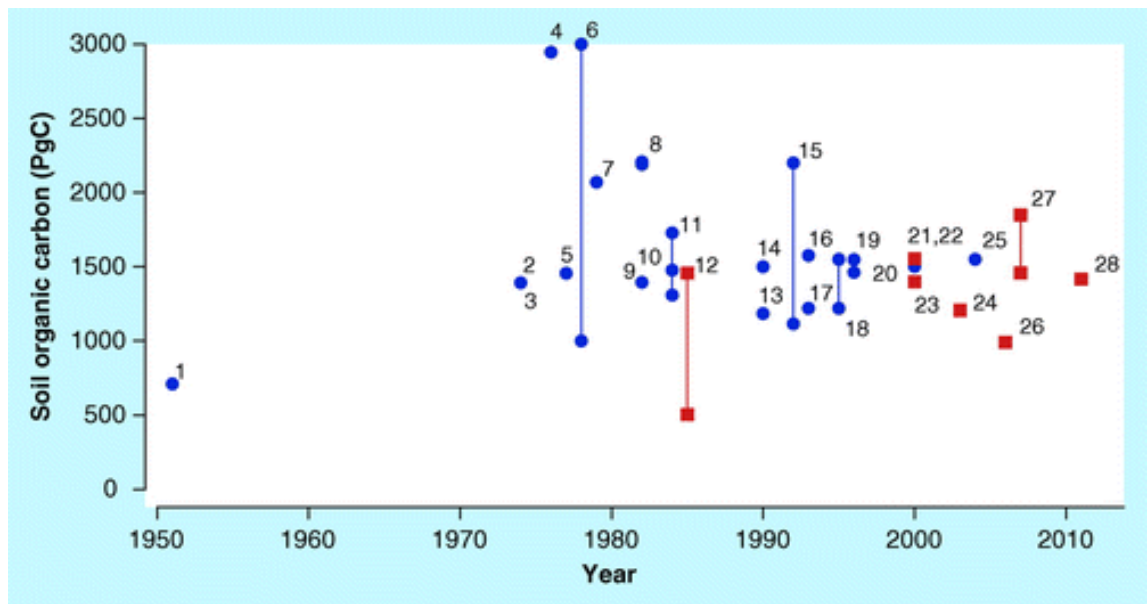


Figure 2.1 Estimates of global soil organic carbon stocks from the literature through time. Median across all estimates 1460.5 Pg C, range 504–3000 Pg C, $n = 27$ studies, based on spatially explicit (red; median 1437 Pg C, range 504–2469.5 Pg C, $n = 7$) and non-spatially explicit methods (blue; median 1388.5 Pg C, range 710–3000 Pg C, $n = 20$). Lines connect minimum and maximum estimates of soil organic carbon reported by the same study (Source: Scharlemann *et al.*, 2014).

Global SOC stock estimates differ substantially depending on the method (and data) used to derive the global estimate (Batjes, 1996; Bohn, 1976; Tifafi *et al.*, 2018). Bohn (1976) used FAO soil maps for South and North America, Asia, Africa, Europe, and Oceania to estimate the global SOC stock of 2207 Pg C, while Batjes (1996) used the World Inventory of Soils Emissions Potentials (WISE) database to estimate a global SOC stock of 1462–1548 Pg C. In a more recent study, Tifafi *et al.* (2018) calculated global SOC stocks to a depth of 1 m using two different databases, and they estimated global values of 3400 Pg using SoilGrids and 2500 Pg using the Harmonised World Soil Database (HWSD). Such disparities highlight the influence of database resolution, land-use cover, and the underrepresentation of C-rich regions, such as peatlands and boreal zones.

Recent studies have sought to refine global SOC estimates using advanced models and high-resolution spatial datasets. Georgiou *et al.* (2022), using a global compilation of 1,144 soil profiles, estimated that mineral-associated SOC in non-permafrost soils to a depth of 1m accounted for approximately 899 Pg C. Padarian *et al.* (2022) developed a semi-mechanistic global SOC model integrating land cover change and climate variables (temperature and precipitation) from remote sensing to estimate a baseline stock of 793 Pg C in the top 30cm for year 2001, with an average annual loss of 1.9 Pg C yr^{-1} from 2001 to 2020 due to land cover conversion.

A comprehensive comparison by Lin *et al.* (2024) assessed five global gridded SOC datasets, the HWSD, World Inventory of Soil Emissions Potentials at 30 arc-second resolution (WISE30sec), Global Soil Dataset for Earth System Models (GSDE), Global Gridded Soil

Information at 250-m resolution (SoilGrids250m) and Global SOC Map (GSOCmap), and reported global SOC stock values ranging from 577 to 1,171 Pg C (mean: 828 Pg C) in the top 30cm, and from 1,086 to 2,678 Pg C (mean: 1,873 Pg C) in the top 1m. Notably, GSDE, GSOCmap, and WISE30sec produced similar estimates, whereas SoilGrids250m and HWSD represented the upper and lower bounds, respectively. These variations reflect the persistent uncertainty surrounding SOC quantification.

Sampling depth has also been found to impact SOC stock estimates significantly. Stockmann *et al.* (2013) reported that 2344 Gt of SOC is stored in the top three metres of soil, with 54% or 1500 Gt of SOC stored within the first metre and about 615 Gt of SOC stored in the first 20cm. The IPCC recommends sampling down to 30cm (IPCC, 2019). However, the SOC content in the upper layer of mineral soil would not be an accurate estimation of the total SOC content, as a large part of C is stored in the subsoil (Maillard *et al.*, 2017). Furthermore, global SOC stock calculations may underestimate SOC stocks beyond a depth of 1 metre due to the difficulties and challenges associated with estimating SOC at depth (O'Rourke *et al.*, 2015). Some global estimates of C stored within the terrestrial ecosystem also include inorganic soil C, which increases the terrestrial pool size and further complicates comparisons (Stockmann *et al.*, 2015).

Other sources of uncertainty include uneven geographical sampling and methodological inconsistencies. Soil samples are not evenly distributed across continents, landscapes or even ecosystems (Scharlemann *et al.*, 2014). Variations in measuring stone content and bulk density further affect SOC estimates (Fenton *et al.*, 2024; Tifafi *et al.*, 2018). The resulting methodological heterogeneity highlights the need for improvements in harmonised data collection and processing to yield more accurate global SOC estimates (Scharlemann *et al.*, 2014).

Anthropogenic emissions from fossil fuel burning and land-use change occur on top of the natural global C cycle, which circulates C between the reservoirs of the atmosphere, the ocean, and the terrestrial biosphere (Friedlingstein *et al.*, 2023). Atmospheric CO₂ levels are not rising in direct proportion to fossil fuel use, indicating the presence of active C sinks (Ciais *et al.*, 2019; Grace, 2004; Prentice *et al.*, 2001). Between 2013 and 2023, fossil fuel and industrial processes contributed an estimated 9.6 ± 0.5 Gt C yr⁻¹, and land-use change added 1.3 ± 0.7 Gt C yr⁻¹. Of this, 5.2 Gt C yr⁻¹ accumulated in the atmosphere, while the ocean and terrestrial biosphere absorbed 2.8 ± 0.4 and 3.3 ± 0.8 Gt C yr⁻¹, respectively, as outlined in Figure 2.2 (Friedlingstein *et al.*, 2023). The uncertainties associated with these figures reflect the imperfect understanding and methods to quantify emissions from the various components of these systems.

The global carbon cycle

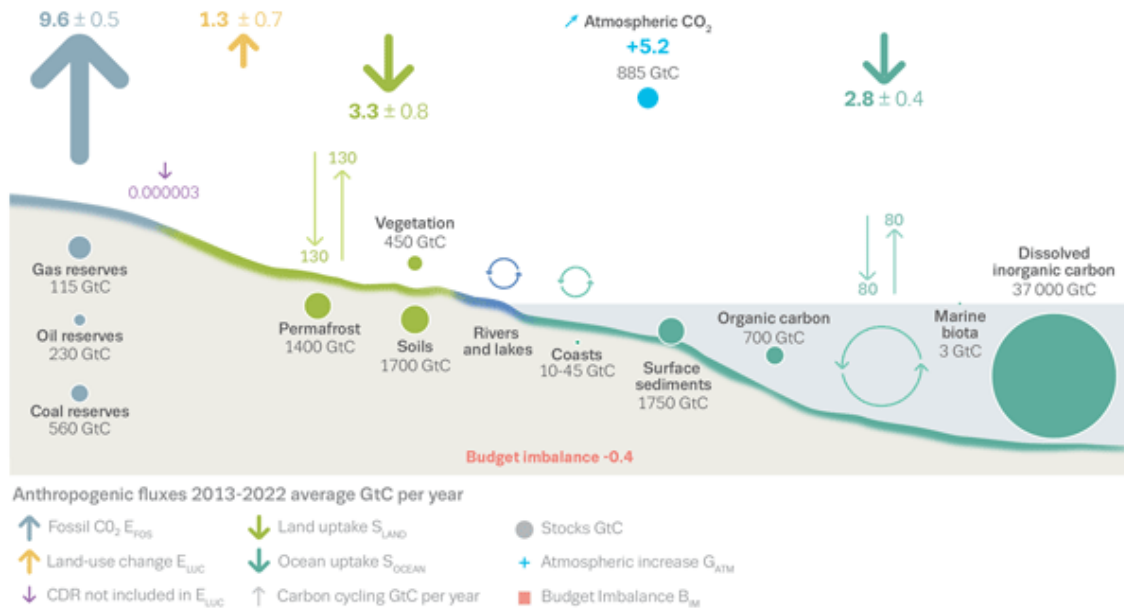


Figure 2.2 Schematic representation of the overall perturbation of the global carbon cycle caused by anthropogenic activities, averaged globally for the decade 2013–2022. The uncertainty in the atmospheric CO₂ growth rate is minimal and is neglected for the figure. Fluxes are in gigatonnes of carbon per year (Gt C yr⁻¹) and reservoirs in gigatonnes of carbon (Gt C). (Source: Friedlingstein *et al.*, 2023).

Direct atmospheric CO₂ concentrations have been measured with high precision since 1957 (Prentice *et al.*, 2001) with the establishment of direct monitoring methods, for example, those established on Mauna Loa by Charles Keeling (NOAA GML, 2025). Pre-1957 atmospheric concentrations are derived from numerous, well-replicated measurements of the composition of air bubbles trapped in ice cores, including Antarctica and Greenland (Grace, 2004; Prentice *et al.*, 2001; Ussiri and Lal, 2017). These records show strong covariation between CO₂ and temperature, linking C cycle dynamics to glacial-interglacial climate transitions (e.g., lowered atmospheric CO₂ during ice age periods) (Falkowski *et al.*, 2000; Ussiri and Lal, 2017).

Numerous other studies have confirmed that the recent and ongoing increase in atmospheric CO₂ concentration is caused by anthropogenic CO₂ emissions, predominantly from the release of C from fossil fuel burning (Friedlingstein *et al.*, 2023; Grace, 2004; IPCC, 2023; Prentice *et al.*, 2001). These emissions are characterised by isotopically ‘old’ carbon, rather than ‘young’ carbon released by vegetation (IPCC, 2023). Although CO₂ is a well-mixed gas in the atmosphere, spatial gradients in CO₂ concentrations exist due to the uneven distribution of sinks and sources, with faster concentration increases observed in the Northern Hemisphere, which is the primary source of most fossil-fuel combustion (Ciais *et al.*, 2019; Malhi, 2002; Prentice *et al.*, 2001). Concurrently, atmospheric oxygen (O₂) is declining at a rate comparable with fossil fuel emissions as combustion consumes O₂ (Prentice *et al.*, 2001). Furthermore, emissions from burning fossil fuels also change the

natural C isotopic composition of the atmospheric CO₂, reducing the ratio of ¹⁴C/C in atmospheric CO₂ (Graven *et al.*, 2020).

The radiative properties of the atmosphere are strongly influenced by the concentration of greenhouse gases (GHGs), primarily carbon dioxide (CO₂), methane (CH₄), and nitrous oxide (N₂O) (Ciais *et al.*, 2013). These polyatomic gases are efficient absorbers and re-emitters of longwave radiation, thereby increasing Earth's radiative forcing, altering the global energy balance. Since the beginning of the Industrial Era, the concentration of CO₂ in the atmosphere has increased by 40% (Ciais *et al.*, 2013), from 280 ppm in 1750 to a progressively faster rate, reaching a value of 367 ppm in 1999 (Ciais *et al.*, 2013; Prentice *et al.*, 2001). Current concentrations of CO₂ are approaching 430 ppm in 2025 (e.g., Friedlingstein *et al.*, 2023; NOAA GML, 2025). This intensification of radiative forcing is the principal mechanism driving anthropogenic climate change.

Climate change is most clearly manifested as an increase in global surface temperatures. During the 2011-2020 period, global surface temperature was approximately 1.1°C warmer than the 1850-1900 pre-industrial period baseline (IPCC, 2023). While a 1.1°C increase may appear modest, even slight shifts in the climate system's mean state can yield disproportionately large increases in the frequency, intensity and duration of extreme weather events (Frank *et al.*, 2015; IPCC, 2023). For example, high northern land areas around the Arctic are warming at almost double the global average, due to Arctic Amplification; similarly, the European continent is warming at a faster rate than evident in the global mean surface temperature (EEA, 2024; IPCC, 2023). These shifts are disrupting ecosystems, reducing agricultural productivity, and amplifying risks to food and water security. Sea level rise, glacier retreat, and ocean acidification are further altering Earth systems, with disproportionate consequences for vulnerable populations and regions (IPCC, 2023).

The terrestrial biosphere has emerged as a critical buffer against climate change, offsetting over one-quarter of anthropogenic CO₂ emissions (Piao *et al.*, 2019). Even minor changes in global SOC stock can have pronounced positive or negative effects on atmospheric CO₂ concentrations (Tifafi *et al.*, 2018). However, human population and economic growth have led to increased exploitation of soil resources to meet the growing demand for food, fibre, and fuel, coupled with urbanisation, which has resulted in the intensification and expansion of available agricultural land (Smith *et al.*, 2016). One of the most notable consequences of converting natural land to agriculture is the loss of SOC stocks (Sanderman *et al.*, 2017).

Given both the magnitude and inherent uncertainty of the global SOC pool, alongside intensifying anthropogenic pressures from agricultural expansion and intensification of soils, soils are increasingly recognised as a critical knowledge gap in national GHG

inventories and our broader understanding of the global C cycle (Bellassen *et al.*, 2022; Sanderman *et al.*, 2017). A comprehensive understanding of terrestrial C stocks, fluxes and feedback mechanisms is essential for accurately predicting and effectively mitigating future climate change. Despite significant advances, critical uncertainties remain in estimating terrestrial C dynamics, highlighting the urgent need for improved observational, modelling, and inventory approaches.

2.2 Policy and legislation and the role of soils

The international legal foundation for recognising and accounting for land use and land-use change (LULUC) as sources and sinks of GHGs was established in 1994 under Article 4.1(d) of the United Nations Framework Convention on Climate Change (UNFCCC). This article obliges all Parties to “*promote sustainable management and promote and cooperate in the conservation and enhancement of sinks and reservoirs of greenhouse gases, including biomass, forests and oceans*” (UN, 1992). This provision forms the basis for the inclusion of terrestrial C sinks in national GHG inventories and has shaped subsequent developments in climate reporting frameworks.

In response to the commitments outlined in the UNFCCC, the Intergovernmental Panel on Climate Change (IPCC) developed the 1996 Guidelines for National Greenhouse Gas Inventories to provide countries with a standardised methodological framework for estimating and reporting GHG emissions and removals (IPCC, 1997). These guidelines marked the first comprehensive effort to harmonise national reporting practices, ensuring transparency, consistency, and comparability across Parties. They included specific methodologies for assessing emissions and removals from the Agriculture, Forestry, and Other Land Use (AFOLU) sectors, recognising the importance of land systems as both sources and sinks of C.

One of the earliest international agreements to formally acknowledge the role of soils in C sequestration was the 1997 Kyoto Protocol to the UNFCCC (UNFCCC, 1998), which established accounting mechanisms for C sinks, including SOC as part of national GHG emission reduction commitments (Smith, 2004). Under the Kyoto Protocol, Annex I countries were required to use the IPCC 1996 Guidelines as part of their mandatory national inventory submissions to ensure consistency and comparability across countries for compliance with emission reduction targets.

The global recognition of soils' capacity for climate change mitigation was further reinforced in 2015, when the UN declared it the International Year of Soils. In the same year, the adoption of the Paris Agreement at COP21 underscored the urgent need to limit global warming to less than 2°C above pre-industrial levels. During this summit, the “4 per 1000 initiative” was launched, proposing an international target to increase SOC stocks by 0.4%

annually as a nature-based solution to climate change and to aid food security (www.4p1000.org). This initiative marked a renewed emphasis on SOC within both scientific and policy communities, accelerating research into its mitigation potential and integration into climate strategies.

The feasibility and practicality of the ambitious 4 per 1000 Initiative have been widely debated (Minasny *et al.*, 2017; Soussana *et al.*, 2019; Wiesmeier *et al.*, 2020). Minasny *et al.* (2017) estimated that the global agricultural soils' SOC sequestration potential in the top 1 metre is 2-3 Gt C year⁻¹ and could potentially offset 20-35% of global anthropogenic GHG emissions. These estimates align with those of Paustian *et al.* (2016), who reported a mitigation potential of 2.2 Gt C yr⁻¹ from improved management practices on agricultural soils.

Minasny *et al.* (2017) highlighted that soil C sequestration is region and context-specific, with the highest C sequestration rates achievable in soils with low initial SOC stock (<30 t C ha⁻¹) and within the first twenty years of implementing best management practices. In contrast, they also acknowledge that high C sequestration rates are not possible for soils with high initial SOC stocks that are close to equilibrium, degraded soils that require long-term management to restore biological functions, peatlands, shallow soils, and arid and semi-arid climates (Minasny *et al.*, 2017). Soussana *et al.* (2019) argued that the 4 per 1000 target, calculated relative to global topsoil SOC stocks, is consistent with literature estimates of technical SOC potential; however, actual achievable sequestration is likely to be substantially lower due to socio-economic constraints.

Wiesmeier *et al.* (2020) tested the feasibility of the 4 per 1000 initiative in agricultural soils in Bavaria, Southeast Germany. They found that the five best management practices, which included cover cropping, improved crop rotation, organic farming, agroforestry, and conversion of arable land to grassland, resulted in annual SOC increases of 0.3-0.4 Tg, or 0.1% of existing SOC stocks. These results support earlier discussions by Minasny *et al.* (2017) and Soussana *et al.* (2019) that suggest that actual sequestration rates fall short of technical estimates.

Another significant challenge associated with SOC sequestration is the issue of non-permanence (Soussana *et al.*, 2019). Most C offset protocols require that the removal and storage of C from the atmosphere be maintained for at least 100 years to be considered permanent (Climate Action Reserve, 2019). This criterion poses a substantial barrier for SOC-based mitigation, as SOC is inherently dynamic and vulnerable to re-emission, making long-term stability difficult to guarantee (Climate Action Reserve, 2019; Smith *et al.*, 2020). Agricultural land managers often require operational flexibility to respond to market fluctuations, climatic variability, and agronomic constraints, which limit their ability to

sustain consistent SOC-enhancing practices over extended periods (Climate Action Reserve, 2019).

Despite these limitations, the 4 per 1000 initiative significantly raised awareness of the role of agricultural soils in climate mitigation (Minasny *et al.*, 2017; Soussana *et al.*, 2019). It is widely seen as a “no-regret” strategy because increasing SOC supports both mitigation and adaptation through improved soil fertility, water retention, and food security (Soussana *et al.*, 2019). As summarised by Lal (2016), the global initiative to improve and protect SOC stocks while reducing atmospheric CO₂ concentrations should be a priority rather than focusing on specific numbers.

In recent years, global, European, and national policies have increasingly acknowledged the critical function of soil in climate regulation, food security, and ecosystem services. As a result, interest in soil policy has surged in recent years, reflected in increased soil research, a widening group of stakeholders and policy integration (Lal *et al.*, 2021). This is particularly evident in the UN Sustainable Development Goals (SDGs) (UN, 2022). Sustainable management of soil health is essential to achieving several SDGs, such as SDG 1: End poverty, SDG 2: Zero hunger, SDG: Good health and wellbeing, SDG 6: Clean water and sanitation, SDG 7: Affordable and Clean Energy, SDG 9: Industry Innovation and Infrastructure, SDG 11: Sustainable Cities and Communities, SDG 12: Responsible Consumption and Production, SDG 13: Climate Action, and SDG 15: Life on Land (see Lal *et al.*, 2021).

In Europe, soil policies are guided by a suite of frameworks, including the European Green Deal (EC, 2019), the European Commission Soil Health and Food Mission (EC, 2020a), the EU biodiversity Strategy for 2030 (EC, 2020b), the EU Soil Strategy for 2030 (Directorate-General for Environment, 2021a) and the European Missions: A Soil Deal for Europe, the EU Soil Health Law (proposed) (EC, 2021b), and Common Agricultural Policy (CAP) (EC, 2023). A summary of these policies and legislation is outlined in Table 2.1.

While not all policies listed in Table 2.1 explicitly target SOC, they collectively support its broader benefits for soil health and climate mitigation. For instance, the European Missions: A Soil Deal for Europe highlights SOC as a central focus within its efforts to enhance soil health and functionality. The European Green Deal, although not directly legislating SOC-specific measurement or monitoring, promotes land-use strategies that encourage soil C sequestration through initiatives such as the Farm to Fork strategy. Similarly, the CAP incentivises management practices, such as maintaining soil cover and preventing erosion, which indirectly promote SOC accumulation.

Table 2.1 Summary of European policies and legislation related to soil health.

Policy	Objective	Relevance to soil
EU Soil Strategy for 2030	To ensure all EU soils are healthy by 2050 through protection, sustainable use, and restoration.	Establishes a policy framework for monitoring, restoring, and legally recognising soil as a vital resource.
EU Soil Health Law (draft)	To introduce legally binding provisions to achieve healthy soils across the EU by 2050.	First legislative instrument explicitly focused on soil; includes mandatory monitoring and restoration targets.
European Green Deal	To achieve a climate-neutral EU by 2050 through systemic sustainability transitions.	Supports sustainable land use and promotes soil carbon sequestration through the Farm to Fork and Biodiversity strategies.
EU Biodiversity Strategy for 2030	To reverse biodiversity loss and restore ecosystems.	Calls for the restoration of degraded soils and recognises soil biodiversity as critical to ecosystem health.
European Missions: A soil deal for Europe	To establish 100 living labs for soil health innovation by 2030.	Promotes applied research and stakeholder engagement to develop and scale sustainable soil management practices.
Common Agricultural Policy	To support farmers and promote sustainable agriculture.	Integrates soil protection through conditionality rules (e.g., maintaining soil cover, preventing erosion).

However, these policies often present internal conflicts. Balancing soil health objectives with agricultural productivity and economic viability remains a persistent challenge (Lal *et al.*, 2021). The conflict between opposing policies under the same banner of soil health has been widely discussed, most commonly between the intensification of sustainable agriculture and the preservation of increased biodiversity on farmlands (Buitenhuis *et al.*, 2020; Henle *et al.*, 2008; Hristov *et al.*, 2020; Pardo *et al.*, 2020).

Agricultural intensification in Europe has resulted in ecosystem loss and continues to threaten farmland biodiversity (Hristov *et al.*, 2020; Pardo *et al.*, 2020). Many CAP policies include environmental goals, such as improving soil quality, enhancing C storage, and supporting biodiversity, but they often lack practical methods to adapt farming practices to achieve these goals (Buitenhuis *et al.*, 2020). Pardo *et al.* (2020) analysed CAP policies that promote or enhance biodiversity practices on farmland and found that many of these policies were mainly related to neutral or negative effects on biodiversity. As a result, there has been a call for a complete reorientation of the subsidy scheme to provide reform proposals that adequately address climate change and biodiversity loss (Heyl *et al.*, 2020). Similar internal conflicts may exist regarding the increase in SOC storage and the sustainable intensification of agricultural soils. However, this topic is less explored than biodiversity, mainly due to the lack of evidence-based measurement, reporting, and verification of SOC changes on farmland.

At a national level, the Government of Ireland has developed several strategies that refer to soil and aim to address these new and incipient EU policies: (1) The Climate Action Plan 2023; (2) a National Soils Strategy under the Programme for Government: Our Shared Future Report (Department of the Taoiseach, 2020); and (3) the Environmental Protection Agency (EPA) Ireland State of the Environment Report 2020 (EPA Ireland, 2020), which aims to provide a cohesive national framework for the protection, restoration, and sustainable management of soil resources. Additionally, the EPA State of the Environment Report 2020 highlights soil as a critical, yet under-protected, component of Ireland's natural capital, calling for enhanced soil monitoring, data collection, and legislative recognition (EPA Ireland, 2020). These initiatives reflect a growing policy awareness of soil's multifunctionality and its foundational role in achieving environmental sustainability and climate resilience.

2.3 The importance of soils

Healthy, high-quality soils are fundamental to sustaining life on Earth and underpin critical ecosystem services essential for human well-being and societal development (Binner *et al.* 2024). Soils are multi-functional and play a crucial role in sustaining and supporting a wide range of critical ecosystem services, including food, fibre, and energy production, as well as climate change mitigation and flood regulation, improved air and water quality, and biodiversity protection (Garsia *et al.*, 2023; Nune *et al.*, 2021; Smith *et al.*, 2016, 2020). Soil is a finite resource, meaning its loss and degradation are not recoverable within a human lifespan (FAO, 2015). Soil organic matter (SOM) plays a key role in maintaining various soil properties and processes, serving as an essential indicator of soil health (Obalum *et al.*, 2017).

Soil organic matter is a heterogeneous pool of C comprised of diverse materials produced by living organisms, including fine fragments of litter, roots, and soil fauna, microbial biomass, products of microbial decay, and simple compounds such as monosaccharides and polysaccharides (Jansson *et al.*, 2010; FAO, 2005). Soil organic carbon is the elementary C and the measurable component of SOM. Soil organic carbon is formed through repeated recycling of new and existing plant and animal residues by soil microorganisms (Wang *et al.*, 2016). The amount of SOC is a balance between the build-up from inputs of new plant and animal materials, and the constant losses where C decomposes and the constituents separate to mineral nutrients and gases, or are leached away (Senapati *et al.*, 2014). A substantial portion of SOC is generally concentrated within the top 40 cm of soil, with the highest concentrations found in the 0-20 cm depth range (Petropoulos *et al.*, 2025).

Soil organic matter represents a chemically and spatially heterogeneous mixture of organic materials that exist along a continuum of various stages of decomposition (Senapati *et al.*,

2014). It is diverse and complex, existing as a single continuous pool with an almost infinite range of turnover times, from minutes to millennia (FAO, 2005; Senapati *et al.*, 2014). Microbial products have been considered the major components of SOC (Paul, 2016). However, we still have incomplete knowledge of SOC formation with essential knowledge gaps associated with the stabilisation of materials (Cotrufo *et al.*, 2013).

Regardless, the soil microbial community plays a significant role in C cycling, and their activity has been considered the primary driver of differences in the potential to store C in soils (Bhattacharyya *et al.*, 2022). Assessing SOC is vital for evaluating soil and ecosystem functions (Stockmann *et al.*, 2015). Soil organic carbon is considered a keystone indicator because of its pivotal role in soil systems, influencing nitrogen (N) and sulphur (S) delivery to the plants and strongly influencing phosphorus (P), iron (Fe) and copper (Cu) for plant availability, improve soil fertility acting as a plant hormone that can increase root growth and the release of organics by the roots, and detoxify harmful elements, and for binding toxic heavy metals making them unavailable to plants roots (Gerke, 2022).

Natural changes in SOC stock are controlled by the balance between C inputs from plant biomass and exogenous organic supplies and C losses mainly through soil respiration (Beillouin *et al.*, 2021; Jobbágy and Jackson, 2000). Soils absorb CO₂ through plant biomass via photosynthesis, which is driven by photosynthetically active radiation, temperature, soil moisture availability, and leaf area index, resulting in the production of organic C biomass (Leahy *et al.*, 2004). Plant inputs drive decomposition and SOC formation and can be viewed as the controlling pump in the terrestrial C cycle (Paul, 2016). A simplified representation of the soil C balance is provided in Figure 2.3.

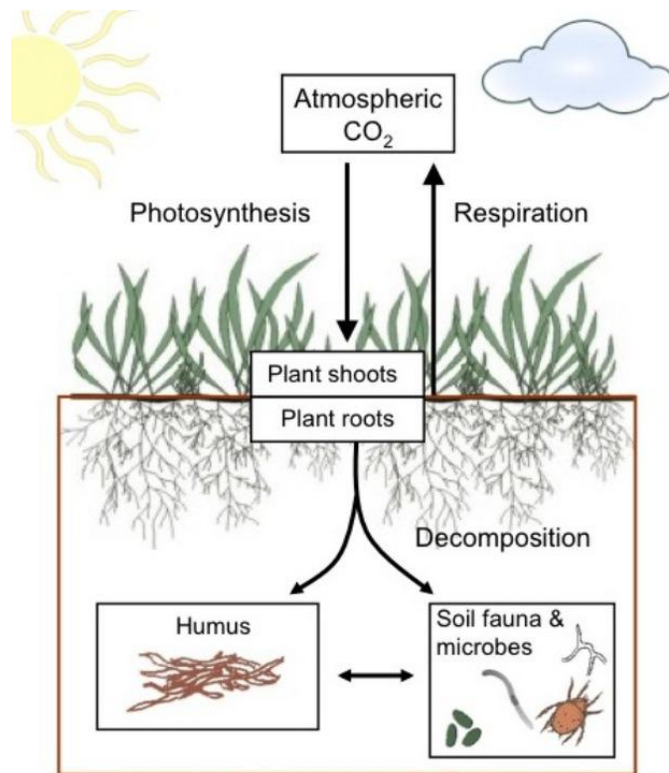


Figure 2.3 A simple diagram of the carbon balance within the soil. Carbon inputs from photosynthesis and carbon losses from respiration control. (Source: Ontl and Schutle, 2012).

Soil respiration is the primary pathway through which CO_2 initially fixed by terrestrial plants via photosynthesis is returned to the atmosphere (Schlesinger and Andrews, 2000). It is commonly defined as the total CO_2 flux from the soil surface, resulting from both autotrophic root respiration and heterotrophic respiration by soil microorganisms decomposing plant litter and SOM (Stockmann *et al.*, 2013). During the decomposition of biomass, most of the C is mineralised and released as CO_2 through soil respiration.

However, a smaller proportion of plant and animal-derived C input is retained in the soil, contributing to the formation and accumulation of SOC (Ontl and Schulte, 2012). Importantly, the processes of photosynthesis and respiration are not perfectly balanced; for SOC to accumulate over long periods, the input of plant residues must exceed the rate of microbial decomposition and mineralisation (Paul, 2016). Agricultural soils are often depleted in C relative to their natural state, primarily due to the export of harvested biomass, intensive soil disturbance, and erosion, which offset C inputs (Paustian *et al.*, 2019b).

Soil carbon sequestration can be defined as the transfer of atmospheric CO_2 into the soil through plants, plant residues and other organic solids, which are stored as SOC (Fuss *et al.*, 2018; Paustian *et al.*, 2019b). It is essential to recognise that soils are unlikely to act as a perpetual sink of atmospheric CO_2 (Smith, 2014) and will eventually reach a steady-state equilibrium, which may fluctuate in response to environmental factors (e.g., climate, management). It is unclear when soil C accumulation might reach a new steady state, mainly because it depends on the interaction between climatic factors, soil type(s) and the

combination of multiple management practices over time (Fornara *et al.*, 2020b; Poulton *et al.*, 2018). However, it is often difficult to distinguish or isolate individual drivers of SOC due to complex interactions of multiple variables within the ecosystem, especially under field conditions (Stockmann *et al.*, 2013).

2.3.1 Climate drivers

Climate conditions, primarily temperature and precipitation, are key direct and indirect drivers of SOC at both global and regional scales. These factors regulate the balance between C inputs, such as plant-derived C inputs and losses, through microbial decomposition and mineralisation (FAO, 2005; Hartley *et al.*, 2021; Wiesmeier *et al.*, 2019). Furthermore, latitude and longitude also influence and govern the general climate conditions, in terms of temperature (e.g., distance from equator) and moisture (e.g., distance from water source) availability, ultimately impacting SOC dynamics (FAO, 2019; Guo *et al.*, 2024; Tang *et al.*, 2018; Zhou *et al.*, 2023).

Several field studies have demonstrated that temperature plays a critical role in controlling the decomposition of plant biomass and microbial activity. Ladd and Amato (1985) reported that the decomposition of leguminous materials in southern Australia followed the same pattern as ryegrass for sites in Nigeria and the United Kingdom, despite differences in plant material and climatic conditions, with the decomposition rates approximately doubling for every 8-9°C increase in mean annual temperature.

Hartley *et al.* (2021) analysed a global dataset consisting of >9,000 soil profiles and found that SOC content in the top 50cm of mineral soil declined significantly with increasing mean annual temperature, declining by a factor of ~1.4 per 10°C (e.g., soil C declines by ~29% for every 10°C increase in mean annual temperature). The impact of temperature on global soil SOC is illustrated in Figure 2.4. Similarly, Okello *et al.* (2023) reported that in situ warming along an elevation gradient led to significant SOC depletion, attributed to enhanced mineralisation and depletion of readily available C, over a two-year warming period. Tan *et al.* (2020), using data from 81 soil samples along a 400 mm isohyet in China, found a negative temperature-SOC relationship, with SOC storage declining at a rate of -0.24 kg m^{-2} per 1 °C increase in mean annual temperature.

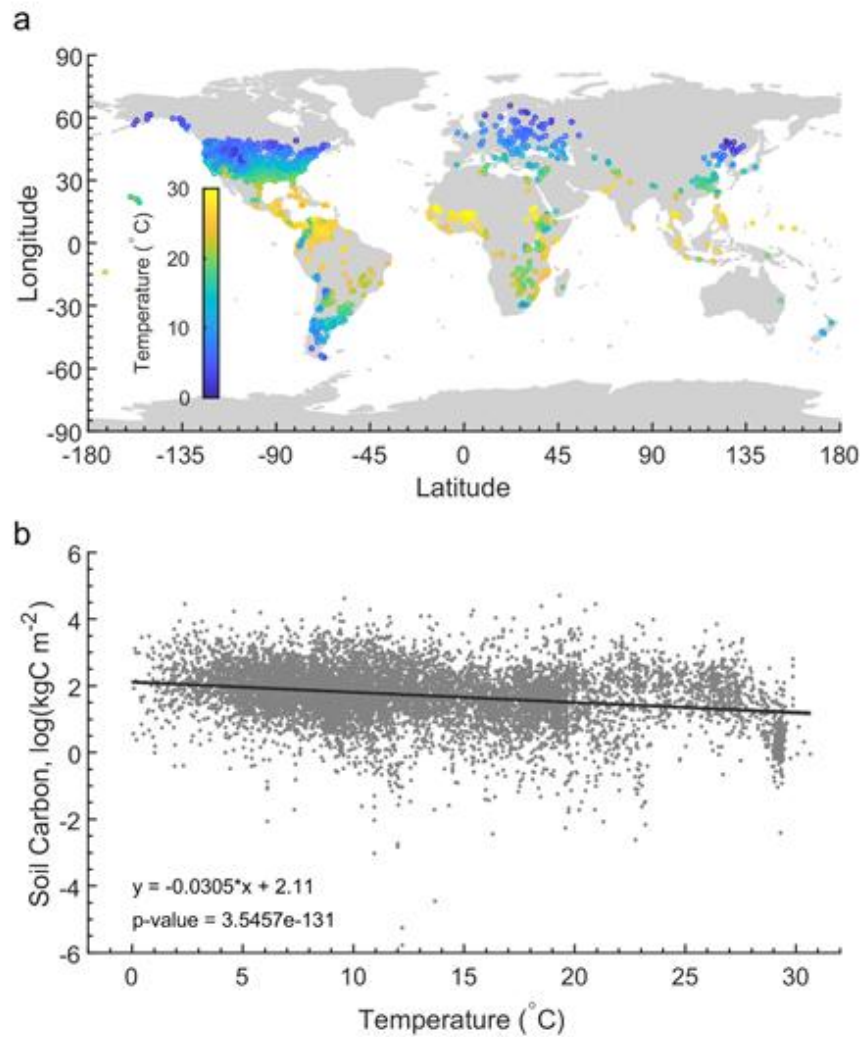


Figure 2.4 Overall effect of temperature on carbon storage. The locations of the soil profiles and temperatures, coloured by annual mean temperature, are outlined in a. The observed relationship between C storage in the top 50cm of mineral soil and mean temperature is outlined in b. (Source: Hartley *et al.*, 2021).

However, temperature's influence on SOC is complex and influenced by soil texture, vegetation type, and depth. For example, Hartley *et al.* (2021) found that the negative relationship between SOC and temperature was more than three times greater in coarse-textured soils, with limited capacities for stabilising organic matter, than in fine-textured soils with greater stabilisation capacities. In contrast, Tan *et al.* (2020) reported that the relationship between SOC and temperature was independent of both soil type and vegetation, suggesting that it may represent a generalizable pattern. Okello *et al.* (2023) further observed that SOC located at high elevations is more vulnerable to increased temperatures due to enhanced mineralisation rates. Overall, these findings suggest that while SOC-temperature relationships may appear broadly consistent in some cases (Tan *et al.*, 2020), their impact can be affected by soil properties and site-specific conditions (Hartley *et al.*, 2021; Okello *et al.*, 2023).

Precipitation is also an important control on SOC dynamics. Soil organic carbon content generally increases with mean annual rainfall due to enhanced plant inputs (in water-limited environments) and reduced decomposition in water-saturated, poorly aerated soils (FAO, 2005; Jobbágy and Jackson, 2000). Wetter climates can promote SOC formation and accumulation by intensifying mineral weathering of the parent material, inducing soil acidification, and enhancing SOC stabilisation, which reduce the rate of SOC decomposition (Wiesmeier *et al.*, 2019). In contrast, arid and semi-arid regions typically exhibit low SOC stocks due to water-limited plant growth and plant-derived C inputs (Han *et al.*, 2024; Jobbágy and Jackson, 2000).

Soil moisture affects SOC directly through its influence on plant photosynthesis and root biomass, and indirectly by altering microbial biomass and enzymatic activities (Han *et al.*, 2024). For instance, in apple orchards in Shaanxi Province, China, Han *et al.* (2024) found that variations in SOC with depth were linked to differences in root dry weight density driven by soil moisture content. Similarly, Peng *et al.* (2023), in a study of 19 North American agricultural sites, identified the Hargreaves climatic moisture deficit (e.g., monthly moisture deficit between Hargreaves evapotranspiration and precipitation for the given area) as the primary climatic determinant of SOC variability under cover cropping systems. However, the degree of soil moisture influence on SOC dynamics is highly variable and dependent on complex interactions between climatic zones, vegetation types and soil characteristics (Han *et al.*, 2024).

In addition, SOM can enhance water availability by increasing aggregate stability and available water-holding capacity (AWHC) (e.g., the water availability for plants to utilise in the soil) due to SOM's hydrophilic properties (Huntington, 2007; Libohova *et al.*, 2018). Libohova *et al.* (2018) found that, in general, a 1% increase in SOM content increased AWHC, on average, up to 1.5% times its weight, depending on soil texture and clay mineralogy. The increase of AWHC was more pronounced for sandy soils, silty clay loam and silt loam soils (Libohova *et al.*, 2018). It demonstrates the complexity of the relationship between moisture and SOC, as moisture can increase SOC accumulation (Han *et al.*, 2024; Peng *et al.*, 2023); however, SOM content can also influence moisture content (Libohova *et al.*, 2018).

Global SOC stocks generally increase in wetter and colder regions and decrease in drier and warmer areas (Stockmann *et al.*, 2013; Wiesmeier *et al.*, 2019). Typically, SOC stocks increase at higher latitudes due to cooler temperatures and lower decomposition rates (Guo *et al.*, 2024) and fluctuate with longitude due to precipitation gradients and regional climate variations (Tang *et al.*, 2018). However, the relationship with longitude appears to be more regionally specific, often influenced by precipitation patterns, which are in turn influenced by unique geographical conditions (Tang *et al.*, 2018).

The climatic drivers of SOC dynamics vary in importance in different regions, scales and depths (Hobley *et al.*, 2015). The influence of climatic drivers on SOC tends to diminish with increasing soil depth, with topsoil SOC being more sensitive to climate variability (Hobley *et al.*, 2015). Spatial scale can also determine the impacts of climate. At larger scales, such as global or regional, climate regulates the metabolic activity of microbes and thus controls large-scale patterns of microbial activity and SOC storage (Bai and Cotrufo, 2022). At the field or farm scale, differences between SOC variability are influenced by other factors such as management (Wiesmeier *et al.*, 2019).

Soil organic carbon stocks are also affected by climate change (Ciais *et al.*, 2005; Frank *et al.*, 2015; Li *et al.*, 2021) by altering the rate of net primary production (NPP) and impacting the type and amount of C inputs into the soil (Stockmann *et al.*, 2013). In the past decade, elevated CO₂ concentrations and rising temperatures have promoted the photosynthesis of European vegetation (Li *et al.*, 2021), which is expected to increase C sequestration (Ciais *et al.*, 2005). However, it remains unclear if increased C sequestration will offset increased ecosystem respiration. Li *et al.* (2021) used a variety of empirical models based on eddy covariance and process-based models, which found no increase in European C uptake from the period 2000 to 2018, as increases in gross primary production (GPP) were offset by the simultaneous increase in ecosystem respiration.

However, the impact of elevated temperatures on SOC varies at specific locations. For example, Siregar *et al.* (2024) found temperate forest ecosystems in New Zealand maintained higher soil respiration rates at higher temperatures without reducing SOC content because higher respiration rates were sustained by higher litterfall rates. In contrast, Soong *et al.* (2021) investigated subsoil (below 20cm) samples from the Sierra Nevada foothills, California, USA, through a whole soil warming field experiment. In this study, soils were artificially warmed by +4°C to a depth of 1m for 4.5 years to simulate future climate change conditions. They observed an in situ decline in SOC stocks despite the increase in plant productivity indicated by CO₂ effluxes. These contrasting results demonstrate the complexities of increased temperatures on forest ecosystems and may indicate that some soils' SOC content may remain stable under increased temperature due to enhanced plant productivity.

Extreme temperature events (e.g., heatwaves) can significantly alter the regional C cycle, causing soils to switch from C sinks to sources (Frank *et al.*, 2015). Ciais *et al.* (2005) used a terrestrial biosphere simulation model to assess continental-scale changes in primary productivity during the European heatwave of 2003. They estimated a 30% reduction in Gross Primary Productivity (GPP) due to rainfall deficits coupled with extreme summer heat over Europe, resulting in a strong net source of CO₂ to the atmosphere and reversing the

effect of four years of C sequestration (Ciais *et al.*, 2005). Additionally, heatwaves in Europe in recent years have resulted in vegetation damage or even death, thereby severely inhibiting the C sink capacity of the terrestrial ecosystem (Li *et al.*, 2021). Moreover, SOC is indirectly affected by climate change, with a higher frequency of fires and pest and pathogen outbreaks during extreme climate events, which indirectly release significant quantities of C into the atmosphere (Frank *et al.*, 2015).

2.3.2 Edaphic and environmental drivers

A wide range of edaphic properties and environmental conditions may directly and indirectly influence SOC dynamics by affecting C inputs, microbial activity and accessibility of C substrates to microbial decomposers (Luo *et al.*, 2021). Luo *et al.* (2021) conducted a global analysis of 141,548 soil profiles to assess the relative impacts of biotic, climatic, and edaphic variables on SOC stocks across four soil depth layers (to 2 m depth). Their findings consistently identified soil-related factors, particularly soil texture, hydraulic properties, and pH, as the dominant controls on the spatial distribution of SOC.

The soil matrix stabilises SOC through a variety of physico-chemical processes (McBratney *et al.*, 2014). Soil organic carbon can be physically protected from decomposition through occlusion within soil aggregates and sorption onto minerals, forming physical and chemical barriers that limit microorganisms' access (Luo *et al.*, 2021). Sand content significantly influences the formation and stability of soil aggregates, thereby regulating SOC stability, soil porosity and oxygen availability, which are critical factors for microbial decomposition (Luo *et al.*, 2021).

Clay is generally considered an important stabiliser that reduces the rate of decomposition (Wei *et al.*, 2014). Prasad and Power (1997) found that organic matter content in fine-textured clay soils was two to four times that of coarse-textured sand soils under similar climate conditions. Similarly, Han *et al.* (2016) reviewed the amount of SOC associated with different soils and textures. They found that the organic C content in soils related to clay, silt, and sand ranged from 0.042 to 12%, 0.012-14%, and 0.010-5.54%, with averages of 3.68%, 3.27%, and 1.93%, respectively. Soils with a high clay content tend to have a higher concentration of SOC because of enhanced soil aggregation and SOC protection by clay minerals, which ultimately increase turnover times and lower decomposition rates (FAO, 2005; Kuśmierz *et al.*, 2023; Schapel *et al.*, 2018).

Parent material also exerts a fundamental influence on SOC dynamics, primarily through its control over soil texture and fertility. Soils derived from nutrient-rich substrates such as basalts are more fertile and typically support greater vegetation biomass, leading to higher C inputs and potentially greater SOC accumulation (FAO, 2005).

Recent developments in soil science have introduced the concept of C saturation, which provides a theoretical maximum potential for SOC sequestration based on mineralogical constraints (Six *et al.*, 2002; McBratney *et al.*, 2014). Angers *et al.* (2011) applied this concept to French Agricultural soils, estimating C saturation deficit as a function of fine particle content (e.g., clay and fine silt). Most agricultural soils were found to be below their SOC saturation potential, indicating additional capacity for SOC storage (Angers *et al.*, 2011).

According to the C saturation concept, the capacity of soils to accumulate stabilised organic C is limited by the number of binding sites on mineral surfaces. However, the concept and application are highly debated (Heinemann *et al.*, 2024; Georgiou *et al.*, 2025). The saturation concept often focuses on mineral-associated organic carbon (MAOC) capacity; however, this is highly debated as the definition of capacity (e.g., lab-based sorption versus field estimates) and divergent methods for quantifying MAOC (Georgiou *et al.*, 2025). Moreover, recent studies challenge the assumption that MAOC content constrains SOC sequestration, suggesting instead that C input rates from biomass are the primary limitation (Heinemann *et al.*, 2024).

Soil pH is a fundamental factor influencing biogeochemical processes in the soil, affecting microbial activity, nutrient availability, and organic matter decomposition (Neina, 2019). Soil pH influences the selective preservation of certain macromolecules during the decomposition of SOC (Wang *et al.*, 2016). The effect of pH on SOC varies among soil types, mineral composition, and sensitivity to pH-driven reactions differ (Kögel-Knabner and Amelung, 2021). For instance, Kuśmierz *et al.* (2023) observed that arable soils in Poland with a neutral to slightly alkaline (6.5-7.2 and >7.2) pH exhibited the highest SOC concentrations, indicating that moderate pH may favour SOC stabilisation. In contrast, Kögel-Knabner and Amelung (2021) reported that alkaline soils may be more prone to SOC losses due to diminished complexation of organic matter with mineral surfaces, as ligand exchange processes are less effective under higher pH conditions. These contrasting findings highlight ongoing uncertainties in understanding pH-SOC interactions, reflecting the broader complexity of edaphic controls on SOC dynamics (Georgiou *et al.*, 2025; Luo *et al.*, 2021).

Furthermore, management has a significant impact on soil pH and its influence on SOC concentration. Ghimire *et al.* (2017) demonstrated that continued application of N fertiliser increased soil acidification and may have negatively impacted SOC, soil N and wheat yields. In contrast, the application of calcium- and magnesium-rich materials to soil (liming) is a common agricultural practice to counteract soil acidity, enhance plant growth and soil C sequestration (Fornara *et al.*, 2011).

Topography and elevation can also influence SOC dynamics. Soil organic matter is often favoured at the bottom of hills or slopes because these areas tend to be wetter, and organic material is frequently transported to the lowest point in the landscape due to runoff and erosion (FAO, 2005). The slope aspect can also influence the dynamics of north-facing slopes (in the northern hemisphere) compared with south-facing slopes because the temperatures are lower (Quideau, 2002). The effects of elevation are highly variable and often dependent on climatic and vegetation interactions (Leifeld *et al.*, 2005; Li *et al.*, 2024), with the relationship between SOC and elevation varying between positive, negative and mixed correlations (Bangroo *et al.*, 2017; Leifeld *et al.*, 2005; Li *et al.*, 2024). In some cases, SOC concentrations increase with elevation due to lower temperatures and higher precipitation, which slows decomposition rates (Leifeld *et al.*, 2005; Li *et al.*, 2024). However, other studies have found negative correlations due to increased soil temperature sensitivity and poorer stabilisation of SOC at higher elevations (Bangroo *et al.*, 2017; Gutiérrez-Girón *et al.*, 2015). Mixed correlations are also common, as elevation effects are often influenced by variations in vegetation, temperature, topography and precipitation at different elevations (Li *et al.*, 2024).

2.3.3 Land-use and management drivers

Land-use and management practices profoundly drive changes in SOC stocks by altering the quantity, quality, and timing of organic matter inputs, which are mediated by both species' composition and broader ecosystem classification (Stockmann *et al.*, 2013). Guo and Gifford (2002), in a review of 74 studies, reported that land-use and land-use change can either deplete or enhance SOC. They found SOC stocks declined after land use changes from pasture to plantation (−10%), native forest to plantation (−13%), native forest to crop (−42%), and pasture to crop (−59%). Soil carbon stocks increase after land use changes from native forest to pasture (+8%), crop to pasture (+19%), crop to plantation (+18%), and crop to secondary forest (+53%).

A global meta-analysis by Beillouin *et al.* (2023) confirmed consistent SOC losses following conversion of forest, grassland, and wetland to cropland, with mean decreases of −25%, −16%, and −25%, respectively. Similarly, Wei *et al.* (2014) found that the largest reduction in SOC stocks from natural forest converted to agricultural land was observed in temperate regions (−52%), followed by tropical regions (−41%) and boreal regions (−31%). Furthermore, Wiesmeier *et al.* (2019) noted that storage in temperate zones typically increases in the order: cropland < forest < grassland, although this order can be altered depending on regional climatic conditions.

It is evident that pastures and forests, whether native or plantation, compared to cropland, are more efficient in storing C in the soil (Söderström *et al.*, 2014). In contrast, SOC depletion

in croplands is driven by erosion, reduced organic inputs, degradation of soil aggregates, and enhanced mineralisation of SOM (Wei *et al.*, 2014; Wiesmeier *et al.*, 2019). Mineralisation is accelerated by increased aeration and elevated soil temperatures following vegetation removal and soil disturbance (Wei *et al.*, 2014; Wiesmeier *et al.*, 2019). However, predicting SOC change after land-use conversion is challenging, as it depends on interactions among ecosystem type, climate, and soil properties (Wei *et al.*, 2014).

Soil management can either enhance or deplete SOC stocks depending on the management practices employed (Gross and Glaser, 2021; Maillard and Angers, 2014). Practices known to promote SOC accumulation include conservation tillage, cover cropping, manuring, integrated nutrient management, and improved grazing (FAO, 2005; Smith *et al.*, 2020; Slessarev *et al.*, 2023). Conversely, decreasing SOC is linked to practices such as burning, overgrazing, residue removal, and bare fallow (FAO, 2005). However, the effectiveness of these interventions depends on edaphic conditions, historical land use, and the initial SOC stock (Stockmann *et al.*, 2013; Slessarev *et al.*, 2023). Two management practices often discussed on a global level to increase SOC content of agricultural soils are tillage management and manure applications.

Tillage is the agricultural preparation of soil by mechanical processes. It is performed because it loosens and aerates the topsoil, facilitates planting and seedbed preparation, mixing of crop residues into the soil and mechanical destruction of weeds (Haddaway *et al.*, 2017). However, conventional tillage may increase compaction of soil below the depth of tillage (e.g., formation of a plough pan), the susceptibility to water and wind erosion, and disturb and aggregate SOC (Angers and Eriksen-Hamel, 2008; Haddaway *et al.*, 2017; Luo *et al.*, 2010). In recent years, less intensive tillage practices, known as reduced tillage and no tillage practices, have been promoted to mitigate some of those negative impacts on soil quality and to preserve SOC (Angers and Eriksen-Hamel, 2008; Haddaway *et al.*, 2017).

Haddaway *et al.* (2017) conducted a systematic review of 351 studies of published research from boreo-temperate regions and found that SOC content was significantly higher in no tillage relative to both intermediate intensity tillage ($1.18 \text{ g/kg} \pm 0.34$) and high intensity tillage ($2.09 \text{ g/kg} \pm 0.34$) in the upper soil layer (0-15cm). Similarly, Angers and Eriksen-Hamel (2008) and Luo *et al.* (2010) found that SOC content in surface layers increased under no-till when compared to full-inversion tillage, and this tendency increases with time. In contrast, cases have also been published where no-till does not increase SOC contents (e.g., Loke *et al.*, 2012) or where no-till with the addition of legume cover crops increased SOC contents (e.g., Boddey *et al.*, 2010).

The influence of management practices on crop residue and SOC decomposition and the distribution with depth remains poorly understood (McBratney *et al.*, 2014). Meta-analyses

on no-till studies in arable systems have found contrasting results for the same management practices when the whole profile is considered (Haddaway *et al.*, 2017; McBratney *et al.*, 2014). Haddaway *et al.* (2017) found that SOC stocks under no-tillage compared to high intensity tillage in the upper 0-30cm soil profile by 4.6 Mg C ha⁻¹ over 10 years, while no effects were detected in the full soil profile. Similarly, Angers and Eriksen-Hamel (2008) and Luo *et al.* (2010) found limiting effects of no-till on SOC stocks when the whole soil profile is considered.

Manure is a collective term for the excreta of different animal species, urine, plant materials, straw, livestock feed residues, and human household waste (Gross and Glaser, 2021). Manure application on agricultural soils is widely regarded as a source of nutrients and a method for maintaining SOC levels to mitigate climate change (Gross and Glaser, 2021; Maillard and Angers, 2014). Milliard and Angers (2014) conducted a global meta-analysis of 42 research articles, totalling 49 sites and 130 observations, and found an overall positive response in SOC stocks, with a significantly larger SOC stock in plots receiving manure compared to control plots (no manure). They calculated an estimated global manure C retention coefficient of 12% for an average study duration of 18 years, meaning 12% of the applied manure is retained in the soil after 18 years (Milliard and Angers, 2014). Similarly, Gross and Glaser (2021) examined 101 studies with a total of 592 manure application treatments on agricultural soils. They found that, on average, the application of manure increased SOC stocks by 35.4%, corresponding to 10.7 Mg C ha⁻¹.

The higher SOC stocks in plots receiving manure are attributed to increased direct C inputs derived from the manure, and indirect C inputs derived from increased NPP and yields (Gross and Glaser, 2021; Maillard and Angers, 2014). Increasing NPP leads to an increase in crop residue inputs and rhizodeposition, which both enhance SOC sequestration (Gross and Glaser, 2021). However, high variation existed among different manure characteristics, soil properties, climate zones and management practices. Manure application was identified as being less effective in tropical climates, sandy soils, soils exhibiting high pH, and soils with initially high SOC stocks (Gross and Glaser, 2021; Maillard and Angers, 2014).

A similar relationship is also observed with mineral fertilisers. Beillouin *et al.* (2023) conducted a second-order meta-analysis comprising over 25,000 primary studies between SOC and various factors, and they concluded that the application of mineral fertilisers resulted in an average increase of +9.4% in croplands and +3.6% in grasslands, which was attributed to increased C inputs from enhanced plant growth.

Soil C's response to land-use change or management can also vary due to legacy effects of the previous or historical land-use or management practices (FAO, 2019). Similar findings suggest that management practices that enhance SOC are most prominent in SOC-poor soils

while having a weak or even negative effect on SOC-rich soils (Gross and Glaser, 2021; Maillard and Angers, 2014; Slessarev *et al.*, 2023). This highlights that the initial SOC condition can determine how effective a management practice will be in increasing the SOC stock.

Furthermore, the longevity of the additional stored C and reversibility of C if retaining practices are not maintained or due to climate variability increases uncertainties in SOC enhancement activities (Rumpel *et al.*, 2020). Management practices that increase SOC stocks can simultaneously increase SOC decomposition. Increased nutrient availability achieved from fertilisation can positively prime dormant microbial activity, which may increase decomposition of old and more stable C (Luo *et al.*, 2016; Stoner *et al.*, 2021).

Regardless, practices that reduce soil disturbance increase the number of organic inputs into the soil, retain plant residues and maintain vegetation to prevent bare soil surfaces are generally understood as practices that can restore or enhance SOC in surface soils by improving soil structure and enhancing nutrition and water retention. There are also other benefits of some management practices that may not directly increase SOC stocks but will increase organic matter quality, enhance structural stability and increase microbial activities, improving soil health (Minasny *et al.*, 2017).

Beillouin *et al.* (2021; 2023) critically assessed and analysed multiple meta-analyses that comprise >25,000 original studies in relation to SOC concentration and stocks. They highlighted the imbalance of SOC studies on specific land uses. Beillouin *et al.* (2021) characterised and assessed 192 meta-analyses of SOC stocks and concentrations, comprising 13,200 original studies conducted from 1910 to 2020 across 150 countries. They observed that most of the meta-analyses focused on croplands (61%), while forest and grasslands accounted for 28% and 23%, respectively. Similarly, Beillouin *et al.* (2023) conducted a second-order meta-analysis comprising over 25,000 primary studies, and from their selection of papers, the number of paired data from each land-use type was as follows: cropland (n=34530), forest land (n=11988), grassland (n=9131), wetlands (n=1267) and other lands (n=4681). Furthermore, in a comprehensive list of global agricultural long-term experiments, only 49 out of >600 experiments were conducted on permanent grasslands (Debreceeni and Korschens, 2003). This highlights that previous research has been more focused on cropland, most likely because they are identified as areas with low SOC stock, and grasslands were often perceived as C-neutral (Poeplau, 2021).

2.4 Importance of global grasslands

Grasslands are ecological communities dominated by grasses with little tree or shrub cover (Dondini *et al.*, 2023). Grasslands are often classified by the intensity of management that occurs on them (e.g., rough, native, improved) or by their climatic region (e.g., temperate,

tropical) (Jones and Donnelly, 2004). Figure 2.5 illustrates the global distribution of grasslands. Natural or native grasslands (often called rangelands) refer to land use dominated by perennial grasses whose species composition has not been altered to improve livestock productivity. In contrast, improved or managed grasslands relate to systems that have been modified to support higher agricultural productivity by sowing more nutrient-rich grass or legumes, using organic and synthetic fertilisation, and improving management practices to support more intensive livestock grazing (Dondini *et al.*, 2023).

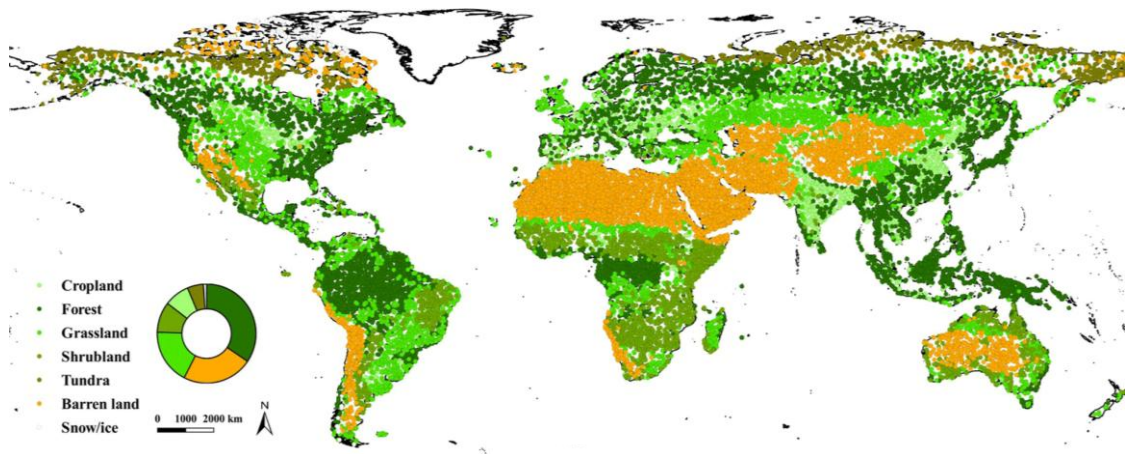


Figure 2.5 Global distribution of grassland, cropland, forest, shrubland, barren land and snow (Source: Liu *et al.*, 2020).

Managed grassland soils can accumulate significant amounts of SOC over time and have the potential to partially mitigate climate change by sequestering atmospheric CO₂ (Fornara *et al.*, 2020b; Stoner *et al.*, 2021). Increases in SOC stocks not only reduce the C footprint of livestock-based systems but also enhance soil health and ecosystem resilience (Fornara *et al.*, 2020b). A defining feature of grassland C cycling is the predominance of belowground C inputs. It is estimated that up to two-thirds of organic matter is contributed through root biomass and decay processes (Quideau, 2002). Root-derived C is more chemically recalcitrant and has a higher stabilisation efficiency than aboveground litter, making it more likely to be incorporated into long-term SOC pools (Bai and Cotrufo, 2022). Furthermore, belowground C inputs tend to have slower turnover rates, increasing their residence time and resistance to decomposition (Jones and Donnelly, 2004).

Despite this potential, many grassland ecosystems have experienced significant SOC depletion due to anthropogenic pressures such as overgrazing, land conversion, and inappropriate management practices (Dondini *et al.*, 2023). However, this trend may be reversible. Practices that enhance plant productivity, particularly root biomass, and that promote the allocation of C from aboveground to belowground pools, can restore SOC stocks and increase long-term C sequestration (Dondini *et al.*, 2023; MacDonald *et al.*, 2018). Common management practices for livestock on grasslands often involve grazing

management and nutrient fertilisation, which can influence SOC dynamics, as outlined in Figure 2.6.

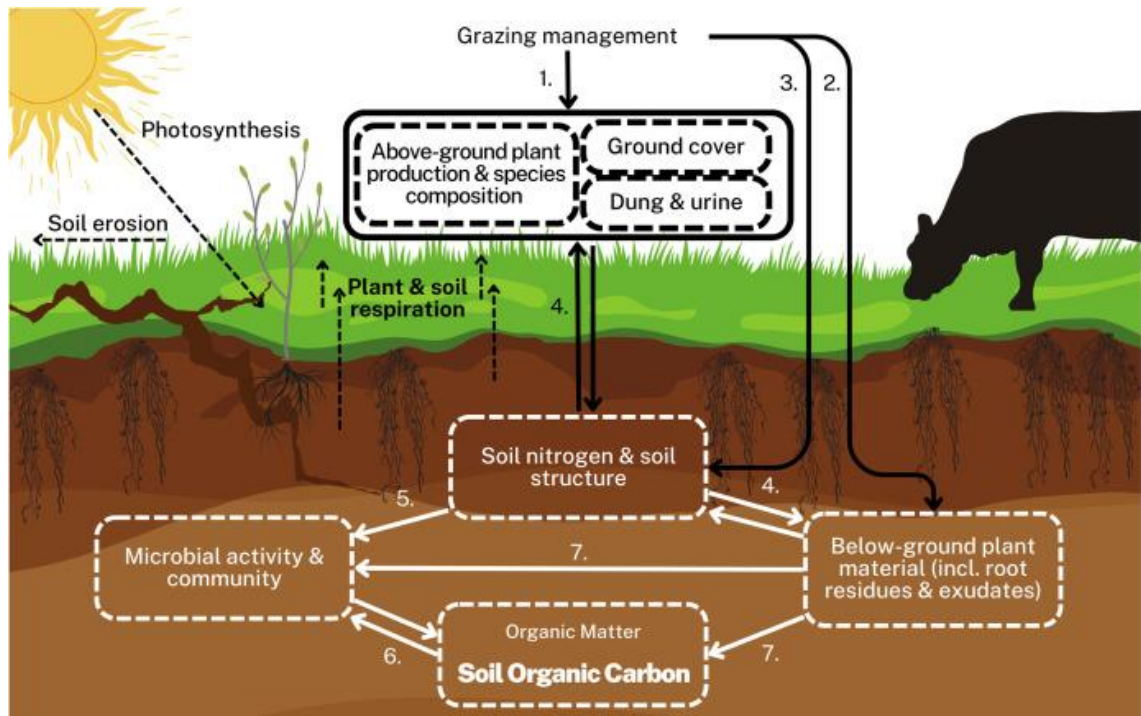


Figure 2.6 Key drivers and processes of soil organic carbon accumulation in grazing systems. 1. Intensity, frequency, timing and duration of stocking impacts above-ground biomass, plant growth rate and species composition, and dung and urine contribution to soil and ground cover. 2. Grazing changes carbon allocation to roots and root growth rate. 3. Management of grazing impacts soil structure, infiltration and potential erodibility. Dung, urine, root carbon allocation and legume composition affect soil nitrogen. 4. Nitrogen increases above-ground plant and root production, and legumes and their symbionts fix atmospheric N. Soil structure impacts above and below-ground plant production. 5. Soil compaction and loss of ground cover reduce soil porosity and infiltration and increase soil temperature fluctuations, leading to changes in microbial activity and communities. N availability impacts the stability of organic matter in soil and soil respiration. 6. Microbes and microbial detritus are components of soil organic matter with various stabilities. 7. Root residues and exudates are significant drivers of microbial activity and contribute directly to soil organic matter (Source: McDonald *et al.*, 2023).

2.4.1 Grazing

Grazing management is a critical determinant of SOC dynamics in grassland ecosystems, with significant implications for C sequestration potential (McSherry and Ritchie, 2013). Grazing intensity has the potential to modify soil structure, function and capacity to store SOC, resulting in both positive and negative outcomes depending on the environmental and management context (Abdalla *et al.*, 2018). The positive effects of well-managed grazing on SOC are typically linked to enhanced root biomass production, the promotion of deep-rooted perennial species, biological nitrogen inputs from legumes, and increased organic matter return through litter and excreta (Jones and Donnelly, 2004; McDonald *et al.*, 2023).

Conversely, overgrazing can lead to SOC losses by reducing vegetative cover, decreasing primary productivity, compacting soils, and enhancing erosion. Additionally, grazing may stimulate microbial turnover and the decomposition of organic matter, which can offset C

gains (Bai and Cotrufo, 2022). Due to the variable and often contradictory impacts of grazing on SOC, a substantial portion of grassland SOC literature has concentrated on grazing-related dynamics (Beillouin *et al.*, 2021).

Numerous meta-analyses have evaluated the impact of grazing intensity, strategy and a wide range of explanatory variables (e.g., soil texture, pH, C/N ratio) on SOC across diverse ecosystems. Byrnes *et al.* (2018), who synthesised 64 studies conducted over temperate and semi-arid grasslands, reported that all grazing intensities and continuous grazing significantly reduced SOC, total N, and the C/N ratio compared with ungrazed systems. Abdalla *et al.* (2018) conducted a global meta-analysis of 83 studies of extensive grazing covering 164 sites and reported that, on average, grazing resulted in a decrease in SOC storage across multiple climatic zones. Similarly, Eze *et al.* (2018) synthesised 341 datasets from five continents and found that, on average, livestock grazing decreases SOC stocks by 15%. Despite methodological differences, a consistent trend emerges across these global syntheses, indicating that continuous and intensive grazing are generally associated with reductions in SOC stocks.

While these global analyses highlight consistent negative trends, many authors emphasise that the relationship between SOC and grazing is highly context-specific (e.g., Abdalla *et al.*, 2018; McSherry and Ritchie, 2013; Phukubye *et al.*, 2022). Abdalla *et al.* (2018) found that all grazing intensity levels increased SOC under a moist warm climate (+7.6%) while there were reductions under a moist cool (-19%). Under dry, warm and dry cool climate conditions, only low (+5.8%) and low to medium (+16.1%) grazing intensities were associated with increased SOC stocks (Abdalla *et al.*, 2018). Eze *et al.* (2018) found the most significant SOC reduction (-22.4%) in the tropics and the smallest reduction (-4.5%) in temperate grasslands due to grazing. McSherry and Ritchie (2013) highlighted that climate and soil can influence the impact of grazers, with an increase in mean annual precipitation of 600mm resulting in a 24% decrease in grazer effect on finer textured soils, while on sandy soils the same increase in precipitation produced a 22% increase in grazer effect on SOC. Together, these findings demonstrate that the impacts of grazing are highly variable but dependent on interactions between climate and soil properties.

Vegetation type also plays a critical role, particularly the distinction between C₃ and C₄ grasslands (Abdalla *et al.*, 2018; McSherry and Ritchie, 2013). McSherry and Ritchie (2013) conducted a multifactorial meta-analysis of grazer effects from 47 independent experiments, and found that increased grazing intensity increased SOC by 6-7% on C₄-dominated and C₄-C₃ mixed grasslands, which are typically located in warmer tropical and subtropical climates, but decreased SOC by an average of 18% in C₃-dominated grasslands, which are more common in cooler temperature regions. Similarly, Abdalla *et al.* (2018)

analysing 164 sites across four climate zones (dry cool, dry warm, moist cool, moist warm), reported the effects of grazing intensity on C₃ and C₄ on SOC were dependent on climate, with C₄-dominated grassland in warm regions generally showing SOC gains, whereas C₃-dominated grassland in temperate and cooler regions tended to show SOC losses.

The form of grazing also impacts the relationship. Byrnes *et al.* (2018) found rotational grazing to have greater SOC content than continuous grazing and was not different from no grazing practices. Other studies indicate that light grazing can show minor adverse effects or even promote soil C storage (Bai and Cotrufo, 2022). In contrast, Phukubye *et al.* (2022) conducted a global meta-analysis of 235 experiment sites in 18 countries in grassland management systems involved in different grazing strategies, intensities, grazers' exclusion, mowing and burning, and indicated that controlled grazing with a high density of grazers increased the average SOC content by 21%, followed by grazing exclusion (SOC increased by 14.9%), and free light grazing (SOC increased by 13.3%), however, grazing exclusion was only beneficial in arid and semi-arid grasslands. McDonald *et al.* (2023) conducted a review of the grazing management impact of SOC in Australia and found no significant impact of stocking intensity or stocking method (e.g., continuous, rotational) on soil C sequestration, but did find positive effects on herbage mass and ground cover with lower stocking rates and resting periods.

The optimal grazing intensity and strategy for SOC are inherently site-specific and must be tailored to local bioclimatic and edaphic conditions (Abdalla *et al.*, 2018; McSherry and Ritchie, 2013). As a result, best practice recommendations vary regionally. For instance, Phukubye *et al.* (2022) recommend the adoption of high-intensity grazing in place of continuous grazing grasslands to mitigate climate change. Whereas, Eze *et al.* (2018) recommended reducing grazing intensity in tropical grasslands to minimise C loss.

2.4.2 Fertilization

Livestock systems receive either organic (e.g., farmyard manure and slurry) or mineral fertilisers, which can contain a combination of macronutrients such as N, phosphorus (P) and potassium (K) to stimulate plant growth (FAO, 2019). Fertilisation affects the coupling of C and nitrogen (C:N ratio) in soils by altering both organic inputs and soil physical structure, thereby modifying SOC dynamics within and across soil aggregate fractions (Fornara *et al.*, 2020a). Nutrient availability can influence SOC cycling in various ways that are not entirely understood and difficult to predict (FAO, 2019).

In Section 2.3.3, we discussed global trends that highlighted that manure and fertilisation application tended to increase SOC stocks. However, these are less effective on soils with initial high SOC stock contents (Gross and Glaser, 2021; Maillard and Angers, 2014). Milliard and Angers (2014) found the average SOC response to manure application was larger when

using control plots (average increase of 9.4 Mg C ha⁻¹) than mineral fertilisers (average increase of 5.6 Mg C ha⁻¹). Furthermore, Gross and Glaser's (2021) results indicated that manure treatments with intermediate initial SOC showed marginal increases in SOC content that often plateau between 11 and 20 years. This has large implications for grasslands as they frequently tend to have relatively high SOC stocks, especially compared to arable soils.

The impacts of organic and mineral fertilisation on grasslands are mixed with varying positive, neutral, and negative impacts, as demonstrated across several long-term field experiments (Bélanger *et al.*, 1999; Hopkins *et al.*, 2009; Poeplau, 2021). Poeplau (2021) investigated several grassland studies examining the effects of management on SOC stocks in Central and Northern Europe and summarised that the addition of 1kg of nitrogen as nitrogen-phosphate-potassium (NPK) consistently led to approximately 1kg of additional SOC. Similarly, Fornara *et al.* (2016) investigated the long-term influence of organic and inorganic fertilisers by examining 43 years of permanent grassland experiments in Hillsborough, Co. Down, Northern Ireland. They found unfertilised control plots showed C sequestrations of 0.35 Mg C ha⁻¹ yr⁻¹ (0-15cm), while high applications of liquid manure increased soil C sequestration to 0.86 Mg C ha⁻¹ yr⁻¹ between 1970 and 2013.

Several studies have reported negligible changes in SOC despite long-term fertilisation. Hopkins *et al.* (2009) found no significant differences in SOC content between 1982 and 2006 for Palace Leas plots in north-east England or between 1959 and 2002 at Park Grass, Rothamsted, under varying long-term management (e.g., no treatment, farmyard addition, N only, P only, N plus K, P plus K). Similarly, Bélanger *et al.* (1999) observed permanent swards in the long-term study in Brunswick, Canada, with four rates of NPK fertiliser and found soil C concentration had remained relatively stable in the 0-15cm layer after 35 years (ranged from 25 to 37 g C kg⁻¹ in 1986 and from 26 to 44 g C kg⁻¹ in 1995). Poulton *et al.* (2018) investigated farmyard manure experimental plots in Park Grass, where 35 t ha was applied every 4 years either with or without additional inputs; they found that over 36 years there was only a modest increase in SOC on two of the treatments and in the following 43 years there was little or no further change (Poulton *et al.*, 2018).

A negative influence on SOC from fertilisation management is less frequently reported but can occur. For example, Sochorova *et al.* (2016) investigated the impact of lime, mineral N and mineral P in a long-term experiment at the Regen Grassland Experiment, Germany, and found that long-term intensive application to maximise hay production significantly reduced (-20%) belowground C storage. Khalil *et al.* (2020) reported a loss of SOC (-3 ± 5%) in Hillsborough long-term experimental plots receiving pig slurry when compared to the unfertilised control and inorganic N fertilisation.

The explanation and potential reasons for SOC increases are inconsistent in these studies. Poeplau (2021) identified that SOC increases were attributed to greater net primary productivity (NPP) and improved microbial anabolic efficiency resulting from increased nutrient availability. Fornara *et al.* (2016) found that enhanced C inputs derived from the liquid manure were the main driver for increased SOC sequestration. In contrast, Bélanger *et al.* (1999) found that the C concentration measured in 1986 and 1995 did not increase with increasing DM yield, but soil C concentrations were greatest in plots with the lowest DM yield.

Potential negative impacts might be explained by slurry-induced priming effects, where high nutrient availability accelerates the microbial mineralisation of native SOC (Fornara *et al.*, 2020b). Furthermore, Sochorova *et al.* (2016) also proposed that fertilisation may shift C allocation from belowground to aboveground biomass, thereby reducing the C in the soil. It is also important to note that any gains in SOC stocks from nitrogen fertiliser could increase N₂O emissions, which could offset gains in SOC sequestration (Oldfield *et al.*, 2021).

Understanding the interactions between increasing inputs and decomposition is essential for informing management decisions to increase soil C stocks (Conant *et al.*, 2017; McSherry and Ritchie, 2013; Stoner *et al.*, 2021). The effects of management on SOC stocks generally decline over time, often requiring long-term field experiments to evaluate the impact (FAO, 2019), however, it is essential to note that management effects on SOC stocks are usually observed from long-term agricultural field experiments, which do not necessarily reflect working farm practices (Oldfield *et al.*, 2021).

2.4.3 Grasslands on organic soils

Global grassland studies predominantly focus on mineral soils, as these represent the most widespread soil type across terrestrial grassland ecosystems. In contrast, organic soils occupy 3% of the global land surface and are largely associated with forested, wetland and tundra regions (FAO, 2020). Grasslands on established organic soils require vastly different management requirements than those on mineral soils.

Organic soils have been artificially drained and degraded over decades for afforestation, peat extraction, agriculture and horticulture, which releases a large amount of emissions due to enhanced decomposition (Tuohy *et al.*, 2023). As a result, the management of grasslands on organic soils typically emphasises restoration rather than productivity enhancement. Site-specific strategies are essential to optimise SOC retention in these systems. In particular, the rewetting of previously drained organic soils, through manipulation of the water table, is increasingly recognised as an effective mitigation strategy to enhance C storage and reduce ongoing emissions (Tuohy *et al.*, 2023).

Although this research predominantly addresses grasslands on mineral soils, acknowledging the unique biogeochemical characteristics and management requirements of organic soils is important. However, detailed exploration of organic grassland systems falls outside the scope of this study.

2.4.4 Sequestration in grasslands

Long-term monitoring of grassland soils has demonstrated their potential to act as significant C sinks. For instance, SOC stocks at the Hillsborough experimental grassland site in Northern Ireland have continued to increase after more than four decades of management, suggesting that these soils have not yet reached C saturation and may continue to sequester C over time (Fornara *et al.*, 2016). In central to northern European long-term experiments demonstrated that increased management intensity (e.g., cutting frequency and mineral fertilisation) led to sufficient sequestration rates that might compensate for increased GHG emissions associated with highly intensive grassland management (Poeplau, 2021).

Estimates of grassland SOC sequestration rates are commonly derived from a combination of empirical observations, process-based SOC models, and eddy covariance flux measurements. Conant *et al.* (2017) estimated the mean sequestration rate of 0.5 tonnes C/ha yr⁻¹ from global grasslands derived from observed SOC increases in managed grassland systems. Similarly, Dondini *et al.* (2023) simulated different management practices that enhance SOC sequestration in global grasslands using the RothC model and estimated a potential increase in SOC content in the top 0-30cm layer by approximately 0.3 t C ha⁻¹ yr⁻¹ after over 20 years. In the USA, conversion to improved grazing has been reported to increase the C sequestration rate by 0.41 to a depth of 50 cm (Conant *et al.*, 2003). In France, using empirical soil data and the RothC model, it was estimated that moderate intensification of improved pasture and planting of hedgerows improved C sequestration rates (0.2 ± 0.25 and 0.1 ± 0.05 , respectively) to a depth of 30cm (Arrouays *et al.*, 2002).

Flux tower studies provide further support for grassland C sink potential. Soussana *et al.* (2007) quantified C budgets across nine European temperate grassland sites under various management regimes using flux towers and found that, on average, these grasslands functioned as net C sinks, with a mean net ecosystem exchange of -240 ± 70 g C m⁻² yr⁻¹, corresponding to a net soil C storage of 104 ± 73 g C m⁻² yr⁻¹. Ciais *et al.* (2010) investigated 20 European grassland sites and found they are acting as a C sink, ranging from 57 to 74 g C m⁻² yr⁻¹ according to the method used for calculation. Byrne *et al.* (2007) integrated eddy covariance flux measurements with detailed farm management records to assess the annual C balance of two Irish dairy farms in 2004. Their analysis revealed that both farms functioned as net C sinks, each sequestering nearly 2 t C ha⁻¹ yr⁻¹. Despite these findings,

significant interannual variability exists in the C balance of grasslands. A 16-year flux tower study on intensively managed grasslands in Switzerland revealed that nine years acted as a C sink and seven as a source, with an average net biome production of $-70 \pm 106 \text{ g C m}^{-2} \text{ yr}^{-1}$, indicating that the system was approximately C neutral (Feigenwinter *et al.*, 2023).

Although several studies have shown that grasslands can function as net CO₂ sinks (e.g., Byrne *et al.* 2007; Conant *et al.*, 2017; Fornara *et al.*, 2016; Soussana *et al.*, 2007), the climate mitigation potential may be limited. For example, Fornara *et al.* (2016) found that increased SOC sequestration in the top 15 cm under intensive management could offset only 9–25% of farm-level GHG emissions. Furthermore, long-term studies at Park Grass (UK) and Brunswick (Canada) have shown SOC stocks in grasslands plateauing over time, indicating saturation and highlighting the need to maintain rather than increase these stocks (Bélanger *et al.*, 1999; Hopkins *et al.*, 2009; Poulton *et al.*, 2018).

Climate change is expected to alter SOC sequestration. In a managed grassland system, SOC stocks will be determined by complex interactions between climate, parent material and the activity of soil microbes, which process C inputs into the rhizosphere and influence the accumulation of C into stable soil organo-mineral pools (Fornara *et al.*, 2020a). Future projected climate change will alter precipitation and temperature events that not only influence SOC dynamics of grassland ecosystems, but also alter plant communities' composition, productivity, C allocation and microbial processes (Bai and Cotrufo, 2022).

Even though there is a growing body of literature demonstrating that improved grassland management can lead to an increase in soil C concentration and stocks, many results do not address several barriers to developing policies intended to bring about increases in soil C stocks as GHG mitigation measures (Conant *et al.*, 2017). Batjes (2019) underlined the large discrepancy between potential and technically achievable SOC sequestration rates, demonstrating that degraded grasslands have the potential to sequester 0.12-0.34 Pg C yr⁻¹, while the currently achievable range was estimated at 0.01-0.05 Pg C yr⁻¹. The potential SOC sequestration rate may not be feasible based on bioclimatic and management constraints (Batjes, 2019).

A significant limitation in understanding global SOC sequestration in grasslands is the paucity of management data. Grassland systems remain underrepresented in global soil monitoring networks relative to forest and croplands (Conant *et al.*, 2017). Knowledge of how the global grazing lands are managed, and the adoption of improved management practices is limited. For example, McSherry and Ritchie (2013) excluded important variables from their grassland meta-analysis, such as fire frequency, soil pH, temperature, type of grazing management, and wild vs domestic grazers, as these variables were rarely measured. Furthermore, information on how grazing land management affects SOC stocks

has been limited to a subset of regions and management practices (Conant *et al.*, 2017), which may restrict insights into SOC processes across the global range of grasslands.

2.5 Quantification of emissions and sequestration

Maximising SOC is crucial for mitigating climate change, ecosystem resilience, and food security. Quantifying SOC stocks and flows within the terrestrial system is an essential element for achieving this. There are several approaches to estimating SOC; the following section will review some of the most common methods.

2.5.1 Direct measurements

Quantifying SOC stocks through direct measurements remains one of the most reliable approaches for assessing terrestrial C storage. This method typically involves field-based soil sampling, in which soil cores are extracted with augers or corers to obtain physical samples for laboratory analysis (FAO, 2019; Kiely *et al.*, 2009). These samples are used to determine bulk density and C concentration, which together facilitate the calculation of SOC per unit area. Standard protocols outlined in the FAO (2019) guidelines specify that SOC measurement requires (i) separation of fine earth (<2 mm) and coarse mineral (>2 mm) fractions, (ii) determination of organic C concentration (%) in the fine earth fraction, and (iii) measurement of bulk density in the fine earth matrix.

Soil C concentration can be measured by either of three methods: dry combustion, loss-on-ignition (LOI), or wet oxidation (Kiely *et al.*, 2009). Dry combustion, typically performed with an elemental analyser, is the most accurate and widely accepted technique, involving the combustion of organic matter at high temperatures to quantify C content. LOI estimates SOC by measuring the mass loss of a soil sample after heating, though it is less precise and can be influenced by soil mineralogy. Wet oxidation, such as the Walkley-Black method, uses chemical oxidants to digest organic carbon, but is considered less reliable due to incomplete oxidation and the hazardous nature of reagents. Each method varies in accuracy, cost, and suitability depending on soil type and analytical objectives (FAO, 2019; Kiely *et al.*, 2009).

Direct measurements rely on appropriate study designs and sampling to deal with the high spatial variability of SOC stocks. Soils must be sampled to capture field-scale variability and provide an unbiased estimate of the mean (Oldfield *et al.*, 2021). Many soil samples are often required at the field scale to provide a reliable estimate of SOC stock with an acceptable error margin (Kuhnert *et al.*, 2022). The FAO (2019) recommends sampling 5-10 soil cores per stratum, with samples collected within a 60-day window and repeated every 4-5 years to monitor temporal changes. However, sampling campaigns will often vary depending on the objective of the research and site conditions (Kuhnert *et al.*, 2022).

However, SOC stock estimates are sensitive to sampling method, especially the approach used for depth stratification. Zhang and Hartemink (2017) present sampling designs for soil profile SOC stock assessment outlined in Table 2.2.

Table 2.2 Summary of profile sampling designs for soil organic carbon (SOC) stock assessment, adapted from Zhang and Hartemink (2017).

Sampling design	Minimum sample size	Summary
Sampling by horizons	2 or 3 transects and horizon-based samples	Soil horizons are accurately delineated, and horizon thickness is measured. Representative samples are collected at the centre of the horizon or bulk samples of the entire horizon.
Vertical transect sampling	2 or 3 vertical transects at fixed intervals	To capture short-range horizontal variations, two or three vertical transects (cores) are required or composited in vertical transect sampling. The depth interval is usually 10 cm when actual soil samples are taken. Smaller increments can be measured in situ or on soil cores.
Depth-based stratified random sampling	10 or 20 samples	It increases the flexibility and estimation accuracy when the horizontal variation is significant, and the SOC concentration decreases with depth.

Wang *et al.* (2017) found sampling by horizon yielded SOC stock estimates 16–22% higher in the top 20 cm and 30–40% higher across the full 0–80 cm profile, relative to vertical transect or fixed sampling approaches. Depth-based sampling is more affordable and easier to implement and often preferred for regional SOC stock sampling campaigns (Gruneberg *et al.*, 2010); however, it ignores the horizontal variation of soil (Zhang and Hartemink, 2017).

Another critical component in estimating SOC stocks is bulk density (Fenton *et al.*, 2024; Li *et al.*, 2019). Bulk density is a basic but important physical soil property related to soil porosity, soil moisture and hydraulic conductivity, which is crucial to soil quality assessment, land-use management and SOC storage estimates (Fenton *et al.*, 2024; Li *et al.*, 2019). Bulk density is often determined or influenced by complex soil-forming processes (e.g., soil types, topography and meteorological factors) and human activities and management (e.g., tillage, machinery, stocking rates, and intensity) (Li *et al.*, 2019). As a result of these influences, bulk density varies with spatial scales and soil depth, contributing to the spatial heterogeneity in SOC (Fenton *et al.*, 2024; Li *et al.*, 2019).

Rock fragments in soils and bulk density are two major sources of uncertainty in depth-based SOC stock calculations, as neglecting rock fragment content can result in systematic overestimation of SOC stocks (Fenton *et al.*, 2024; Poeplau *et al.*, 2017). For instance, Poeplau *et al.* (2017) reported that in stoney soils (rock fragments >30% volume) SOC stocks could be overestimated by more than 100%. Similarly, Fenton *et al.* (2024) compared five different methods to calculate bulk density and found the average relative difference in SOC stocks ranged from 7.7% to 18.9%. However, in some samples, the maximum difference reached as high as 388% (Fenton *et al.*, 2024).

Repeated soil surveys or sampling campaigns rely on resampling locations after varying periods of time. These surveys have the advantage of repeated SOC measurements over large spatial scales and long periods (Smith *et al.*, 2020). The main disadvantage of repeated SOC sampling is that the land management between the sampling intervals is mainly unknown, making it difficult to determine the specific drivers from changes in observed measurements (Smith *et al.*, 2020).

The financial cost associated with sampling is another issue. Mäkipää *et al.* (2008) estimated that a reliable SOC stock change inventory for Finnish forest soils with repeated SOC sampling would take ten years and cost €8 million. The estimated cost of direct SOC measurements in the United States of America (USA) was calculated at \$32 per hectare, and at the same time, the price of C credits for many emerging C crediting organisations suggests \$10-\$15 per credit, demonstrating the financial restrictions on large-scale testing (Oldfield *et al.*, 2021).

Other uncertainties also exist with direct SOC measurements. Soils are heterogeneous, and even at the plot level, measurements have high coefficients of variation in SOC concentration (Luo *et al.*, 2016; Smith *et al.*, 1997). Soils tend to have significant spatial variability and relatively slow C gains, making detecting SOC changes challenging (Smith *et al.*, 2020). Most SOC changes require many years to be detectable by present analytical methods, so long-term experiments are needed (Söderström *et al.*, 2014). Furthermore, every resample represents a new soil sample in time and space, and temporal differences observed through repeated soil sampling are always spatially biased (Hoffmann *et al.*, 2017). Long-term datasets of agricultural field trials do not necessarily capture the natural heterogeneity of SOC, as researchers often implement treatments across replicated field blocks to reduce soil variability (Oldfield *et al.*, 2021).

Point source measurements of SOC stocks are often scaled up to broader spatial extents by scaling the measured value by the area of interest. Upscaling point-based SOC measurements to regional or national scales introduces further error. Multiplying local measurements by landscape area assumes spatial homogeneity, which is rarely the case. Hobley and Willgoose (2010) found that the coefficient of variation in SOC stocks can increase sevenfold when extrapolated to broader scales, underscoring the importance of representative spatial sampling.

Despite these limitations, upscaled SOC data are frequently used in land management and climate policy. These policies typically follow two strategic approaches: (1) identify areas of high SOC and prioritise their conservation to avoid future C losses, and (2) identify areas of low SOC stock and target them for improved land management practices that enhance SOC sequestration, thereby creating a net C sink (FAO, 2019; Smith *et al.*, 2020).

Direct measurements of SOC provide high-quality and accurate estimates of SOC stocks at the site scale. However, their application at larger spatial scales is limited by logistical and financial constraints, including high costs, the need for destructive sampling, and challenges related to standardisation across sites (Scharlemann *et al.*, 2014; Smith *et al.*, 2020). While direct measurements are critical for benchmarking and validation, they are subject to uncertainties stemming from variability in bulk density estimates (Luo *et al.*, 2016) and inconsistencies in sampling methodologies (Zhang and Hartemink, 2017). Furthermore, such measurements yield limited insight into the underlying mechanisms driving SOC dynamics due to infrequent temporal resampling and a lack of integration with process-based information (Chen *et al.*, 2014).

2.5.2 Flux measurements

The flux measurement approaches account for the initial uptake of C through photosynthesis and its subsequent partial losses through soil respiration to measure the net ecosystem exchange (NEE) (Smith *et al.*, 2020). Indirect SOC stock changes can be derived from NEE using two standard methods. Net ecosystem carbon balance (NECB) and trace gas exchange chambers (hereafter referred to as chambers) both measure the gaseous exchange of C inputs and C exports to create a C budget (Hoffmann *et al.*, 2017; Smith *et al.*, 2020). The difference between C uptake and loss determines whether an ecosystem is a net emitter or sequester of CO₂ over short (seasonal) and long (inter-annual) periods (Chen *et al.*, 2014).

Soil Chambers

Chamber systems quantify fluxes over a relatively small surface ($\sim 1 \text{ m}^2$) (Chen *et al.*, 2014). They are typically employed for plot-size field experiments and CO₂ partitioning studies (Chen *et al.*, 2014). They offer an advantage where the exchange rate is highly variable locally (Hutchinson and Livingston, 1993). Chambers provide other benefits, including low cost and ease of use, and they represent the measurement technique of choice in process-level studies and other research requiring replicate measurements in space or time (Hutchinson and Livingston, 1993). Chambers can be open or closed systems. Hutchinson and Livingston (1993) define open chambers as forced flow-through air circulation with air outside the enclosure. Closed chambers have a closed-loop or no forced air exchange in which the emitted gases can accumulate, making these systems more favourable.

Chamber measurement techniques have improved, eliminating pressure inconsistencies between the inside and outside of the chamber at various wind velocities (Riederer *et al.*, 2014). Differences in mean air pressure inside and outside the chamber can generate disturbances, causing pressure fluctuations associated with turbulence, which impact results due to loss of trace gases (Hutchinson and Livingston, 1993). Modern chambers are automatic systems that increase the temporal resolution and allow for the detection of

small-scale spatial differences and treatment comparisons regarding the gaseous C exchange (Hoffmann *et al.*, 2017).

Net ecosystem carbon balance (NECB)

Net ecosystem carbon balance requires flux towers that measure CO₂ continuously without disturbing the environment around the vegetation (Chen *et al.*, 2014). The most commonly used instrumentation is based on the eddy covariance technique. The eddy covariance technique relies on the principle that CO₂ is transported by turbulent eddies (Malhi, 2002). By measuring both the vertical wind velocity and the CO₂ concentration at a high frequency (~10 Hz), required to capture these eddies accurately, the covariance of these two measurements will reflect the vertical flux of CO₂ at that location (Malhi, 2002). Eddy covariance flux towers are applied to measure NEE on a large scale (hundreds of meters to kilometres). As a result, C fluxes based on eddy covariance measurements are integrated over a larger footprint area (Hoffmann *et al.*, 2017).

This method's accuracy is dependent on stable atmospheric conditions, flat terrain, and homogeneous surfaces, as theoretical assumptions must be made (Riederer *et al.*, 2014). However, the values obtained from net C fluxes estimated by flux towers need to be validated against measurements of soil and biomass C stocks (Malhi, 2002). The eddy covariance technique provides the most robust measure of net ecosystem exchange and gross primary production at large scales (FAO, 2019).

Uncertainties associated with eddy covariance towers can be highlighted with tower sites measuring CO₂ fluxes as part of the Large-scale Biosphere-Atmosphere (LBA) experiment in Amazonia Forest in Brazil that measured C uptake rates between 5 and 10 t C/ha yr⁻¹ (Malhi, 2002). However, if such rates were upscaled to the entire Amazonia Forest, it would be sequestering ~10 Gt C yr⁻¹ (Malhi, 2002), which is inconsistent with the global terrestrial C sink of 3.3 ± 0.8 Gt C (Friedlingstein *et al.*, 2023). These inconsistencies are most likely derived from a combination of unmeasured loss of C in the form of dissolved organic C, volatile hydrocarbon emissions, and changes like the air movement at night (Malhi, 2002).

Flux measurements can provide a detailed mechanistic understanding of the process controlling C uptake and release (Malhi, 2002). Coupling flux measurements with direct measurements is a valuable technique for understanding both the principal drivers' short- and long-term effects on ecosystem functioning (Smith *et al.*, 2020). Regardless of the indirect measurement used, estimates of C sequestration from flux measurements remain somewhat uncertain due to the necessary assumptions with data processing, point-in-space measurement (e.g., variable footprint of sensor), and net changes in soil C pools are relatively small compared to C stored in biomass when measured over short periods (Smith

et al., 2020). Furthermore, flux towers are high-cost technologies that often require experts for installation, data processing, analysis and maintenance (Malhi, 2002; Smith *et al.*, 2020).

2.5.3 Remote sensing techniques

Remote sensing (RS) techniques offer a potentially low-cost, fine-scale and global approach to estimating SOC dynamics (Paustian *et al.*, 2019a). Remote sensing methods often rely on the reflectance of light on soil in the infrared region, with organic bonds and minerals in the soil absorbing light at specific wavelengths, resulting in soil content-specific absorbance and reflectance spectrum (Smith *et al.*, 2020). The recommended wavelength for these measurements is the visible near-infrared shortwave between 700 and 2500nm. It shows a good signal-to-noise ratio and is a cost and time-effective option for spectroscopy (Kuhnert *et al.*, 2022). Remote sensing is applied at various scales, from laboratories and small plots to entire fields, using a range of platforms from handheld devices and drones to satellite platforms (Kuhnert *et al.*, 2022).

Remote sensing has seen growing interest as a potential tool for SOC mapping in recent years using satellite technologies. Yuzugullu *et al.* (2024) attribute the growing international interest to four main reasons: 1) Satellite data offers the advantage of efficiency and cost-effectively of monitoring large areas and rapid assessment of SOC distribution; 2) Satellite data can provide information on regions where collecting ground data is challenging or even impossible; 3) High temporal resolution of satellite data facilitates the tracking of SOC dynamics over time, improving our understanding; and; 4) Remote sensing techniques are non-invasive requiring no direct soil interaction.

Remote sensing techniques are relatively new and rapidly improving, but they have many limitations. These include measurements that can be affected by plant cover on the ground, the availability of spectral libraries, and the fact that only the top centimetre can be measured (Kuhnert *et al.*, 2022; Paustian *et al.*, 2019a; Smith *et al.*, 2020). To date, many RS techniques are currently being developed and refined and often applied to limited test areas (Paustian *et al.*, 2019a).

2.5.4 Methods for estimating carbon

The challenges associated with direct measurements, including more indirect flux methods, have led to the development of alternative techniques to estimate SOC. One popular alternative is the use of SOC models. A model is a simplified mathematical representation designed to meet different objectives. Soil organic carbon models represent the turnover or decomposition of SOC and its transformation in the soil-plant-atmosphere system (Senapati *et al.*, 2014). Soil organic carbon models are generally used to scale up short- and long-term field experiments and can provide accurate estimates of SOC stocks and soil carbon

sequestration, provided the model(s) used are correctly calibrated and constrained. Models range in complexity from simple empirical-based stock change models to dynamic complex ecosystem models (Campbell and Paustian, 2015; FAO, 2019; IPCC, 2019). Many countries use the former, which may under- or over-estimate SOC (Bellassen *et al.*, 2022; Goglio *et al.*, 2015).

The IPCC produce guidelines for national GHG inventories and provides a standardised internationally agreed framework for methodologies intended for use by countries to estimate GHG inventories to report to the United Nations Framework Convention on Climate Change (UNFCCC) (IPCC, 2006). Even though there is no universally agreed-upon approach to estimating SOC stocks using model-based approaches, the IPCC guidelines are one of the most popular approaches (Del Grosso *et al.*, 2016; Paustian *et al.*, 2019a). The IPCC guidelines represent SOC models within a multi-tier methodology, which determines the data requirements of the model used to derive the SOC estimate. Tier 1 is the most basic method, tier 2 is intermediate, and tier 3 is the most demanding regarding complexity and data requirements (Del Grosso *et al.*, 2016; IPCC, 2006, 2019).

IPCC Tier 1 Approach

The IPCC Tier 1 approach, which is an accounting-based method, combines information on the extent of human activity (called activity data or AD) with coefficients estimating emissions or removals per unit activity (emission factors or EF). The basic equation is therefore:

$$Emissions = AD \times EF \quad (2.1)$$

Equation 1 is standard for all Tier 1 methods. The IPCC guidelines include standard reporting tables covering all relevant categories and provide an application method for the most basic (or Tier 1) estimation methodology (IPCC, 2006). However, variations of this equation exist and often depend on the sector.

Tier 1 methods are empirical-based models for estimating SOC stock change (Paustian *et al.*, 2019a). This method estimates SOC stock change in the Agriculture, Forestry and Other Land Use (AFLOU) sector by first assigning a reference SOC value based on scale, climate, soil type and other factors (IPCC, 2006). The reference value is multiplied by factors representing the quantitative effect of changing grassland management on SOC storage (FAO, 2019). Stock change factors are derived from global, regional, or national experiments (IPCC, 2006). Soil organic carbon stocks under the Tier 1 approach are estimated as follows:

$$\Delta C_{Mineral} = \frac{(SOC_0 - SOC_{(0-T)})}{D \text{ or } T} \quad (2.2)$$

$$SOC_{Mineral} = \sum_{c,s,i} SOC_{REF_{c,s,i}} \times F_{LU_{c,s,i}} \times F_{MG_{c,s,i}} \times F_{I_{c,s,i}} \times A_{c,s,i} \quad (2.3)$$

(Note: T is used in place of D in equation 2 if T is ≥ 20 years)

where,

$\Delta C_{Mineral}$ = annual change in organic C stock in mineral soils (tonnes C yr⁻¹)

SOC_0 = mineral SOC ($SOC_{Mineral}$) in the last year of an inventory period (tonnes C)

$SOC_{(0-T)}$ = $SOC_{Mineral}$ at the beginning of the inventory time period (tonnes C)

T = number of years over a single inventory time period (year)

D = time dependence of mineral SOC stock change factors, the default time period for transition between equilibrium SOC values. It is commonly 20 years, but it depends on the assumptions made in computing the factors. If T exceeds D, use the value.

c = represents the climate zones included in the inventory

s = represents the soil types included in the inventory

i = represents the set of management systems included in the inventory

$SOC_{REF_{c,s,i}}$ = the SOC stock for mineral soils in the reference conditions

$F_{LU_{c,s,i}}$ = stock change factor for land-use system or sub-system for a particular land-use.

$F_{MG_{c,s,i}}$ = stock change factor for management regime, dimensionless

$F_{I_{c,s,i}}$ = stock change factor for the input of organic amendments

$A_{c,s,i}$ = the land area of the stratum being estimated, ha

Tier 1 methods are simple in design and use default parameter values derived from global data sources. Hence, they tend to be spatially coarse and general in nature, meaning they often group diverse soil types, land uses and climate zones into generalised categories rather than accounting for regional or site-specific variability (Paustian *et al.*, 2019a). The IPCC (2019) recognise the limitations of Tier 1 approaches and advocates for more complex Tier 2 and Tier 3 approaches. The Tier 1 method is meant to represent average SOC changes over large land areas that integrate many different cropping systems and practices that are not explicitly defined in the method and should not be applied to plot-level observations (Del Grosso *et al.*, 2016).

IPCC Tier 2 Approach

Tier 2 methods can use the same methodological approach as Tier 1 (IPCC, 2006) but apply national and regional activity data and emission factors. Tier 2 methods follow the same framework as Equations 2 and 3 but utilise nationally derived SOC_{REF} , F_{LU} , F_{MG} , and F_I from country-specific studies. Tier 2 methods are expected to be more accurate than Tier 1 methods and accurate at the national level (Bellassen *et al.*, 2022). Differences and comparisons between Tier 1 and Tier 2 approaches are outlined in Table 2.3.

Table 2.3 Summary of IPCC Tier 1 and 2 methods for calculating soil C changes adapted from Laamrani *et al.* (2021).

	Tier 1	Tier 2
Scale and Required Data	This corresponds to the default method with emission or stock change factors listed in the guidelines. It corresponds to very large-scale approaches, with average emission factors for major climate zones (e.g., boreal, tropical, and temperate).	It uses the same calculation methods as tier 1, but uses national or country-representative data in the derivation of emissions and stock change factors. It uses specific data linked to a state, region, landscape, or even a project. It requires more accurate emission factors, usually obtained by intensive field measurements at the required scale.
Carbon stocks in soil	Changes in soil C from both organic and mineral soils are used using default coefficients, and the land areas are stratified by climatic region.	Based on direct measurements of soil C stocks. Mutually organic and mineral soils use a mixture of default and country-specific coefficients, and area estimates of increasingly high spatial resolution.

Both empirical-based Tier 1 and 2 approaches often fail to reflect SOC dynamics accurately as they are based on static emissions factors, consider SOC changes linearly over a fixed transition period, and typically only register SOC change following land-use conversions (Bellassen *et al.*, 2022; Goglio *et al.*, 2015; IPCC, 2006, 2019). As a result, SOC reporting for mineral soils has remained relatively stable since 1990 despite three decades of changes in weather and management, as illustrated in Figure 2.7 (Bellassen *et al.*, 2022). A further limitation is that Tier 1 and 2 approaches assume SOC stocks reach equilibrium within 20 years, whereas long-term experiments show that grasslands can require more than a century to stabilise (Poulton *et al.*, 2018). Tier 3 model approaches aim to overcome these constraints by dynamically representing SOC processes, and many authors have advocated for the development of country-specific Tier 3 methods (Bellassen *et al.*, 2022; Del Grosso *et al.*, 2016; IPCC, 2019).

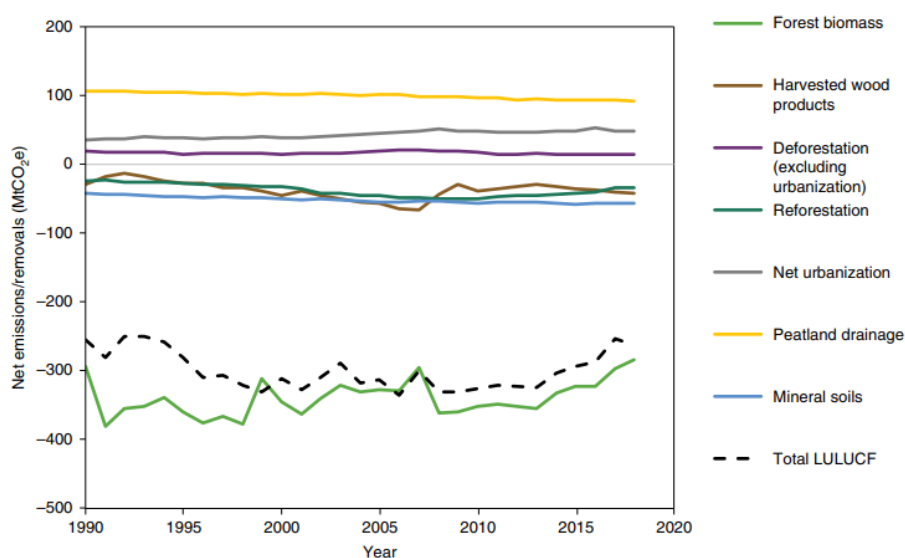


Figure 2.7 Land-related emissions in the EU 27 as reported in national GHG inventories. A negative value indicates a net carbon storage. (Source: Bellassen *et al.*, 2022).

IPCC Tier 3 Approach

Tier 3 SOC models are dynamic and partition SOC into a series of conceptual, functional pools, with flows between them that are governed by first-order kinetics decomposition and regulated by climatic and edaphic rate modifiers (Campbell and Paustian, 2015; Paustian *et al.*, 1997; Sierra *et al.*, 2012; Stockmann *et al.*, 2013). These models have played a crucial role in soil C research by providing a mathematical framework to improve our understanding of soil functioning and processes, supporting hypothesis testing by estimating soil C dynamics across space and time (Campbell and Paustian, 2015; FAO, 2019).

Several models have been developed to simulate soil C (e.g., Campbell and Paustian, 2015; Sierra *et al.*, 2012; Smith *et al.*, 2020). Even within the classification of Tier 3 models (e.g., RothC, CENTURY, ECOSSE, C-Tool, PaSim), there is a broad range of options, including simple C models (that are much more complex than empirical models) to more complex soil-plant-atmosphere models that simulate SOC dynamics along with other environmental processes (e.g., plant growth, soil respiration, soil moisture).

The general applications of SOC models are as follows: 1) to gain a deeper understanding of SOC turnover processes; 2) to support agronomic yield predictions and strategic nutrient management; 3) to aid policy decisions regarding C sequestration strategies; and 4) to investigate the impacts of climate change and land-use change on SOC (Falloon and Smith, 2000). They can be used for interpolation and extrapolation of experimental data, both in time and space, providing a mathematical testing bed for projections of SOC under a diverse range of scenarios. They provide a valuable basis for investigating and exploring SOC interactions, which is sometimes impossible in experimental field studies, once validated. Validating the quantity estimated by SOC models requires well-defined long-term field experiments and a benchmark site to evaluate and validate their predictions (Smith *et al.*, 2020).

2.6 Measuring, reporting and verification

Nature-based solutions such as soil C sequestration have been widely advocated as cost-effective and scalable means of addressing climate change (Brummitt *et al.*, 2024). Agricultural soils have the potential to sequester C and help mitigate climate change. However, there is a pressing need to develop a system to evaluate emerging SOC measurement, reporting and verification (MRV) frameworks (Kuhnert *et al.*, 2022; Oldfield *et al.*, 2021). Land-based GHG emissions and soil C changes are challenging to measure, report and verify (Campbell and Paustian, 2015). Soils are utilised for different purposes and managed by various users with different interests and management practices (Kuhnert *et al.*, 2022). To determine if these different interests are increasing SOC stocks, it is important to rely on a functional and applicable MRV system (Kuhnert *et al.*, 2022).

To date, there is still no global standardised MRV approach. However, there has been development and discussion of generic concepts (e.g., FAO, 2019; Kuhnert *et al.*, 2022; Paustian *et al.*, 2019a; Smith *et al.*, 2020), and recent initiatives have produced early prototypes at national to global scales, including the GSOC-MRV Protocol and GSOCseq map developed by the FAO (Dondini *et al.*, 2023; Peralta *et al.*, 2022). These frameworks combine global datasets, process-based models, and national contributions, offering a harmonised modelling framework.

Despite these advances, most MRV frameworks operate at coarse landscape scale (e.g., gridded approaches that operate at $\geq 1 \times 1 \text{ km}^2$) (e.g., Dondini *et al.*, 2023; Oyesiku-Blakemore and Dondini, 2022; Peralta *et al.*, 2022). While such scales enable broad spatial coverage, they often fail to represent processes at the farm level, the smallest unit of land management and the scale at which most SOC-relevant management practices are implemented. Addressing this scale mismatch is essential for ensuring that MRV frameworks accurately reflect management impacts on SOC. Brummitt *et al.* (2024) identified three critical challenges for MRV systems for management practices that increase SOC stocks, which are: 1) efficiently monitoring field-level activities at large scales and addressing gaps in data; 2) demonstrating that a specific project has an impact that will persist over time, and 3) managing uncertainty and accounting for the variability in inherent agricultural soils.

Measurement, reporting and verification frameworks are based on a combination of methods, outlined in Section 2.4. A central component of MRV frameworks is field measurements, which often constitute high-quality data and can determine an appropriate baseline (Kuhnert *et al.*, 2022). A baseline SOC stock is the SOC stock under 'business as usual' scenarios, which is used to determine changes in SOC from different land-use, management practices and weather or climate scenarios (Dondini *et al.*, 2023; FAO, 2019; Peralta *et al.*, 2022).

Smith *et al.* (2020) outlined a generic concept for an MRV framework as a combination of different approaches to quantify SOC change over time. They list seven components of an MRV framework, including long-term experiment sites, field experiments, site-specific SOC modelling, spatial re-sampling, spatial analysis combined with modelling, collection and aggregation of activity data, and remote sensing techniques (Smith *et al.*, 2020).

Similarly, Paustian *et al.* (2019a) outlined a generic concept for a global soil information system, focusing on a detailed framework that overlaps with Smith *et al.*'s (2020) MRV framework components. Paustian *et al.* (2019a) outlined the central components of a global soil information system that requires the collaboration of soil monitoring networks that consist of long-term field experiments, repeated spatial SOC measurements, SOC models,

spatial data inputs, remote sensing, and collection and aggregation of activity data, as outlined in Figure 2.8.

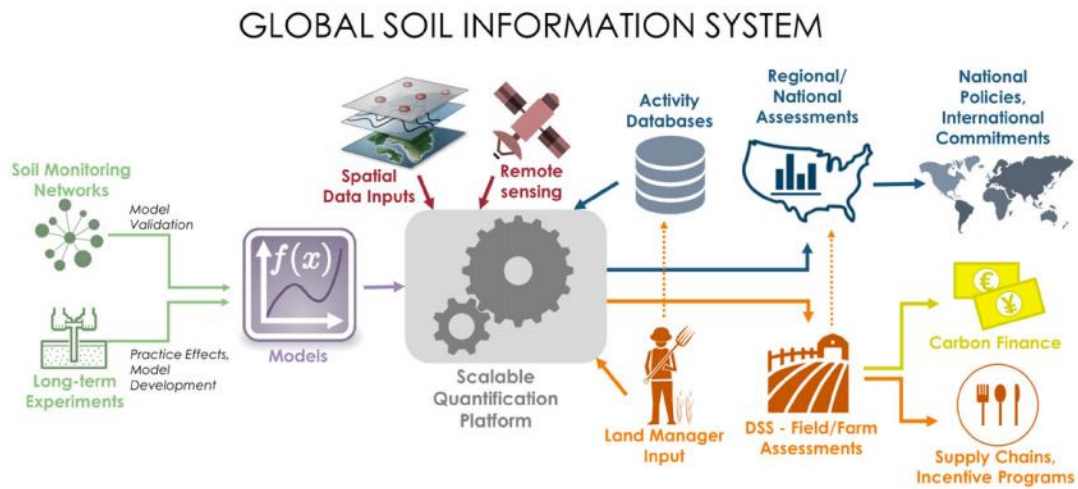


Figure 2.8 Overview of the components and information flow for quantifying SOC stock changes from field to national scale. DDS: Decision support system. (Source: Paustian *et al.*, 2019a).

Both Paustian *et al.* (2019a) and Smith *et al.* (2020) recognise the advantages and disadvantages of the different components. Only the combination of all or at least several of these methods will provide good MRV outcomes (Kuhnert *et al.*, 2022). For example, a combination of direct and indirect measurements (at site-specific scales) and soil carbon modelling (at larger spatial scales) can significantly reduce the cost related to measuring SOC and improve the efficiency of land management (Smith *et al.*, 2020).

As there are limitations to field measurements and indirect measurements, modelling often becomes the most prominent alternative to provide inputs for MRV applications (e.g., Dondini *et al.*, 2023; Paustian *et al.*, 2019a; Peralta *et al.*, 2022; Smith *et al.*, 2020). Models contribute to MRV frameworks in different ways, such as providing baseline information, interpolating measurements and projections, estimating SOC changes and providing information for an optimised measurement plan (Kuhnert *et al.*, 2022).

Both approaches outlined by Peralta *et al.* (2022) and Dondini *et al.* (2023) seek to establish reliable, transparent, and cost-effective mechanisms to monitor and verify changes in SOC stocks in agricultural areas. Both authors agree that the chosen SOC model (in this case, the RothC model) should be continually extended, improved, and updated to better reflect local SOC dynamics and enhance the model's performance.

However, there is little evidence to suggest that existing models can accurately represent SOC dynamics at the field scale for all proposed management practices, soil type and climate combinations (Oldfield *et al.*, 2021). Country-driven approaches using country-specific data and expert knowledge are fundamental to model development and improvements (Peralta *et al.*, 2022). Peralta *et al.* (2022) recommend using a SOC model from the country of interest

or parameterising a model that has been designed for a region with similar climatic and soil conditions. A significant disadvantage of both approaches is that the methodology applies a uniform approach to allow direct comparison between countries, but this will fail to represent country-specific ecosystems, management regimes, climate, and soil types.

National approaches to estimate SOC stocks do exist and are often applied to GHG national inventories, but very few countries have established or implemented Tier 3 methods. National inventories that incorporate Tier 3 methods include Australia, Canada, Denmark, Finland, Japan, Sweden, Switzerland, the United Kingdom (UK) and the United States (Richards, 2001; Shiratio and Taniyama, 2003; Smith *et al.*, 2020). However, most countries listed only apply the Tier 3 method to specific land use types.

The evaluation of Tier 3 models is highly context-dependent (Forrester *et al.*, 2024). Validating national Tier 3 approaches becomes increasingly challenging with the increased complexity of modelling (Bellassen *et al.*, 2022). In addition, many countries do not conduct repeated soil inventories (Bellassen *et al.*, 2022), a critical component for validating SOC models (Paustian *et al.*, 2019a; Smith *et al.*, 2020), which hampers improvements that most national Tier 3 approaches require. Furthermore, the model's performance relies heavily on the quality and quantity of data used in evaluating and validating its performance (FAO, 2019; Peralta *et al.*, 2022). However, modelling approaches must strike a balance between complexity and accuracy to accommodate national utility (Kuhnert *et al.*, 2022).

To date, no universally standardised approach exists for estimating SOC stocks (Kuhnert *et al.*, 2022; Paustian *et al.*, 2019a; Smith *et al.*, 2020). This reflects two primary challenges. First, soil C accounting is a relatively recent focus in both scientific and policy domains, resulting in a diverse range of methods and limited methodological convergence (Bellassen *et al.*, 2022; Smith *et al.*, 2020). Second, and more fundamentally, SOC dynamics are inherently complex and context-specific, governed by interactions among climate, soil properties and land management (Paustian *et al.*, 2019a; Stockmann *et al.*, 2013). Given this heterogeneity, it is unlikely that a single SOC model can capture SOC dynamics across all ecosystems (Peralta *et al.*, 2022). Instead, the future of SOC monitoring will likely rely on a suite of nationally adapted models that are integrated into harmonised reporting systems. This underscores the need for flexible and modular MRV frameworks that can accommodate both the diversity of local conditions and enable credible SOC accounting while accommodating regional variability.

2.7 Summary

Global SOC stocks represent a critical yet highly uncertain component of the global C cycle. Grasslands are one of the most extensive land-use types globally, and play a pivotal role in terrestrial C storage. Despite this, historical research has predominantly focused on arable

and forest soils, resulting in a relative underrepresentation of grassland systems. Grasslands can hold substantial quantities of SOC, particularly where they are intensively managed, underscoring the need for systematic monitoring to support both soil health and climate change mitigation strategies.

While direct measurements of SOC provide high-quality data, their global application is constrained by logistical, financial, and temporal limitations. In this context, SOC modelling provides a robust theoretical framework for estimating SOC dynamics at multiple scales, provided the models are appropriately calibrated and validated. SOC models are a key component of most MRV frameworks and are widely used for large-scale spatial assessments. Numerous SOC models are available, each varying in complexity, data requirements, and suitability depending on research objectives. The RothC model is a popular choice for Tier 3 GHG inventories due to its modest data requirements, and it can be applied across a diverse range of conditions.

Chapter 3: Soil carbon model evolution: generalised model framework

3.1 Introduction

Biogeochemical models play a critical role in soil carbon (C) research, providing a mathematical framework to test and evaluate hypotheses leading to improved understanding of soil processes and their relationship to environmental drivers, and ultimately, enabling soil C dynamics to be estimated across space and time (Campbell and Paustian, 2015). However, numerous biogeochemical models exist; at present, there are estimated to be more than 250 different models and sub-models (LeNoë *et al.*, 2023; Manzoni and Porporato, 2009; Sierra *et al.*, 2012).

Biogeochemical models encompass a variety of frameworks that simulate the biological, chemical, and physical processes regulating C dynamics, nutrient cycling and greenhouse gas (GHG) emissions, with differing levels of complexity. Among these, a subset of models specifically focus on simulating SOC, often called SOC models. In contrast, more comprehensive models such as CENTURY, DNDC and ECOSSE include SOC subcomponents but extend their simulations to broader nutrient cycles and biogeochemical interactions. This chapter predominantly focuses on SOC models, examining both dedicated SOC models and the SOC-related components within the broader biogeochemical models available.

Despite the apparent large number of available models, many SOC models are functionally similar and are designed around a common set of principles. While early reviews of SOC models revealed that many models shared common elements and indicated a convergence of model approaches (McGill, 1996), other studies have demonstrated significant variability in SOC estimates between models (e.g., Smith *et al.*, 1997; Riggers *et al.*, 2019). Understanding the underlying concepts and model structure is necessary to understand why some models exhibit similarities, while others diverge. To demonstrate the similarities and differences between SOC models, we focus the discussion here on 1) Model structure and 2) Model processes.

3.2 Model Structure

Soil organic matter represents a diverse mixture of chemically and spatially heterogeneous organic materials that exist along a spectrum of decomposition stages (Senapati *et al.*, 2014). Consequently, SOC cannot be easily separated into discrete pools, as it is one continuous pool with an almost infinite range of turnover times from minutes to millennia (Senapati *et al.*, 2014). Soil organic carbon models cannot represent this level of complexity within the soil system and therefore simplify it into a set of conceptual pools, each with distinct turnover rates, inputs and decomposition dynamics (Smith *et al.*, 2002; Zimmermann *et al.*, 2007).

Many of the current models have their origins in older models and therefore share common elements. To fully understand current methods, it is important to consider these earlier developments and how various models have co-evolved, often converging towards similar architectures and implementations.

3.2.1 Single pool SOC models

One of the earliest and simplest soil models is Jenny's (1941) model, which is described as:

$$\frac{dX}{dT} = -kX + A \quad (3.1)$$

where, dX/dT represents the rate of change of the state variable (e.g., soil C or N), k is a first-order constant (t^{-1}), and A is the addition rate (mass t^{-1}), which is independent of both loss and amount present, describing C accumulation (McGill, 1996). Jenny (1941) provided one of the first model frameworks to conceptualise SOC dynamics and represents one of the first single-pool SOC models.

Single-pool models consider all SOC within the soil profile as one homogeneous pool and often assume static conditions, where environmental variables remain constant over time (Senapati *et al.*, 2014). However, SOC is inherently heterogeneous, consisting of various pools exhibiting different levels of stability (McGill, 1996). Consequently, single-pool SOC models fail to capture this heterogeneity, as they do not differentiate between SOC pools with distinct decomposition rates and stability levels (Sierra *et al.*, 2012).

One approach to overcoming these limitations was the development of statistical single-pool models. These models incorporate a stochastic component to account for soil heterogeneity (Clifford *et al.*, 2014). However, this approach is only viable if adapted correctly (Clifford *et al.*, 2014) and remains a niche advancement in single-pool C modelling frameworks.

3.2.2 Two-pool SOC models

To account for the varying decomposition rates of SOC, a conceptual framework was developed to better represent actual soil conditions. It involved the introduction of multiple pools, each characterised by its own decomposition rate. Initially, this focused on an additional pool to form a two-pool SOC model to capture the decay dynamics of plant materials in soil (e.g., Henin and Dupuis, 1945; Jenkinson, 1990). Henin and Dupuis (1945) proposed a simple two-pool model, where the annual input of plant carbon (A_c) decomposes very rapidly, forming a quantity of humus carbon (fA_c) that is identical to that already in the soil. The factor f is the isohumic coefficient. This model is expressed as:

$$C = \frac{fA_c}{k} + \left(C_0 - \frac{fA_c}{k} \right) e^{-kt} \quad (3.2)$$

where C is the total SOC at time (t), k is the fraction of C decomposing each year, and C_0 is the initial SOC stock. This model accounted for an initial phase of rapid decomposition followed by a slower, prolonged decay phase

Similar to single-pool models, two-pool models are relatively simple and assume static conditions as environmental variables remain constant (Senapati *et al.*, 2014). Despite their simplicity, two-pool SOC models offer a more complex representation of SOC dynamics than their predecessor single-pool models.

One of the most notable two-pool SOC models is the Introductory Carbon Balance Model (ICBM), proposed by Andren and Kätterer (1997). This model is akin to that proposed by Henin and Dupuis (1945) but includes a term for the dependence of decomposition rates on temperature and moisture; critically, this model implementation opened the pathway for the inclusion of dynamic environmental variables rather than the previously employed static or constant environmental variables. Figure 3.1 outlines a simple flowchart of the ICBM.

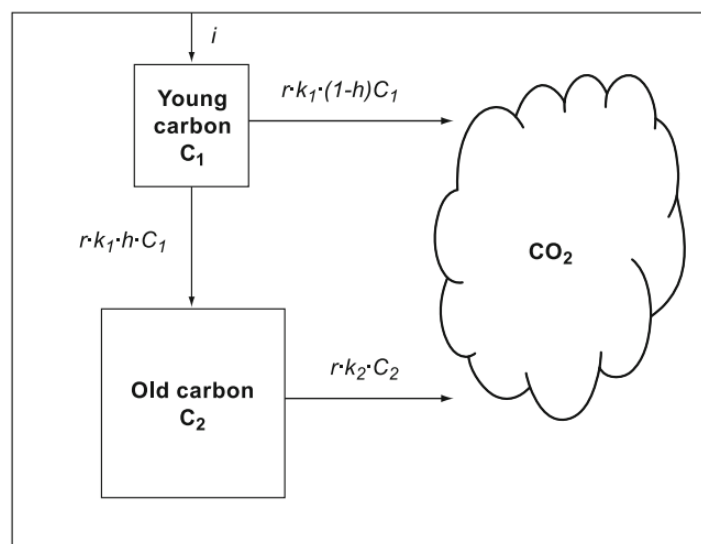


Figure 3.1 The structure of the Introductory Carbon Balance Model (ICBM). There are two pools: young and unstable (C_1), and old and stable (C_2). The decomposition of the two pools depends on climatic factors (r), pool-specific decay rate (k) and the initial carbon pool size (C). The inputs (i) and the pool transfer coefficient (h) are other factors. (Source: Reichstein *et al.*, 2009).

The original implementation of ICBM has been successfully used for several decades to simulate SOC stock across temperate, tropical and humid regions of the world (Riggers *et al.*, 2019). Furthermore, Kröbel *et al.* (2016) proposed an updated model version by segregating C inputs into above and below-ground sources, crop residues and manure with specific humification rates for these fractions.

3.2.3 Multi-pool SOC models

Multi-pool SOC models are broadly categorised into two main groups: organism-oriented and process-oriented SOC models.

3.2.3.1 Organism-oriented SOC models

Organism-oriented models estimate C and N flow through food webs (McGill, 1996). These models are dynamic, accounting for different trophic levels or functional groups of soil biota (Senapati *et al.*, 2014) and are primarily used to describe soil biology in agricultural systems (McGill, 1996). A popular model is the Allison-Wallenstein-Bradford (AWB) model to study the influence of soil microbial processes on C stocks (Allison *et al.*, 2010). The AWB model represents pools of microbial biomass, extracellular enzymes produced by microbes, polymeric SOC that is not available for microbial uptake, and a pool of available dissolved organic carbon (DOC) produced from enzymatic depolymerisation of SOC (Schwarz *et al.*, 2024). A schematic of the AWB model is outlined in Figure 3.2.

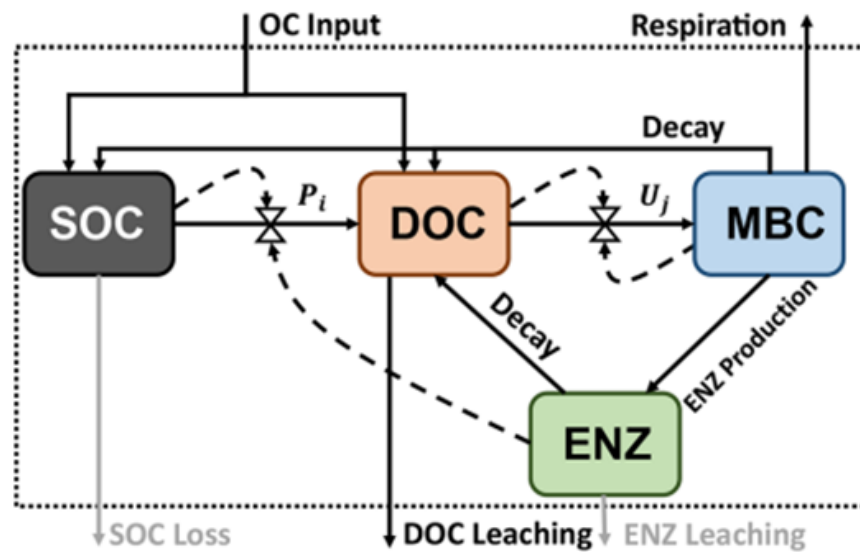


Figure 3.2 Schematic of the Allison-Wallenstein-Bradford (AWB) SOC model. Coloured boxes indicate the state variables of soil organic carbon (SOC), dissolved organic carbon (DOC), microbial biomass carbon (BMC), and extracellular enzymes (ENZs). Solid arrows indicate fluxes, and dashed arrows connected to value symbols indicate controls over the non-linear kinetics. Grey arrows indicate processes neglected in some analyses. The dotted line delineates the system boundary. P_i and U_j are the general depolymerisation and uptake kinetics, respectively. (Source: Schwarz *et al.*, 2024).

However, organism-oriented models simulate the complete soil food web, leading to highly complicated models that tend to be very site-specific (Manzoni and Porporato, 2009), due to the input data requirements. They also face limitations concerning calibration and validation due to the high cost and difficulty of estimating detailed parameters such as feeding preferences, nitrogen content, life cycles, assimilation efficiencies, decomposability, and population sizes (Manzoni and Porporato, 2009; Stockmann *et al.*, 2013).

Organism-oriented models often operate at plot scale with a daily timestep, but this can introduce significant scale-related uncertainties in the representation of microbial and SOC dynamics (Manzoni and Porporato, 2009; Schwarz *et al.*, 2024; Stockmann *et al.*, 2013). These models often exhibit oscillatory behaviour and potential instability at very small spatial and temporal scales, which can emerge from non-linear microbial interactions

between microbial biomass, extracellular enzymes, and substrate pools, as well as substrate-resource dependencies (Manzoni and Porporato, 2009; Schwarz *et al.*, 2024). Such oscillations can realistically capture microscale ecological processes occurring at the soil aggregate or pore scale, including microbial population dynamics and enzyme-mediated substrate degradation (Manzoni and Porporato, 2009).

When organism-oriented models are applied beyond their intended resolution, such as at field, landscape, or regional scales, the intrinsic oscillatory behaviour they simulate can lead to unrealistic outcomes. While plausible at the microscale, these oscillations are generally not observed at broader spatial or temporal scales, because the biological and environmental heterogeneity that drives such dynamics tends to be averaged out, effectively dampening these fluctuations when aggregated across larger extents or over longer timescales (Schwarz *et al.*, 2024). Furthermore, resolving microbial dynamics at such fine resolutions imposes high computational costs and data requirements, limiting more widespread adoption of these models for large-scale ecosystem assessments.

3.2.3.2 Process-oriented models

Process-oriented models are more prevalent in the study of SOC dynamics (Campbell and Paustian, 2015; Senapati *et al.*, 2014; Stockmann *et al.*, 2013), and the remainder of this chapter focuses exclusively on these models. Process-oriented models incorporate both the biological and physical processes governing the movement and transformation of C within soil systems (Senapati *et al.*, 2014). Multi-pool process models typically represent SOC as a finite number of pools, each well-mixed and homogeneous. Differences between pools are characterised by the model structure and pool-specific decay rates (e.g., Campbell and Paustian, 2015; Jenkinson, 1990; Post *et al.*, 1996; Senapati *et al.*, 2014). These models typically feature interactions between pools, with process-based models representing a sequence of C moving from plant and animal debris to microbial biomass and eventually into SOC pools of increasing stability (Senapati *et al.*, 2014). Different stability levels are incorporated through distinct pool-based decay rates, which can be modified by external environmental factors at each time step (Campbell and Paustian, 2015; Post *et al.*, 1996; McGill, 1996; Sierra *et al.*, 2012).

Nearly all multi-pool SOC models include a combination of several types of pools. Typically, incoming plant material is first divided between two pools depending on the assumed decomposition rate (Coleman and Jenkinson, 1996; Parton *et al.*, 1987). Most models will incorporate one or more labile pools, and between one and three physically and chemically protected pools, and finally one passive or inert pool (Zimmermann *et al.*, 2007). The outputs from these decomposable pools usually move into a microbial biomass pool and an anaerobic pool that resists decomposition (Senapati *et al.*, 2014).

In practice, many SOC models opt for a balance that includes three to five pools (e.g., RothC, CENTURY). This aims to provide sufficient complexity to sufficiently represent SOC dynamics while avoiding the over-generalisation of model parameters. A graphical representation of model complexity and the number of pools is outlined in Figure 3.3, which demonstrates how additional pools can increase model complexity by altering the processes of C transfers.

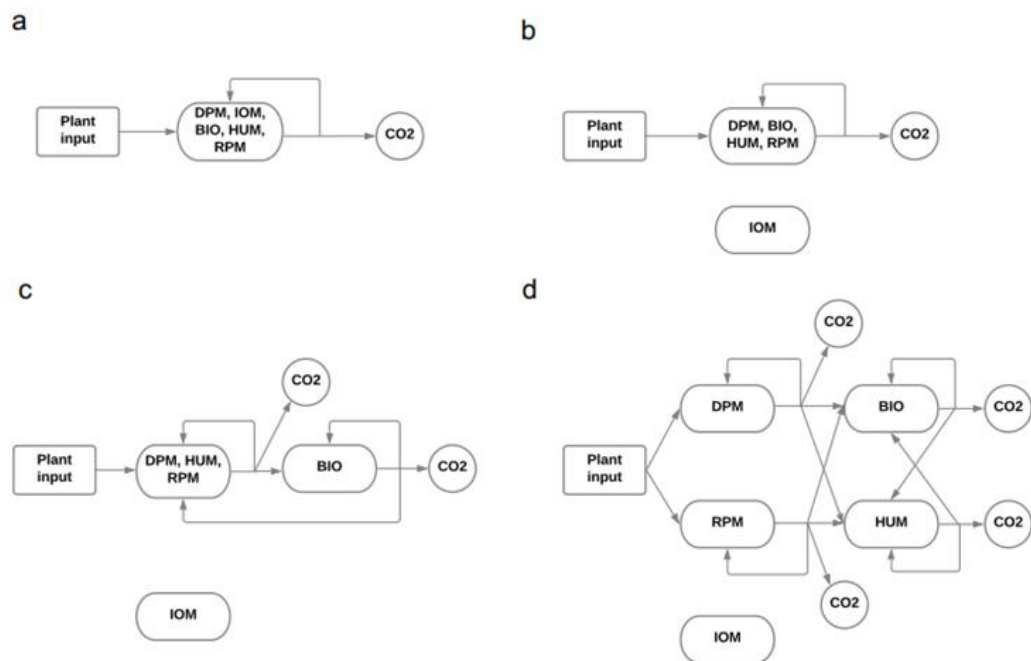


Figure 3.3 Graphical representation of the carbon emissions in (a) one-pool model, (b) two-pool model, (c) three-pool model, and (d) five-pool model. The five-pool model is a flowchart of the RothC model, with the other models being different amalgamations of the same pools. As the number of pools increases, so does the model complexity as there are more parameters and interactions between parameters (Source: Davoudabadi *et al.*, 2024).

While the RothC and CENTURY models differ in scope and complexity, they share common concepts and assumptions (Coleman and Jenkinson, 1996; McGill, 1996; Parton *et al.*, 1987). For example, in the RothC model, C inputs from plant biomass are divided into resistant plant material (RPM) and decomposable plant material (DPM) pools (Coleman *et al.*, 2024). In the CENTURY model, these inputs are split into structural C and metabolic C pools (Parton, 1996a). Both models apply pool-specific decomposition rates influenced by climate and edaphic modifiers to simulate and regulate SOC dynamics. Additionally, both models operate on a monthly timestep and transfer C between pools of increasing stability. A schematic of the CENTURY model is outlined in Figure 3.4, which can be compared to RothC in Figure 3.3d.

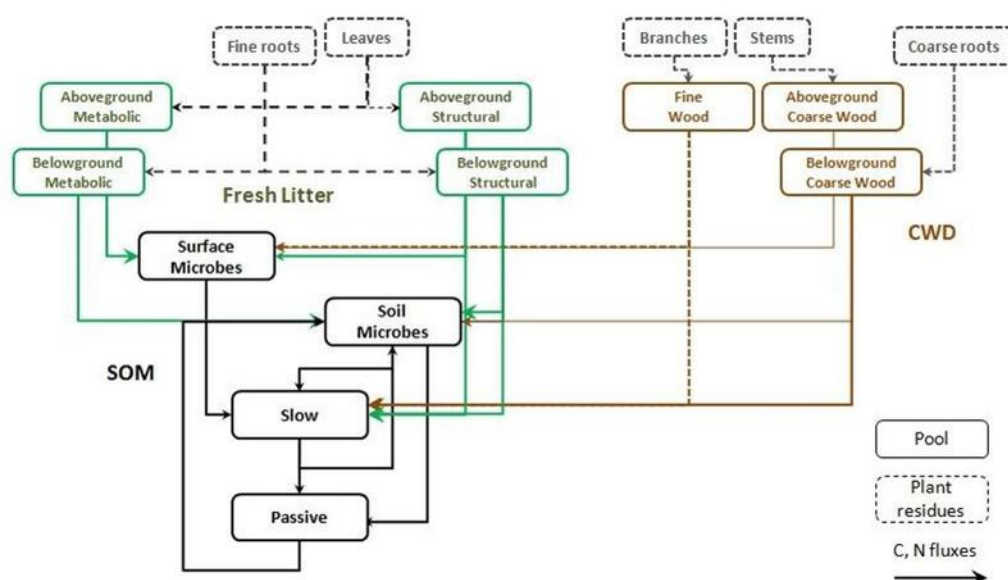


Figure 3.4 Flow diagram of the C flows in the CENTURY model. The flowchart for the CENTURY model is much larger, as it includes additional sub-modules for plant growth, coarse woody debris (CWD) and fresh litter. The graphics in black are the soil organic matter sub-model. (Source: Biondo *et al.*, 2020).

Most present-day models are multi-pool process-based models, with 30 out of the 33 available models on the Global Change and Terrestrial Ecosystem (GCTE) and Soil Organic Matter Network (SOMNET) database being multi-pool process-oriented models (Senapati *et al.*, 2014). Despite the numerous SOC models available, a small selection of specific models has tended to dominate the literature. For example, many authors have noted that the CENTURY and RothC models are two of the most widely utilised models in this field of research (e.g., Campbell and Paustian, 2015; Falloon and Smith, 2002; Sierra *et al.*, 2012). Figure 3.5 demonstrates the popularity via total citations of the most popular soil biogeochemical models.

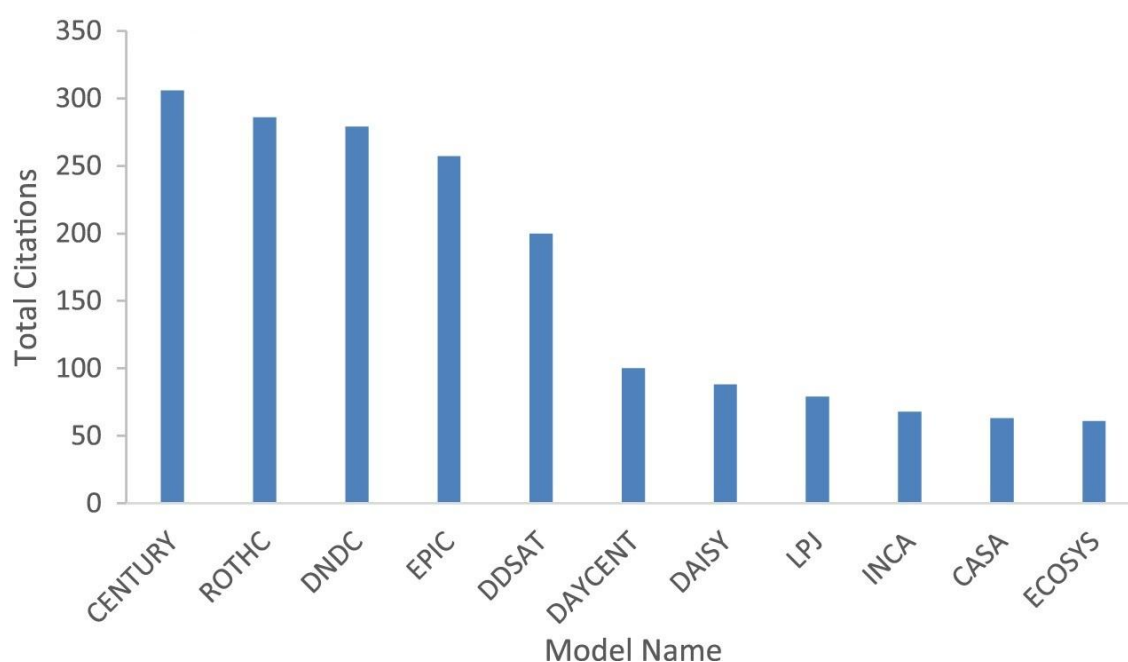


Figure 3.5 Total citations of soil organic carbon models in Web of Science Literature for named models with >50 citations from 1970-2010. EPIC = Environmental Policy Integrated Climate Model. DSSAT = Decision Support System for Agrotechnology Transfer. LPJ = Lund-Potsdam Jena Model. INCA = Integrated Catchment Model. CASA = Carnegie-Ames-Stanford Approach. Source: Campbell and Paustian (2015).

Despite the widespread use of multi-pool SOC models, recent studies have explored model simplification to enhance the predictive accuracy under data-limited conditions. For instance, Davoudabadi *et al.* (2024) developed a novel two-pool RothC model, reducing the original five pools to lower model complexity and thereby reducing the number of required parameters. Their findings suggest that in contexts with limited or sparse time-series data, simplified two-pool models can outperform more complex model structures.

3.2.4 Pool uncertainties

Soil organic carbon models are generally calibrated using field measurements of total C values, with the number and structure of the pools inferred to best represent observed C dynamics (Falloon and Smith, 2000). Carbon pools in models are mostly conceptual; however, some pools can be measured (Christensen, 1996; Zimmermann *et al.*, 2007). For example, most models often contain a microbial biomass pool that can be physically related to field measurements (Christensen, 1996; Coleman *et al.*, 1997). Validating model outputs is essential for reliable SOC estimation (Zimmermann *et al.*, 2007). Measurable SOC pools have been recommended for use in SOC models to replace the conceptual SOC pools approach, which would enhance the confidence of SOC models and reduce some of the uncertainties related to the initialisation of the different pools (Luo *et al.*, 2014; Zimmermann *et al.*, 2007).

Relating modelled to measurable pools is achieved by fractionation. This often involves the physical fractionation of soil samples (however, chemical fractionation is possible but less utilised) to separate them into non-composite fractions (Christensen, 1996; Smith *et al.*, 2002; Zimmermann *et al.*, 2007). A non-composite fraction refers to a fraction that may be composed of many different chemical species, but the decomposition properties are uniform throughout the fraction (Smith *et al.*, 2002).

New fractionation methods are being evaluated to relate models' conceptual pools to measurable pools (e.g., Luo *et al.*, 2014; Smith *et al.*, 2002; Zimmermann *et al.*, 2007). For example, Zimmermann *et al.* (2007) proposed a soil fractionation scheme to derive initial C fractions in soil for initialising the RothC model. Their method combines physical and chemical procedures to isolate five fractions: dissolved organic carbon (DOC), sand and stable aggregates (S+A), particulate organic matter (POM), silt and clay (s+c), and resistant organic carbon (rSOC). In their procedure, POM and DOC are assumed to correspond to RothC's decomposable plant material (DPM) and resistant plant material (RPM) pools, respectively. The humified organic matter (HUM) and microbial biomass (BIO) pools are

inferred as the C remaining in s+c fraction after subtracting rSOC and S+A. The fractionation method of Zimmermann *et al.* (2007) is represented in Figure 3.6.

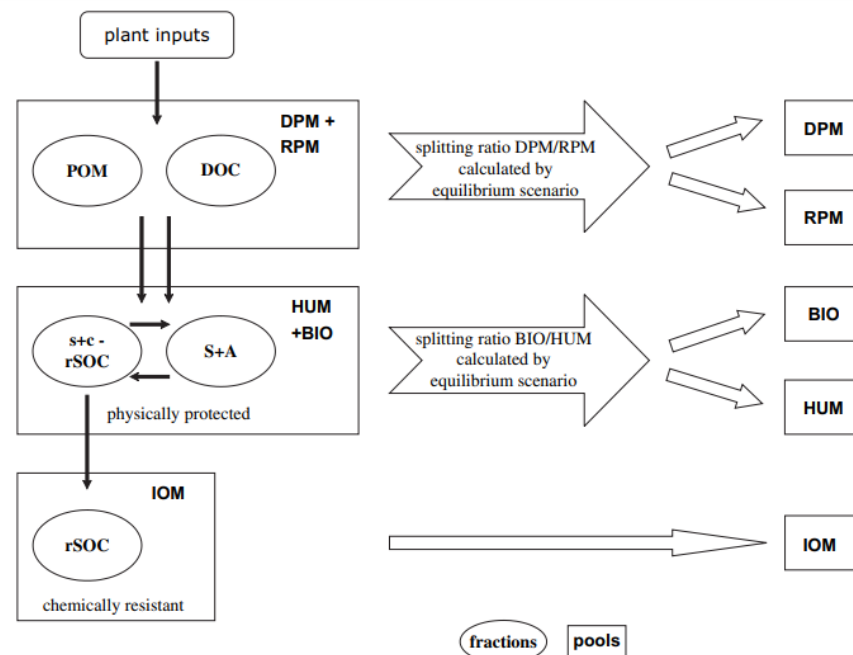


Figure 3.6 Diagram representing the concept of splitting SOC fractions and pools (Source: Zimmermann *et al.*, 2007).

However, Smith *et al.* (2002) suggested that if a model were constructed entirely from measurable pools, simulations would become unreliable in environments different from those where the model was initially developed. Furthermore, Luo *et al.* (2014) demonstrated that the same measurable pool maximum potential decomposition rate varies significantly between sites, supporting the suggestion from Smith *et al.* (2002).

The assignment of fractions is often difficult, requiring more data collection for validation (Stockmann *et al.*, 2013). Many authors have identified the lack of data as a hurdle for model validation (LeNoë *et al.*, 2023; Luo *et al.*, 2014; Smith *et al.*, 2002); increasing data requirements is likely to further prevent uptake.

3.3 Model Processes

It is challenging to compare individual models according to their mathematical formulation because of the large number of different model structures (e.g., number of pools), complexity (e.g., number of variables and processes) and reaction terms (e.g., linear vs nonlinear kinetic laws) (Manzoni and Porporato, 2009). However, most models incorporate similar processes (e.g., climatic, edaphic and management influences) that control SOC dynamics (Post *et al.*, 1996; Manzoni and Porporato, 2009; McGill, 1996). Differences between models typically arise from their structure, their processes and how the underlying complexity is conceptualised and codified (Manzoni and Porporato, 2009; Sierra *et al.*, 2012).

3.3.1 Representation of processes

A clear example of how SOC models differ in their representing of similar pools is the inclusion of a pool that is either inert (e.g., inert organic matter, IOM) or decomposes extremely slowly (e.g., refractory soil organic matter, RSOM) (Falloon and Smith, 2000; McGill, 1996). The IOM pool is assumed to be a small organic pool within the soil that is immune to biological attack (Jenkinson, 1990). It is uncoupled from the active pools and remains static throughout the simulations (Falloon and Smith, 2000). In contrast, some models do not contain any truly inert pool and instead represent a very stable pool, such as the RSOM, which is assigned turnover times ranging from 400-2000 years (Falloon and Smith, 2000; Parton, 1996a). In addition, a number of models include proportions of decomposition products entering the RSOM that increase with clay content (Parton, 1996a). Both approaches have distinct advantages and limitations. If truly inert organic carbon exists (e.g., coal or charcoal), excluding an IOM pool may lead to underestimation of total SOC stocks (Falloon and Smith, 2000). Conversely, models lacking a very stable RSOM component may fail to capture the persistence of long-lived organic carbon in mineral soils.

More sophisticated and complex SOC models often include more pools, intended to enhance the model's ability to represent additional processes that govern the loss or accumulation of SOC (Famiglietti *et al.*, 2021; Sierra *et al.*, 2012). However, the impact of increased structural complexity on the accuracy of model outputs remains unclear. While adding more processes can theoretically enhance the realism of the model, it can also diminish effectiveness by introducing poorly constrained or overly generalised pools and parameters, potentially leading to overfitting (Famiglietti *et al.*, 2021) and limiting the potential application of the model where data may not be available to run a more complex model.

3.3.2 Environmental modifiers

Environmental modifiers typically refer to an environmental factor that alters the decomposition rate and is often applied equally to all pools. Modifiers are typically derived from long-term field data that include gas fluxes, temperature and soil water content measurements collected along a gradient, fitting the observations to the best equation or model (e.g., linear, Arrhenius) and are subsequently parameterised within the model (Del Grosso *et al.*, 2005). For example, temperature modifiers alter decomposition rates based on air or soil temperature (Sierra *et al.*, 2012, 2015). Broadly speaking, environmental modifiers in SOC models are typically based on air temperature and moisture, with rainfall and evaporation employed as surrogates for soil water; these are typically available meteorological measurements (Sierra *et al.*, 2012, 2015). However, soil and management can also be represented through modifiers, altering the transfer coefficients between pools.

3.3.2.1 Temperature modifiers

Temperature modifiers are estimates of potential rather than actual microbial response to soil temperatures (Post *et al.*, 1996) and are often implemented as exponential in form (Campbell and Paustian, 2015; Kirschbaum, 1995). However, one of the most widely used and well-known equations that relates temperature to heterotrophic soil respiration is the Q_{10} , which represents a proportional and linear change in respiration with a 10°C increase in temperature (Campbell and Paustian, 2015; Kirschbaum, 1995; Lloyd and Taylor, 1994). While this relationship is easy to use and provides a ready indication of the temperature sensitivity of the system, it lacks a theoretical justification (Kirschbaum, 1995). The constant Q_{10} equation is considered too simplistic over a wide range of ecosystems; hence many authors have tried to improve the Q_{10} equations (Foley, 1995; Harmon and Domingo, 2001; Lloyd and Taylor, 1994) or by developing soil respiration rates from long-term field experiments (Burke *et al.*, 2003; Jenkinson, 1990; Kelly *et al.*, 2000; Kirschbaum, 1995).

There are several different temperature modifiers, such as Q_{10} , RothC (Jenkinson, 1990), Lloyd and Taylor (LandT) (1994), Demeter (Foley, 1995), Kirschbaum (1995), Daycent (Kelly *et al.*, 2000), Standcarb (Harmon and Domingo, 2001), and Century (Burke *et al.*, 2003; Adair *et al.*, 2008). Different temperature modifiers reflect the range of sensitivities of measuring respiration rates during seasonally varying temperatures and the compounding effects of water availability, litter quality and root respiration (Lloyd and Taylor, 1994; Kirschbaum, 1995). Table 3.1 lists a range of temperature modifiers commonly used within SOC models. These temperature modifiers differ in their functional forms, parameters and complexity, which can be observed through their mathematical representations.

Table 3.1 List of temperature modifiers in the SoilR package (Sierra *et al.*, 2012, 2015) in chronological order. These modifiers are commonly used in SOC modelling studies. In all cases, temperature (T) is expressed as °C. Variables include the temperature sensitivity coefficient (Q_{10}), soil temperature (T_s), maximum temperature (T_{max}), and optimum temperature (T_{opt}).

Name	Temperature modifier	Reference
Q10	$Q_{10}^{\frac{T-10}{10}}$	(3.3)
RothC	$\frac{47.9}{1 + \exp\left(\frac{106}{T + 18.3}\right)}$	(3.4) Jenkinson <i>et al.</i> (1990)
LandT	$\exp\left(308.56\left(\frac{1}{56.02} - \frac{1}{(T + 273) - 227.13}\right)\right)$	(3.5) Lloyd and Taylor (1994)
Demeter	$\exp\left(\left(\frac{\ln(Q_{10})}{10}\right)(T - 20)\right)$	(3.6) Foley (1995)
Kirschbaum	$\exp\left(-3.764 + 0.204T\left(1 - \frac{0.5T}{36.9}\right)\right)$	(3.7) Kirschbaum (1995)

Daycent (1)	$0.8 \exp(0.095T_s)$	(3.8)	Kelly <i>et al.</i> (2000)
Daycent (2)	$0.56 + \frac{1.46 \arctan(\pi 0.0309(T_s - 15.7))}{\pi}$	(3.9)	Parton <i>et al.</i> (2001); Del Grosso <i>et al.</i> , (2005)
Standcarb	$\exp(-T(T_{opt} - T_{lag}))^{T_{shape}} Q_{10}^{\frac{T-10}{10}}$	(3.10)	Harmon and Domingo (2001)
Century (1)	$(\frac{T_{max} - T}{T_{max} - T_{opt}})^{0.2} \exp(\frac{0.2}{2.63} (1 - (\frac{T_{max} - T}{T_{max} - T_{opt}})^{2.63}))$	(3.11)	Burke <i>et al.</i> (2003)
Century (2)	$3.439 \exp(\frac{0.2}{2.63} (1 - (\frac{T_{max} - T}{T_{max} - T_{opt}})^{2.63})) (\frac{T_{max} - T}{T_{max} - T_{opt}})^{0.2}$	(3.12)	Adair <i>et al.</i> (2008)
Linear	$0.198 + 0.036T$	(3.13)	Adair <i>et al.</i> (2008)

To demonstrate the impact of the various temperature modifiers on decomposition rates, the same theoretical temperature range was applied to each modifier shown in Figure 3.7.

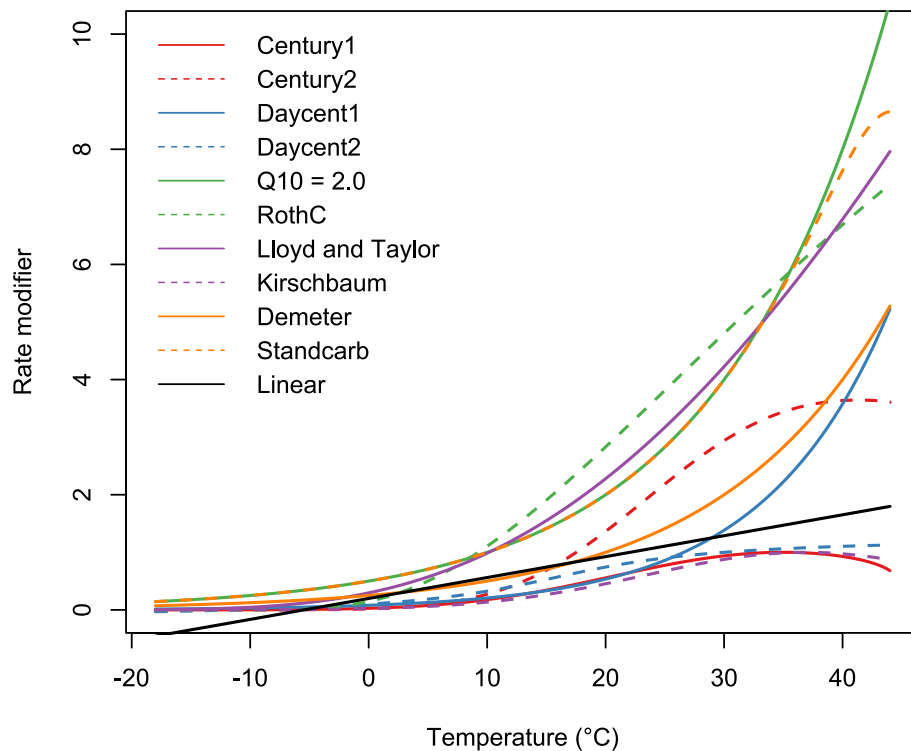


Figure 3.7 The effect of different temperature modifiers on identical artificial data. The graph was created using the SoilR work package developed by Sierra *et al.* (2012, 2015) and their online resources (<https://www.bgc-jena.mpg.de/TEE/basics/2016/04/14/Decomposition-Modifiers/>).

From Figure 3.7, it is evident that the various temperature modifier rates can be summarised into three broad categories of responses: low, intermediate and high, when applied to temperatures above 0°C. Critical differences in the temperature modifiers occur above 0°C as many modifiers indicate little or no impact at or below 0°C, except the linear modifier.

The low response temperature modifiers consist of Century (1), Kirschbaum, linear and Daycent (2). The Century (1) temperature modifier uses maximum and optimum temperatures to capture increasing and decreasing microbial activity around an optimum temperature. Similarly, the Kirschbaum temperature modifier added non-linear temperature dependence; once a certain temperature threshold is exceeded, the rate modifier remains unchanged. Century (1) is the only temperature modifier in the low response category that limits respiration rates once a maximum threshold is reached. The Kirschbaum does not implement a decrease but prevents the rate modifier from exceeding a maximum threshold. The linear temperature modifier is linear with temperature but is often only applied where temperature sensitivity is less complex (Adair *et al.*, 2008). The Daycent (2) temperature modifier uses an arctangent function to capture a smooth response to temperature and does not grow indefinitely. Both the linear and Daycent (2) temperature modifiers do not have a threshold limit.

The temperature modifiers with an intermediate response are Century (2), Daycent (1) and Demeter. The Century (2) temperature modifier is similar to Century (1) but modified for additional scaling to increase adaptability for more temperature ranges. Daycent (1) temperature modifier is a simple exponential function of soil temperature, capturing general temperature sensitivity, and the Demeter temperature modifier uses a logarithmic scaling factor based on Q_{10} . Even though the Daycent (1) and Demeter are slightly different in their formulation, they produce a similar response. The Daycent (1) and Demeter follow an upward curve with no threshold limit. In contrast, within the intermediate response, the Century (2) temperature modifier has a threshold where the decomposition rate no longer increases, exhibiting a downward curve after this threshold.

The temperature modifiers with a high response are Q_{10} , Lloyd and Taylor, Standcarb, and RothC. The Q_{10} temperature modifier is a simple exponential modifier based on a constant coefficient, in which the modifier rate doubles for every 10°C in temperature. The Lloyd and Taylor modifier is a modified Arrhenius-type modifier that captures temperature dependence by considering activation energy. The RothC temperature modifier is exponential and parameterised from long-term field experiments. The Standcarb temperature modifier combines the Q_{10} exponential modifier based on optimal and lag temperatures. These temperature modifiers show a rapid increase in decomposition rates as temperature increases. They also assume that there is no upper temperature limit to respiration. This means they assume a proportional increase in decomposition rates with increasing temperatures, potentially leading to unrealistically high decomposition rates if given extreme temperature inputs.

Consequently, the impact of temperature changes on SOC dynamics remains an area of significant uncertainty, mainly because isolating temperature effects in natural settings is challenging. Furthermore, the controlled conditions of laboratory incubations, where such temperature effects are often studied, do not always accurately reflect field conditions (Campbell and Paustian, 2015). This issue is compounded by many experimental studies focusing on theoretical optimal temperature ranges, which may not capture the full variability of temperature effects in natural environments (Sierra *et al.*, 2015). Moreover, most models apply a uniform temperature modifier to decomposition rates across all SOC pools. This approach may not be fully representative, as some studies suggest that more resistant organic C is more sensitive to temperature than more labile organic C (Stockmann *et al.*, 2013). This may pose an issue when simulating future climate change scenarios with increased temperatures.

3.3.2.2 Moisture modifiers

Moisture modifiers in SOC models are typically more complex than temperature modifiers, and their effects on decomposition rates are even less consistent (Sierra *et al.*, 2015). Moisture modifiers, although very different from temperature modifiers, share the same concepts. Moisture modifiers are estimates of potential microbial activity and response rather than direct measurements of actual processes (Post *et al.*, 1996) and are typically applied uniformly across all SOC pools.

While temperature modifiers generally only require temperature data, moisture modifiers use a range of inputs required to represent soil moisture. These inputs include precipitation (P), actual or potential ET (Jenkinson, 1990; Parton *et al.*, 2001), water-filled pore space (Kelly *et al.*, 2000), volumetric water content (Del Grosso *et al.*, 2005), soil moisture content (Foley, 1995; Harmon and Domingo, 2001) or a combination of these moisture parameters.

Moisture modifiers were developed using different concepts to estimate soil moisture, which is reflected in the modifier data requirements. For example, the Standcarb modifier represents soil moisture as volumetric content of water relative to the maximum amount of water the soil can hold (Harmon and Domingo, 2001). The Daycent modifier represents soil moisture as water-filled pore space (Kelly *et al.*, 2000). The Century modifier represents soil moisture as the ratio of precipitation to potential evapotranspiration (Parton *et al.*, 2001). Each method provides a different way to reflect how moisture influences microbial activity and decomposition processes.

Due to the variety of data inputs used for moisture modifiers, we use a homogenised variable defined as a moisture index (W_i) developed by Sierra *et al.* (2015) to allow for practical comparison between modifiers. Commonly utilised moisture modifiers are outlined in Table 3.2.

Table 3.2 List of moisture modifiers in the SoilR package (Sierra *et al.*, 2012, 2015) presented chronologically. These modifiers are commonly used in SOC modelling studies. Coefficients a, b, c, and d are empirical parameters that define the shape and behaviour of the moisture modifiers. Variables $W_{\min}$ and $M_{\max}$ represent the minimum and maximum soil moisture levels. *RothC moisture modifier can not be represented by the moisture index (W_i), therefore, it is represented as normal using accumulated (acc.) topsoil moisture deficiency (TSMD) and maximum (max) TSMD (Coleman *et al.*, 2024). (Adapted from Sierra *et al.*, 2012; 2015).

Name	Moisture modifier		Source
Myers	$bW_i + (1 - b)W_i^2$	(3.14)	Myers <i>et al.</i> (1982)
Demeter	$0.25 + 0.75(W_i)$	(3.15)	Foley (1995)
RothC*	$\begin{aligned} & \text{if } acc.TSMD < 0.444 \max.TSMD, \quad b = 1 \\ & \text{otherwise,} \\ & b = 0.2 + (1.0 - 0.2) \times \frac{(\max.TSMD - acc.TSMD)}{\max.TSMD - 0.444 \max.TSMD} \end{aligned} \quad (3.16)$		Coleman and Jenkinson (1996)
Daycent	$\left(\frac{W_i - b}{a - b}\right)^{d\left(\frac{b-a}{a-c}\right)} \left(\frac{W_i - c}{a - c}\right)^d$	(3.17)	Kelly <i>et al.</i> (2000)
Standcarb	$(1 - \exp(-(3/W_{\min})(W_i + a)))^b \exp(-(W_i/M_{\max} + c))^d$	(3.18)	Harmon and Domingo (2001)
Century	$\frac{1}{1 + 30 \exp(-8.5W_i)}$	(3.19)	Parton <i>et al.</i> (2001) & Adair <i>et al.</i> (2008)
Gompertz	$\exp(-\exp(a - bW_i))$	(3.20)	Janssens <i>et al.</i> (2003)
Candy	$4W_i(1 - W_i) \text{ if } W_i \leq 0.5; 1 \text{ if } W_i > 0.5$	(3.21)	Bauer <i>et al.</i> (2008)
Moyano	$aW_i - bW_i^2$	(3.22)	Moyano <i>et al.</i> (2013)

To demonstrate the difference in moisture modifiers, we implemented a theoretical moisture range on decomposition rates as depicted in Figure 3.8.

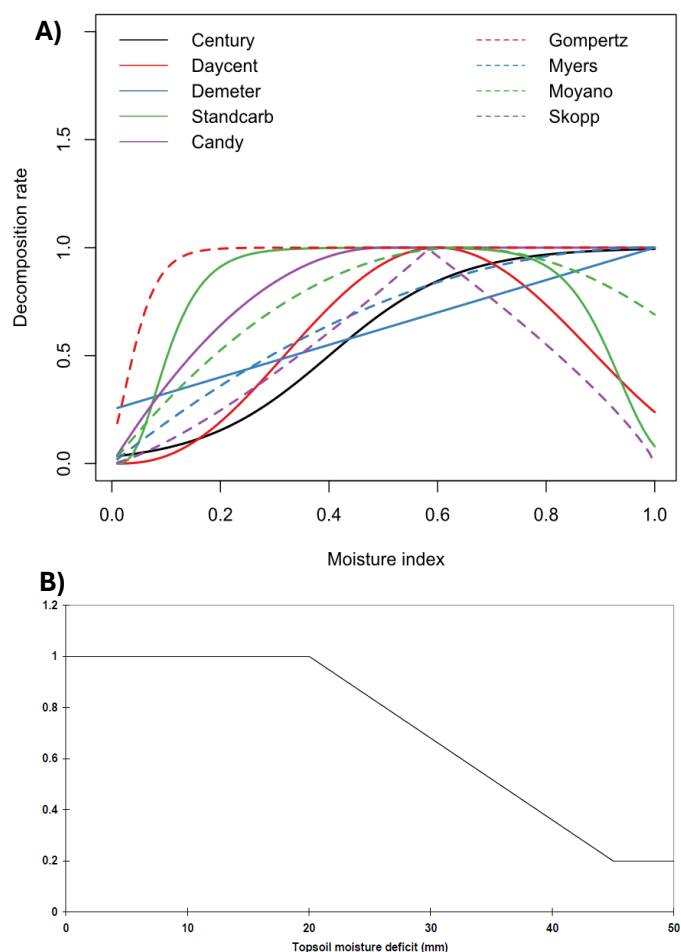


Figure 3.8 Decomposition rate as influenced by moisture modifiers A) quantified with a unitless homogenized moisture index (W_i) and artificial data. The graph was created using the SoilR package developed by Sierra *et al.* (2012, 2015; <https://www.bgc-jena.mpg.de/TEE/basics/2016/04/14/Decomposition-Modifiers/>) (top) and B) moisture modifier from RothC (bottom) (Coleman *et al.*, 2024).

The diverse range of moisture modifiers is attributed to differing conceptualisations and representations of soil moisture and its influence on decomposition rates (Del Grosso *et al.*, 2005; Foley, 1995; Harmon and Domingo, 2001; Jenkinson, 1990; Parton *et al.*, 2001). Despite these differences, the moisture modifiers can be broadly categorised into three groups based on the decomposition response to increasing moisture: low response, monotonic response, and non-monotonic response. The low response group consists of Gompertz and Candy moisture modifiers. Both achieve the maximum decomposition value of 1.0 relatively early with low W_i levels compared to other moisture modifiers. Once the maximum value is reached, it remains constant and does not fluctuate.

The monotonic group consists of Myers, Demeter, and Century moisture modifiers. These moisture modifiers assume a maximum decomposition rate of 1.0 is reached when the W_i approaches its maximum. However, the trends of these lines differ to achieve the maximum

values. The Demeter is a linear increase, the Century is an S-shaped curve increase, and the Myers is an upward curve to the maximum.

The non-monotonic group consists of Skopp, Daycent, Moyano, and Standcarb. These moisture modifiers contain both an increase and a decrease in decomposition rates. These moisture modifiers achieve the maximum rate of 1.0 in the intermediate range of the W_i . Once the maximum decomposition rate is reached, these moisture modifiers decrease as W_i approaches a maximum. These modifiers also represent a decline post maximum, indicating an inhibition in decomposition at high soil moisture levels.

A further complication with using different moisture modifiers is the variability in methods used to calculate their data requirements (Maas and Lal, 2023). For example, the RothC and CENTURY moisture modifier requires measurements or estimates of open water evaporation or potential evapotranspiration. However, there are multiple ways to estimate ET. For example, Maas and Lal (2023) demonstrated that different methods to estimate ET can result in variation in the RothC moisture modifier decomposition rates, ultimately impacting SOC estimates. The impact of different ET on model outcomes will be addressed in Chapter 5.

Another important shortcoming regarding the moisture modifiers is that none account for the changes in water phases. The transition from water to ice alters water and oxygen availability while modifying the soil structure (Sierra *et al.*, 2015) and soil temperature, which could significantly change the decomposition rates. Incorporating and accurately representing water phase dynamics into SOC models is difficult. There are significant challenges in obtaining relevant data from experimental sites where soil freezing is infrequent. As a result, this aspect of moisture dynamics is often overlooked in current moisture modifier approaches.

3.3.2.3 Management and edaphic modifiers

Land use and management practices directly affect SOC dynamics by altering the quantity and quality of carbon inputs. Soil organic carbon models incorporate these alterations by adjusting the allocation of carbon between different pools, a process that relies on the model's structural ability to differentiate inputs based on their quality. For example, plant quality can determine the proportions of plant input into specific pools, often in a ratio (e.g., decomposable to resistant ratio). A higher ratio indicates greater decomposability, with more plant material entering the faster-decomposing pool and less entering the slower resistant pool (Coleman *et al.*, 2024; Jenkinson, 1990).

More complex SOC models further differentiate the types of carbon inputs by separating above and below-ground plant residues. This distinction is important because aboveground residues (e.g., leaves and stems) and belowground residues (e.g., roots) decompose at

different rates and contribute differently to soil carbon dynamics (Parton, 1996a). By accounting for these inputs separately, models can more accurately represent different decomposition processes and carbon sequestration potential.

Some models account for the presence of a soil cover (e.g., soils under vegetation), which generally experience lower decomposition rates than fallow soils (Jenkinson, 1990). SOC models reflect this by applying a reduction factor to reduce decomposition across all carbon in cropped soils. For example, the RothC and ECOSSE models employ a reduction factor of 0.6 for soils under crops, while a factor of 1.0 is used to represent bare soils (Coleman *et al.*, 2024; Jenkinson, 1990; Smith *et al.*, 2010). The factor of 0.6 reduces the overall rate modifier, leading to lower decomposition rates, while the factor of 1.0 represents no reduction in decomposition rates, resulting in higher decomposition rates (Jenkinson, 1990; Smith *et al.*, 2010).

SOC models also generally account for soil texture, primarily focusing on clay content (McGill, 1996; Stockmann *et al.*, 2013). Clay particles play an important role in forming organo-mineral complexes, stabilising organic C in the soils, reducing microbial activity (McGill, 1996; Post *et al.*, 1996). As a result, heavy clay soils often contain more organic C than light-textured sandy soils (Jenkinson, 1990).

The approach of SOC models accounting for more resistant forms of C stored in the system varies. Some SOC models account for soil texture by altering the transfer coefficients of C within specific pools. For example, clay content increases the stabilisation of C within the HUM pool by changing the transfer coefficient between the BIO and HUM pools, increasing C's long-term storage within the RothC and ECOSSE models (Jenkinson, 1990; Smith *et al.*, 2010). The CENTURY model decreases the rate constant as clay content increases (Parton *et al.*, 1987). Similarly, the DNDC model reduces the decomposition rate depending on the clay content (Li *et al.*, 1992).

3.4 Model comparison

Having reviewed different models' structures and processes, we can demonstrate how these impact model outputs. This type of comparison provides a quantitative comparison of simulated results from different models or compares the ability of models to simulate observed data from common sites (Parton, 1996b).

Smith *et al.* (1997) evaluated nine SOC models using twelve datasets from seven long-term experiments representing grassland, arable and woodland. The nine SOC models were CANDY, CENTURY, DAISY, DNDC, ITE, NCSOIL, RothC, SOMM and Verberne. The authors determined that the model's performance could be classified into two groups. The CANDY, CENTURY, DAISY, DNDC, NCSOIL and RothC performed well with an RMSE between 6.5 and

10 Mg C ha⁻¹ and did not differ significantly from each other. In contrast, the SOMM, ITE and Verberne performance was poor, with an RMSE between 17–22 Mg C ha⁻¹ and demonstrated more significant model errors (Smith *et al.*, 1997). However, the main difference between the two groups was that all those in the poorer performance group were less developed for application to a broader range of land use (Smith *et al.*, 1997).

Palosuo *et al.* (2012) simulated SOC dynamics of an Austrian conifer forest with CENTURY, Coup-model, Forest-DNDC, Q, ROMUL, RothC, SoilCO₂/RothC and Yasso07. The CENTURY, Coup-Model and Forest-DNDC are plant-SOC models, and the remaining are SOC models. No statistical analysis between models was conducted, making it difficult to quantify the model differences. However, the study did plot the differences between the models, providing a visual aid to assess the differences in model estimates. The differences in simulated SOC stocks are demonstrated in Figure 3.9. Palosuo *et al.* (2012) showed that almost all models produced a similar SOC simulation trend that is relatively stable with minor fluctuations. The difference between the model's output is the estimated initial starting point and the estimated SOC stock, with most of the model-estimated SOC stocks in the 75 to 115 Mg C ha⁻¹ range. This extensive range reflects the variability in SOC stock estimates by the different models.

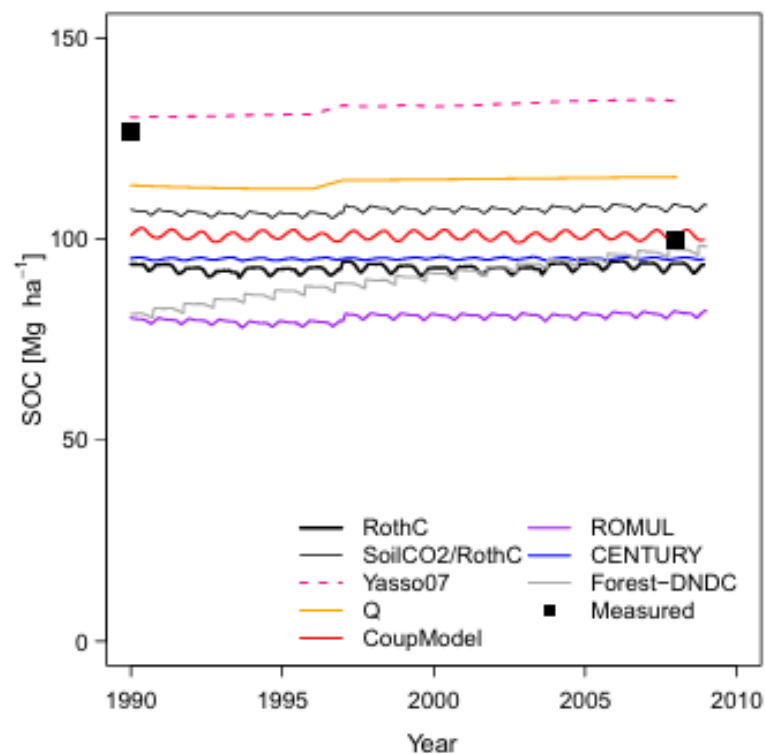


Figure 3.9 Soil organic carbon stocks in the organic layer and the uppermost 30cm in the mineral soil layer of the Murau study site from 1990 to 2008 were estimated with different models. The measured SOC stocks in 1990 and 2008 are also shown (Source: Palosuo *et al.*, 2012).

Falloon and Smith (2002) used datasets from six long-term experiments to evaluate the performance of the RothC and CENTURY models. In this study, they supplied the RothC model with two different C input estimates. The first method used the RothC inverse C method, which generates the monthly C input for a known combination of soil, site and weather data (Coleman *et al.*, 2024). RothC used in the inverse mode estimates how much C must enter the soil each year to maintain the measured SOC stock (Farina *et al.*, 2013). The second approach involved supplying the RothC model with the CENTURY-derived C input estimates. The RMSE for the simulations were: CENTURY model with CENTURY-derived C inputs ranged from 1.83 to 16.35 Mg C ha⁻¹, with an average of 6.64 Mg C ha⁻¹; the RothC model with RothC inverse C inputs ranged from 1.25 to 29.20 Mg C ha⁻¹, with an average of 9.9 Mg C ha⁻¹, and the RothC model with CENTURY-derived C inputs ranged from 1.06 to 60.93 Mg C ha⁻¹, with an average of 19.20 Mg C ha⁻¹. In general, the performance of both models was good across all the datasets (Falloon and Smith, 2002).

Simulations using the RothC model with inverse-estimated C inputs tended to show the best agreement with measured SOC data; however, this method depends on optimising C input values rather than simulating the process. RothC C input estimates were generally lower than those derived from the CENTURY model, as CENTURY applies higher decomposition rates, which are offset by correspondingly higher assumed C inputs. As a result, when RothC is run using CENTURY-derived inputs, it tends to overestimate SOC due to its inherently lower decomposition rates and the inappropriately high C input values (Falloon and Smith, 2002).

In a similar study, Cerri *et al.* (2007) demonstrated a better model agreement relative to Falloon and Smith (2002) when comparing RothC and CENTURY under different field conditions. They applied both models to simulate SOC dynamics following a land-use change from forest to grassland across sites in Brazil. Under these conditions, RothC and CENTURY produced comparable RMSE values of 17 and 16 Mg C ha⁻¹, respectively, indicating a more consistent performance between the two models in this context.

Singh and Benbi (2020) evaluated the performance of the DNDC and RothC models in simulating SOC dynamics under rice-wheat, maize-wheat and cotton-wheat cropping systems against multiple independent long-term field experiments (9 to 34 years) in Punjab, India. Validation of the models for long-term studies on rice-wheat systems showed good agreement ($R^2=0.935$ for DNDC, $R^2=0.920$ for RothC, $n=22$). Similarly, soils under the maize-wheat system showed similar agreement ($R^2=0.895$ for DNDC, $R^2=0.967$ for RothC, $n=11$).

Similarly, Li *et al.* (2016) applied the RothC and DNDC models to simulate SOC dynamics under wheat-maize rotation systems in China, across a range of fertilisation and residue management treatments. Both models demonstrated reasonable agreement with measured

SOC stock values, with comparable performance across most treatments. The RMSE values for each model and treatment scenario are presented in Table 3.3, providing a quantitative assessment of model accuracy.

Table 3.3 Root-mean-square-error (RMSE; Mg C ha⁻¹) of simulated soil organic carbon (SOC) stocks using RothC and DNDC models across eight treatment plots in North China. Treatments include Nil (no fertiliser), NPK (mineral fertiliser), NPK-straw (NPK with straw amendment), and NPK-manure (NPK with manure amendment). The RothC model was applied using measured biomass-derived carbon inputs (RothC-M) and, alternatively, using DNDC-estimated carbon inputs (RothC-D). Data adapted from Li *et al.* (2016).

Site	Model	RMSE (Mg C ha ⁻¹)			
		Nil	NPK	NPK-straw	NPK-manure
Changping	RothC-M	8.74	7.83	7.02	5.76
	DNDC	9.76	8.12	5.31	7.19
	RothC-D	8.76	8.30	8.61	6.42
Zhengzhou	RothC-M	14.27	13.19	9.00	8.31
	DNDC	14.40	14.28	8.07	6.99
	RothC-D	13.69	12.88	9.13	8.20

Heikkinen *et al.* (2014) used the Yasso07 and RothC model to estimate SOC changes from a cropland conversion to a grassland site in Pushchino, Russia. Both Yasso07 and RothC models predicted the overall increase in SOC stock relatively well compared to measured SOC stock values, with model efficiencies of 0.60 and 0.73 (on a scale of 0-1, with a model efficiency of 1.0 indicating an identical comparison). Yasso7 underestimated the change, whereas RothC overestimated the change in C stocks (Heikkinen *et al.*, 2014).

3.4.1 Model comparison challenges

Model comparisons are valuable for evaluating different approaches; however, they do not provide a quantitative basis for assessing models' relative strengths and weaknesses (Parton, 1996b). The variability in model outputs is case-specific, influenced by the choice of models, data availability, and assumptions made during the modelling process (Palosuo *et al.*, 2012). Some models undergo site-specific calibration, adjusting model parameters to best fit empirical data (LeNoë *et al.*, 2023). While calibration enhances predictive accuracy for a given site, it may reduce the model's ability to simulate SOC dynamics at other locations, necessitating further validation on independent, non-calibrated sites (LeNoë *et al.*, 2023; Smith *et al.*, 1997). Despite the many similarities between models, differences in input data and parameterisation can complicate direct comparisons, potentially leading to biased evaluations (Parton, 1996b).

Model validation metrics often rely on measured SOC stock values for model comparison (LeNoë *et al.*, 2023; Powlson *et al.*, 1996; Smith *et al.*, 1997, 2020). Long-term field experiments are often the ideal means of detecting and quantifying slow changes in SOC stocks (LeNoë *et al.*, 2023; Powlson *et al.*, 1996; Smith *et al.*, 2020). Many long-term experiments were not initially designed with SOC models at the focal point. Consequently, many experimental plots undergo treatments involving multiple variables, making it difficult to isolate them individually (Powlson *et al.*, 1996). For example, treatments are often altered between experiments, making it difficult to assess the statistical significance of any discrepancy between modelled and measured data (Coleman *et al.*, 1997). Statistical analysis, such as the RMSE, can be susceptible to a limited number of substantial errors, especially in small datasets. This can skew model performance and comparison efforts.

In some cases, the numerical results of the model simulation are not of prime importance but rather the model's predictive behaviour in estimating trends or aiding policymakers (Powlson *et al.* 1996). Furthermore, decades of regular climate patterns determined the SOC stocks of many long-term experiments. Climate change is already occurring, and weather patterns are altering. Models calibrated for previous climate conditions may be unreliable under today's altered climate patterns, compounded by lag effects in the soil response to extreme events.

A prominent issue with model comparison is the lack of a common modelling framework (Flattery *et al.*, 2018; Manzoni and Porporato, 2009; Parton, 1996b; Sierra *et al.*, 2012). Development of a general framework would enable users to review and explain the differences and similarities between the various formulations of decomposition (Manzoni and Porporato, 2009). A common framework would promote analysis of conceptual differences among models and determine the consequences of these differences (Parton, 1996b), which would allow for standardised intercomparisons between models (Manzoni and Porporato, 2009; Sierra *et al.*, 2012).

3.5 Generalised SOC modelling framework

As outlined in this chapter, most SOC models share a common mathematical framework representing specific cases of linear dynamical systems with SOC as a state variable (Manzoni and Porporato, 2009; Sierra *et al.*, 2012). Each pool undergoes first-order decay, where the flux of material from the pool is linearly related to the quantity of material in that pool (Campbell and Paustian, 2015) and the decomposition rate constant is a function of environmental modifiers and variables (Sierra *et al.*, 2012; Stockmann *et al.*, 2013). Sierra *et al.* (2012) developed a generalised model structure in the R environment called 'SoilR' for most linear dynamical models, which can be expressed as:

$$\frac{dC(t)}{dt} = I(t) + \xi(t)AC(t) \quad (3.22)$$

where $C(t)$ is a vector of carbon stores in m pools at a given time (t) ; $I(t)$ is a time-dependent column vector describing the amount of inputs to each pool m ; $\xi(t)$ is a time-dependent column scalar containing environmental effects on decomposition rates; A is a $m \times m$ square matrix containing constant decomposition rates and transfer coefficients between pools. The matrix A can be used to determine different model structures. Pool-based models can be designed by a diagonal matrix in the form:

$$A = \begin{pmatrix} -k_1 & a_{1,2} & 0 & \dots & 0 \\ a_{2,1} & -k_2 & a_{2,3} & \dots & 0 \\ 0 & a_{3,2} & -k_3 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & -k_{j,m} \end{pmatrix} \quad (3.23)$$

where entries in the diagonal represent the decomposition rate for each pool (k_j) for each pool (k) once the requirement is met (all $k_j \geq 0$); a_{ij} are the transfer coefficients of material from pool j to pool i , once the requirement is met (all $a_{ij} \geq 0$). More complex structures can replace the zero entries in the matrix A representing transfer between different pools, i and j .

The decomposition rate constant in multi-pool models is almost always altered by temperature, moisture and/or other edaphic conditions (Campbell and Paustian, 2015). In SoilR, these factors are represented by $\xi(t)$, which is a scalar value that can be directly multiplied by the matrix A . Which can be expressed as:

$$\xi(t) = f(x_1(t), \dots, x_n(t)) \quad (3.24)$$

The values of x_i are determined by different environmental functions, often referred to as temperature and moisture ‘modifiers’, which are time-dependent.

The generalised framework requires two more structures. Firstly, the initial C value (C_0), where C_0 is an $m \times 1$ vector with the C content in the different pools i . Secondly, C inputs are represented by $I(t)$, which can be expressed as:

$$I(t) = I(t) \begin{pmatrix} Y_1 \\ \vdots \\ Y_i \\ \vdots \\ Y_m \end{pmatrix} \quad (3.25)$$

where $I(t)$ is a time-dependent scalar representing the total amount of inputs, and the coefficients Y_i represent the partitioning among the different pools.

This theoretical framework allows any linear dynamical SOC model to run in the R environment, once the $I(t)$, matrix structure and $\xi(t)$ are accurate to the source model. Therefore, all components in a common framework can be represented as such:

$$\frac{dC}{dt} = I(t) \begin{pmatrix} Y_1 \\ \vdots \\ Y_i \\ \vdots \\ Y_m \end{pmatrix} + \begin{pmatrix} -k_1 & a_{1,2} & 0 & \cdots & 0 \\ a_{2,1} & -k_2 & a_{2,3} & \cdots & 0 \\ 0 & a_{3,2} & -k_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & -k_{j,m} \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ \vdots \\ C_m \end{pmatrix} \quad (3.26)$$

The carbon release from organic C decomposition, leaving the system over time, is represented with the general term r , which is given by:

$$r = RC(t) \quad (3.27)$$

where r is an $m \times 1$ vector containing the release of C for all pools, and R is an $m \times m$ diagonal matrix with the release coefficients r_j in its diagonal, calculated from

$$r_j = 1 - \sum_i a_{i,j} \quad (3.28)$$

Adapting models within a common programming language also has auxiliary benefits. This allows for easier upgrades, increases the model's applicability, and enables greater adaptability by allowing the user to exclude non-essential components (e.g., calculations for tracing of radioactive ^{14}C in soils), which can increase processing efficiency (Coleman *et al.*, 2006).

3.6 Conclusion

Generalised model frameworks such as SoilR offer a potential pathway forward for MRV development by providing a unifying mathematical structure for representing SOC models as systems of linear or nonlinear differential equations (Sierra *et al.*, 2012). Through its standardised, matrix-based formalism, SoilR enables explicit comparison of model structures and supports the construction of hybrid configurations, such as substituting decomposition functions or environmental modifiers, and reduced-form models by selectively removing components (Coleman *et al.*, 2006; Flattery *et al.*, 2018; Manzoni and Porporato, 2009; Parton, 1996b). This flexibility represents a crucial step toward harmonising model development, testing, and evaluation in SOC modelling research.

However, the value of generalised frameworks depends on rigorous benchmarking against well-established models like RothC, CENTURY, and DNDC. It is essential to verify that the implementation of these models within SoilR faithfully reproduces their original behaviour. Once validated, SoilR could provide a platform for transparent model intercomparison, facilitate complex scenario analyses by removing hard-coded constraints, and enable the

development of novel model architectures, including chains of interconnected sub-models. In doing so, it holds promise for advancing both theoretical understanding and practical applications of SOC modelling.

Chapter 4: Evaluation of the SoilR implementation of the RothC model to estimate SOC stocks in mineral grasslands.

Abstract

The RothC model is one of the most widely used models to estimate SOC dynamics. However, it was developed using the Windows visual basic interface, which requires significant user interaction and is labour-intensive, ultimately limiting the user experience and application of the model. As a result, RothC has been replicated and implemented in several different coding languages (e.g., MATLAB, R, Python, Fortran) or software environments (e.g., MS Excel) to facilitate ease of use. One of the most recent RothC implementations is in the R environment, known as SoilR. However, this implementation is based on a generalised model structure, and its performance regarding the original Windows version of RothC has not been thoroughly evaluated. Therefore, it is essential to have a robust comparison between both models to ensure they behave as expected.

To evaluate model consistency, all simulations were conducted using data from the long-term Rothamsted Park Grass Experiment, which provides an established benchmark for SOC model evaluation. The SoilR model implemented with the RothC modifiers (RothC_R_{def}) performed poorly compared to the original Windows RothC version, with annual differences of $\sim 30 \text{ Mg C ha}^{-1}$. In contrast, when RothC_R was modified (RothC_R_{mod}) to account for land cover impacts on SOC dynamics, results were consistent with the Windows Roth C version. RothC_R_{mod} reproduced similar outputs, with only negligible differences ($< 1 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$). To validate we utilised data from the long-term Rothamsted Park Grass experiment to simulate SOC dynamics, which demonstrated good model performance based on the evaluation metrics employed. We emphasise that all researchers should outline code amendments for any model implementation to increase the model's faithfulness to the source model and contribute to the wider use and development of generalised SOC modelling frameworks.

4.1 Introduction

The Rothamsted Carbon (RothC) model is one of the most popular and widely used SOC models used to estimate SOC dynamics (Campbell and Paustian, 2015; Sierra *et al.*, 2012; Smith *et al.*, 1997, 2020). The RothC model has been utilised to simulate SOC stocks in grasslands on many different scales, including field (Coleman *et al.*, 1997; Jebari *et al.*, 2021; Heikkinen *et al.*, 2014; Moll-Mielewicz *et al.*, 2023), regional (Doblas-Rodrigo *et al.*, 2023; Fallon and Smith, 2002), national (Oyesiku-Blakemore and Dondini, 2022; van Wesemael *et al.*, 2010) and global scales (Gottschalk *et al.*, 2012; Morais *et al.*, 2019). As a result of its widespread use, its performance has been extensively validated across various management practices, soil types, and climatic conditions (Coleman *et al.*, 1997; Falloon and Smith, 2002;

Smith *et al.*, 1997, 2020). Furthermore, the RothC model (or modified versions) has been used to estimate CO₂ emissions and removals in different GHG national inventories (e.g., Australia's FullCAM model, Japan's modified RothC model) (see Smith *et al.*, 2020).

The original RothC model is freely accessible from Rothamsted Research, where the RothC Windows visual basic interface can be downloaded (Rothamsted Research, n.d). Despite its popularity, the architecture and design of the RothC Windows visual basic interface limit the model's utilisation, making it challenging to graph the output, undertake statistical analysis (Janik *et al.*, 2002), generate multi-model ensembles (Riggers *et al.*, 2019) or evaluate different model modifications (Jebari *et al.*, 2021). Critically, the model cannot be modified as it comes as a precompiled executable file.

Limitations around the ease of use have been cited as a significant constraint on the broader use and uptake of SOC models more generally (Sierra *et al.*, 2012) and have led to the development and implementation of the RothC model in other programming languages. For example, the RothC model has been implemented in Microsoft Excel (Jebari *et al.*, 2021; Richards, 2001), the R environment (Sierra *et al.*, 2012), MATLAB (Heikkinen *et al.*, 2014), and C++ (Dechow *et al.*, 2019). In recognition of the limitations, Rothamsted Research has recently released an official version of RothC in both the Python scripting and Fortran programming languages (Rothamsted Research, n.d).

Of the various implementations, the SoilR package, which was developed by Sierra *et al.* (2012) and implemented in the R software environment, has been widely cited in the published literature (e.g., Boone *et al.*, 2018; Geremew *et al.*, 2024; Hyun and Yoo, 2024; Lefebvre *et al.*, 2020; Moll-Mielewczik *et al.*, 2023; Oyesiku-Blakemore and Dondini, 2022; Riggers *et al.*, 2019; Spotorno *et al.*, 2024). Its success is partly attributable to the fact that it was built for a widely used software environment, provides an open-source platform and employs a generalised matrix-based structure or framework representative of several different soil organic matter (SOM) decomposition models (Sierra *et al.*, 2012; 2015). The RothC model operated through the R environment will be referred to hereafter as RothC_R, to distinguish it from the original RothC model.

Several factors contribute to the popularity of RothC_R as an alternative to RothC: 1) R is a high-level programming language favoured by statisticians, data analysts, and researchers; 2) RothC_R was one of the first publicly available open-source implementations of RothC; 3) it enhances the potential scope for model exploration, improved model usability and model comparisons (Boone *et al.*, 2018; Coleman *et al.*, 2006; Riggers *et al.* 2019); and 4) non-essential components (e.g., calculations for tracing of radioactive ¹⁴C in soils in the RothC model) for SOC dynamics simulation can be excluded, which can increase processing efficiency (Coleman *et al.*, 2006).

However, there are known differences between RothC and the model implementation in SoilR. For instance, the RothC model requires C residue inputs prescribed every month (Coleman *et al.*, 2024), while SoilR uses annual estimates of C residue inputs (Sierra *et al.*, 2012). Models implemented in different programming languages also exhibit variations in processes due to differences in their underlying software architectures, potentially leading to discrepancies in model outputs. Other authors have observed that the RothC_R requires amendments to reproduce outputs consistent with the original model (Lefebvre *et al.*, 2020; Moll-Mielewicz *et al.*, 2023; Spotorno *et al.*, 2022).

While RothC has already undergone extensive validation in previous studies (e.g., Coleman *et al.*, 1997; Falloon & Smith, 2002; Smith *et al.*, 1997), our evaluation of the RothC_R model goes beyond relying on these prior assessments. In addition to a rigorous model comparison, we replicate a long-term RothC simulation study and directly compare model outputs with measured SOC stock values. The subsequent analysis allows us to evaluate the fidelity of the RothC_R implementation and its ability to reproduce real-world observations under established conditions. Successful validation of RothC_R against the RothC model would pave the way for expanded research possibilities that can leverage the benefits of the SoilR, such as enabling the model to be applied more efficiently and readily adapted to different scenarios (e.g., unique land-use or management scenarios, local parametrisation, additional sub-models).

4.2 Data and methods

4.2.1 Model description

The RothC model version 26.3 was originally developed at the Rothamsted Station in the UK. The model operates on a monthly time step and simulates SOC turnover in non-waterlogged mineral soils ranging from a few years to a few centuries. Similar to other SOC models, the RothC model requires various inputs, ranging from site-specific to more general model parameters. These inputs include monthly rainfall (mm), average monthly temperature, potential evapotranspiration (ET, mm) or monthly open-pan evaporation (OPE, mm), clay content (as %), an estimate of the decomposability of the incoming plant material, referred to as the DPM/RPM ratio, soil cover, sampling depth, and monthly input of plant residues (t C ha⁻¹), and farmyard manure (t C ha⁻¹) if applicable.

The RothC model structure allocates available SOC into four active pools and a small pool of inert organic matter (IOM) resistant to decomposition. The four active pools are Decomposable Plant Material (DPM), Resistant Plant Material (RPM), Microbial Biomass (BIO) and Humified Organic Matter (HUM). The RothC model allocates incoming plant residues into DPM and RPM. Both pools decompose to form BIO, HUM, and CO₂. These four

pools decompose by first-order kinetics and have a pool-specific decomposition rate. The rate constants are DPM:10.0, RPM:0.3, BIO:0.66, and HUM:0.02 year⁻¹. The pool-specific decomposition rate and the influence of moisture, temperature, and plant cover factors determine the model-simulated rate of decomposition. The final pool is the IOM pool, which remains constant and does not decompose. The clay content of the soil affects the apportioning of SOC between the evolved CO₂, BIO, and HUM pools.

The RothC model does not contain a plant sub-model or algorithms for generating carbon input estimates, and the model must be supplied with C input to generate estimates of SOC. Alternatively, the RothC model can be operated in inverse mode using a known SOC stock, climate, and soil data to derive an estimated C input required to achieve the prescribed SOC stock value. For more information about the RothC model, see Coleman *et al.* (2024) and the official website: <https://www.rothamsted.ac.uk/rothamsted-carbon-model-rothc>.

4.2.2 Site description

The site selected for the model evaluation and validation was Park Grass, the oldest continuous experiment on permanent grassland, located in Rothamsted, Harpenden, England (51°48' N, 0°22' W; elevation 133m) (MacDonald *et al.*, 2018; Rothamsted Research, 2006; Silvertown *et al.*, 2006). The site of the experiment comprises approximately 2.8 ha of almost level land that has been in grass for more than a century, since the experiment began in 1856 (MacDonald *et al.*, 2018; Silvertown *et al.*, 2006). The Park Grass site is in a temperate climate region with a recorded long-term (from 1991-2020) average annual temperature (MAT) of 10.2°C and average annual rainfall of 763.5mm (Perryman *et al.*, 2021). The topsoil (0-23cm) is classified as a silty clay loam overlying clay-with-flints and is moderately well drained (Silvertown *et al.*, 2006).

From 1856 onwards, the site was developed to investigate the effects of inorganic and organic fertilisers on hay yields (Rothamsted Research, 2006). Long-term measurements from this site have also been used to calibrate and validate SOC models, specifically the RothC model (e.g., Coleman *et al.*, 1997; Smith *et al.*, 1997). Comprehensive land management and weather data for Park Grass are available from the electronic Rothamsted Archive (e-RA), which has maintained a detailed database for the long-term field trial, including meteorological data, since 1853 (Perryman *et al.*, 2018).

For the model evaluation, sub-plots 3d and 14d were selected as they were previously employed by Coleman *et al.* (1997) and Smith *et al.* (1997) to evaluate RothC. Both plots have been previously described by MacDonald *et al.* (2018). Briefly, they received consistent and uniform management every year. Plot 3 is a control plot and received no fertilisers or manure. In contrast, plot 14 received 35 kg N as sodium nitrate, 225 kg K as potassium sulphate, 15 kg Na as sodium sulphate, and 10 kg Mg as magnesium sulphate. Sub-plots a, b,

and c received a certain amount of lime when necessary to achieve or maintain a soil pH of 7, 6, and 5, respectively, while sub-plot d received no lime. The mean annual yield of grass dry matter (DM) (t ha^{-1} , 2012-2016) for the Park Grass experiments showed a wide range, with the lowest grass yields in plot 3d (2.7 t DM ha^{-1}) and some of the highest in plot 14d (6.9 t DM ha^{-1}). A schematic of the layout of the Park Grass experimental plots is outlined in Figure 4.1. Table 4.1 summarises the main parameters Coleman *et al.* (1997) utilised in their RothC simulation.

Table 4.1 Summary of the RothC parameters Coleman *et al.* (1997) used in the Park Grass plot 3d and 14d simulations.

Parameter	Value
Soil thickness	23cm
Clay	23.4%
IOM pool size	6.9 Mg C ha^{-1}
DPM/RPM ratio	1.44
Long-term C input	$3 \text{ t C ha}^{-1} \text{ yr}^{-1}$
Annual 3d C input	$3 \text{ t C ha}^{-1} \text{ yr}^{-1}$
Annual 14d C input	$2.7 \text{ t C ha}^{-1} \text{ yr}^{-1}$
Temperature	Monthly average ($^{\circ}\text{C}$)
Rainfall	Monthly average (mm)
Evaporation	Monthly average open-pan measurements (mm)

		a	b	c	d	
			FYM/PM			13/2
			(FYM/Fishmeal)			13/1
			Nil			12
18d			N3 P K Na Mg Si			11/2
			N3 P K Na Mg			11/1
18c			N2 P Na Mg			10
18/2	N2K Na Mg		N2 P K Na Mg			9/2
			(N2) PK Na Mg			9/1
18b			P Na Mg			8
18a			P K Na Mg			7/2
19/1			(P) K Na Mg			7/1
19/2			N1 PK Na Mg			6
19/3	FYM		These areas used for microplot experiments			5
20/1						
20/2	FYM N*PK		N2P			4/2
20/3			P			4/1
			Nil			3
			Nil			2/2
			K since 1996			2/1
			N1			1
			N*2 PK Na Mg			14/2
			(N*2) PK Na Mg			14/1
			N*3 PK Na Mg			15
			N*1 PK Na Mg			16
			N*1			17

Figure 4.1 Overview of Annual fertilization treatments for selected plots in the Park Grass experiment. Nitrogen was applied as ammonium sulfate (N1, N2, N3) or sodium nitrate (N*1, N*2, N*3) at 48, 96, and 144 kg N ha⁻¹ yr⁻¹, respectively. Treatments (N2) and (N*2) received their final application in 1989. Other annual mineral applications included triple superphosphate (17 kg P ha⁻¹ yr⁻¹), potassium sulfate (225 kg K ha⁻¹ yr⁻¹), sodium sulfate (15 kg Na ha⁻¹ yr⁻¹), magnesium sulfate (10 kg Mg ha⁻¹ yr⁻¹), and sodium silicate (450 kg Si ha⁻¹ yr⁻¹). Organic amendments were farmyard manure (FYM) at 35 t ha⁻¹ yr⁻¹ and pelleted poultry manure (PM) supplying 65 kg N ha⁻¹ yr⁻¹. (Source: MacDonald *et al.*, 2018).

4.2.3 Model inputs

All model input parameters were held identical for the model comparison. RothC model parameters such as soil thickness, clay content, IOM pool size, DPM/RPM ratio and C input were obtained from Coleman *et al.* (1997) (Table 4.1). However, meteorological inputs were not provided in their study. To address this, we utilised long-term 30-year (1961-1990) average monthly temperature, rainfall and evaporation data (Perryman *et al.*, 2021) to initialise the pool size, followed by 21 years (1991) of monthly meteorological data from the Rothamsted meteorological records, accessed via the e-RA database.

The e-RA database provides estimates of evaporation over water following Berry's (1964) methodology with additional refinements from Allen *et al.* (1998). Berry's (1964) evaporation over water method is a refinement of Penman's (1948) natural evaporation from open water. These refinements included a Fourier approximation for solar radiation, empirical adjustments for aerodynamic and energy terms, and explicit modelling of long-wave radiation (Berry, 1964). These empirical adjustments were further optimised by incorporating modern empirical constants from Allen *et al.* (1998). The Berry evaporation over water equation can be expressed as:

$$Evap_{water} = \frac{(h_j \times ev_1) + (0.66 \times EA)}{\delta + 0.66} \quad (4.1)$$

where,

Evap_{water}: Evaporation over water in mm per month

h_j : Net available energy for evaporation

ev_1 : Net radiation at the water surface (MJ/m²/day)

EA: Aerodynamic evaporation term (mm/day)

δ : Slope of vapour pressure curve (mm Hg/°C)

0.66: Psychrometric constant (mm Hg/°C)

For additional details on this implementation of Berry (1964), refer to https://www.era.rothamsted.ac.uk/info/met/derived_variables. The evaporation over water estimates were obtained from the Rothamsted meteorological station via the e-RA database.

For the Park Grass replication simulation, we used multiple data sources to ensure direct comparability with previous work. Coleman *et al.* (1997) provided site-specific soil information, including soil thickness, clay percentage, and the DPM/RPM ratio; these values were 23cm, 23.4% and 1.44, respectively. Furthermore, plots 3d and 14d received no farmyard manure, so these values were set to zero. However, meteorological inputs and measured SOC stock values were not provided by Coleman *et al.* (1997).

To address this, meteorological measurements from the Rothamsted weather station were employed. The Rothamsted weather station has measured precipitation since 1853 and temperature since 1878. Coleman *et al.* (1997) utilised actual open-pan measurements. However, these measurements are not available from the e-RA database and are not commonly utilised in SOC modelling studies (Allen *et al.*, 1998). We employed two alternative approaches: an evaporation over water estimate (Allen *et al.* 1998; Berry, 1964) and Penman-Monteith ET (Monteith, 1965). Evaporation over water was employed as a surrogate for open-pan evaporation.

The Penman-Monteith (Monteith, 1965) method is considered the most complex and accurate for estimating ET and is recommended by the Food and Agriculture Organization (FAO) (Allen *et al.*, 1998). It is expressed as:

$$ET_{PM} = \frac{0.408\Delta(R_n - G) + \gamma \frac{900}{T + 273} u_2 (e_s - e_a)}{\Delta + \gamma(1 + 0.34u_2)} \quad (4.2)$$

where,

ET_{PM}: Penman-Monteith ET in mm per month

R_n: Net radiation at crop surface (MJ/m²/day)

G: Soil heat flux density (MJ/m²/day)

u₂: Wind speed at 2 meters height (m/s)

e_s: Saturation vapour pressure at air temperature (kPa)

e_a: Actual vapor pressure (kPa)

Δ: Slope of the saturation vapour pressure curve (kPa/°C)

γ: Psychrometric constant (kPa/°C)

T: Mean air temperature (°C)

To calculate Penman-Monteith, the R package 'FAO56' (Ahani and Nadoushani, 2023) was employed, which implements equations from Allen *et al.* (1998). Coleman *et al.* (1997) determined the long-term evaporation average from 1960 to 1993 and used it for monthly values before 1960. We employed the same approach for evaporation over water and Penman-Monteith (ET_{PM}) estimates.

As the SOC data was not directly available, we employed a data extraction software tool to extract the reported measured SOC stock values from plot 3 and plot 14 SOC based on the figures contained in Coleman *et al.* (1997). The data extraction software tool employed in this study was WebPlotDigitizer (Rohatgi, 2024), which has proven to be reliable and accurate (Drevon *et al.*, 2017).

Coleman *et al.* (1997) estimated carbon inputs for the RothC model using an inverse modelling approach constrained by site-specific SOC measurements, weather, soil characteristics, and management practices. In their study, achieving the initial SOC equilibrium required annual carbon inputs of 3.0 t C ha⁻¹. For plots 3d and 14d specifically, the inverse-modelled annual C inputs were 3.0 t C ha⁻¹ and 2.7 t C ha⁻¹, respectively. As the

original weather files were unavailable, and to maintain methodological consistency with Coleman *et al.* (1997), we calculated site-specific C inputs using the same inverse modelling technique with climatic data sourced from the e-RA database. This yielded annual C input estimates of 1.98 t C ha⁻¹ for model spin-up, and 2.57 t C ha⁻¹ and 2.27 t C ha⁻¹ for plots 3d and 14d, respectively.

An additional investigation of C input was undertaken to understand potential impacts on the model-estimated values. The RothC model requires monthly C inputs, while the SoilR implementation requires annual C inputs. The RothC model was operated using three different monthly C input distributions to highlight any differences between the timing of C inputs. The first approach involved allocating the total annual C input into the first month of the year (Single). The second approach utilised the default Park Grass management file, which varied C input across the 12 months of the year (Default). The third approach evenly distributed the total annual C input each month (Equal). Appendix A.1 contains a detailed table of the monthly C inputs employed.

4.2.4 Environmental modifiers

SoilR provides environmental modifiers for a range of SOC models. For the purposes of this evaluation, the RothC environmental modifiers in SoilR were selected.

The RothC temperature modifying factor (*fT*) is calculated using the equation:

$$fT = \frac{47.9}{1 + e^{\frac{106}{T + 18.3}}} \quad (4.3)$$

where, *T* is the average monthly air temperature (°C).

The RothC moisture modifier (*fW*) is more complex and requires a number of inputs. Initially, the topsoil moisture deficit (TSMD) is determined as the difference between total monthly precipitation (*P*, mm) and total monthly evaporation (*E*, mm). The RothC model is primed to run on open pan evaporation (OPE), which is then multiplied internally by 0.75 to derive an estimate of ET, meaning the RothC model SOC stock estimates are based on ET values (Coleman *et al.*, 2024). In the original RothC model, the initial input ET values must be converted to OPE by dividing the values by 0.75 before running the model. In the model implementation in SoilR, it contains an evaporation coefficient (*pE*) that can be adjusted to 0.75 for OPE and 1.0 for ET. Therefore, TSMD can be expressed as:

$$TSMD = P - (E \times pE) \quad (4.4)$$

The maximum TSMD (TSMD_{max}) is a fixed value derived from the clay content and is given by:

$$TSMD_{max} = -(20.0 + 1.3(\%clay) - 0.01(\%clay)^2) \quad (4.5)$$

When the soil is bare, the $TSMD_{max}$ is divided by 1.8 to give bare TSMD to compensate for the reduced evaporation.

The fW modifier is then defined as:

$$fW = 1, \quad \text{if } TSMD_{acc} < 0.444(TSMD_{max}),$$

Else,

$$fW = 0.2 + 0.8 \times \frac{TSMD_{max} - TSMD_{acc}}{TSMD_{max} - 0.444(TSMD_{max})} \quad (4.6)$$

where $TSMD_{acc}$ is the monthly accumulation of TSMD limited by $TSMD_{max}$ calculated from the sum of monthly precipitation and evaporation differences.

In SoilR, the decomposition rate modifier (ξ) accounts for external environmental and edaphic effects. By default, ξ (ξ_{def}) is calculated as the product of RothC's temperature and moisture modifier, expressed as:

$$\xi_{def} = fT \times fW \quad (4.7)$$

The RothC model reduces decomposition by 0.60 if the soil is vegetated (Coleman and Jenkinson, 1996). The ξ rate modifiers in SoilR were consequently amended to account for a soil cover factor (SCF) of 0.60. The amended ξ rate modifier (ξ_{mod}) is described by:

$$\xi_{mod} = fT \times fW \times SCF \quad (4.8)$$

where ξ_{mod} accounts for temperature, moisture and vegetation cover, which is a simplified representation of the influence of the modifiers on decomposition in each active pool at the given time-step. For clarity, simulations using the original RothC model are referred to as 'RothC', simulations using RothC_R (SoilR implementation) with ξ_{def} (Eqn 4.7) are referred to as 'RothC_R_{def}', and simulations using RothC_R with ξ_{mod} (Eqn. 4.8) are referred to as 'RothC_R_{mod}'.

4.2.5 Model initialisation

Initialisation of RothC and RothC_R was conducted using a model 'spin-up' period. This involves starting the model with the active C pool set to zero and running it under constant, long-term average C inputs and climate until an equilibrium is reached for each SOC pool, where a stable SOC value is reached that results from the balance between the inputs and outputs. The spin-up determines the initial SOC stock value of a simulation. The RothC model's default spin-up run is 10,000 years (Coleman *et al.*, 2024), which cannot be

modified. Therefore, we also employed a 10,000-year spin-up period for both RothC_R models. Once the initial pool sizes are determined, based on the prescribed climatology, the model is run using monthly meteorological data for the period of interest and a constant C input.

4.2.6 Model comparison and evaluation

This study employed two approaches to investigate two different research objectives: model comparison and simulation replication.

Model comparison

All three models (RothC, RothC_R_{def}, RothC_R_{mod}) were prescribed identical inputs for the initial model comparison to ensure a standardised comparison. The model's spin-up run utilised the long-term average (LTA) climate from 1961 to 1990. Each model received 3 t C ha⁻¹ yr⁻¹, consistent with Coleman *et al.* (1997). Once the initial pool sizes were determined, all models were run with monthly meteorological data from 1991 to 2011 with the same C input of 3 t C ha⁻¹ yr⁻¹. An additional model comparison was conducted, which started each model from the same initial pool sizes to identify if differences in initial pool size resulted in differences between the model simulations. Every effort was made to ensure uniform model operation, required to ensure that output differences arose from model structure rather than variations in inputs or parameters. The R code used to operate RothC_R_{def} and RothC_R_{mod} is provided in Appendix A.2.

Model evaluation

Following the model evaluation, the best performing RothC_R model configuration was selected to replicate the Park Grass plot 3d and 14d experiments. A spin-up simulation of 10,000 years was conducted using a default weather file (Rothamsted Research, n.d) to establish the initial total pool size of 74.5 Mg C ha⁻¹. Once initial pool sizes were determined, three variants were implemented.

Variants 1 and 2 applied the model parameterisation reported by Coleman *et al.* (1997), differing only in their evaporation method. Variant 1 used evaporation over water, while Variant 2 employed Penman-Monteith estimates. Variant 3 also used Penman-Monteith, but incorporated C inputs estimated inversely to optimise the fit between modelled and observed SOC. All simulations were driven by monthly meteorological data from 1856 to 1993. Modelled SOC outputs were compared against the SOC measurements reported in Coleman *et al.* (1997) for evaluation. An overview of the simulation variants is provided in Table 4.2.

Table 4.2 An overview of the different variants of the Park Grass plot 3d and 14d simulations that utilise different evaporation methodologies and C input estimates.

Parameter	Variant 1	Variant 2	Variant 3
Soil thickness	23cm	23cm	23cm
Clay	23.4%	23.4%	23.4%
IOM pool size	6.9 Mg C ha ⁻¹	6.9 Mg C ha ⁻¹	6.9 Mg C ha ⁻¹
Total initial pool size	74.5 Mg C ha ⁻¹	74.5 Mg C ha ⁻¹	74.5 Mg C ha ⁻¹
DPM/RPM ratio	1.44	1.44	1.44
Temperature	Monthly average	Monthly average	Monthly average
Rainfall	Monthly average	Monthly average	Monthly average
Evaporation	Evaporation over water	Penman-Monteith	Penman-Monteith
Annual 3d C input	3 t C ha ⁻¹ yr ⁻¹	3 t C ha ⁻¹ yr ⁻¹	2.57 t C ha ⁻¹ yr ⁻¹
Annual 14d C input	2.7 t C ha ⁻¹ yr ⁻¹	2.7 t C ha ⁻¹ yr ⁻¹	2.27 t C ha ⁻¹ yr ⁻¹

4.2.7 Statistical analysis

Statistical tests were employed to evaluate the performance between models and measured SOC data: root mean square error (RMSE) and mean absolute difference (MAE). The smaller value from our performance metrics indicates better model performance (e.g., a zero value for RMSE and MAE indicates an identical match between measured and modelled). The RMSE and MAE can be described as:

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (P_i - O_i)^2}{n}} \quad (4.7)$$

$$MAE = \frac{1}{n} \sum_{i=1}^n |P_i - O_i| \quad (4.8)$$

where O_i is the observed value, P_i is the predicted value, $\bar{O}$ is the mean of the observed data, and n is the number of paired values. These outputs will indicate the model's performance. The RMSE and MAE units are always expressed in the same units as the parameter.

4.3 Results

4.3.1 Carbon inputs distribution

Figure 4.2 illustrates the simulated SOC stocks from RothC using different C input distribution methods. The Single distribution produced a sawtooth pattern, with sharp increases in January followed by gradual declines, while the Default (monthly) distribution displayed a more seasonal cycle consistent with the timing of carbon inputs. The Equal distribution generated the smoothest annual trajectory. Although these input distributions did not affect long-term annual SOC stocks, the Equal method was selected for model

comparison, as it minimises within-year variability and most closely aligns with the annual C input structure used in SoilR.

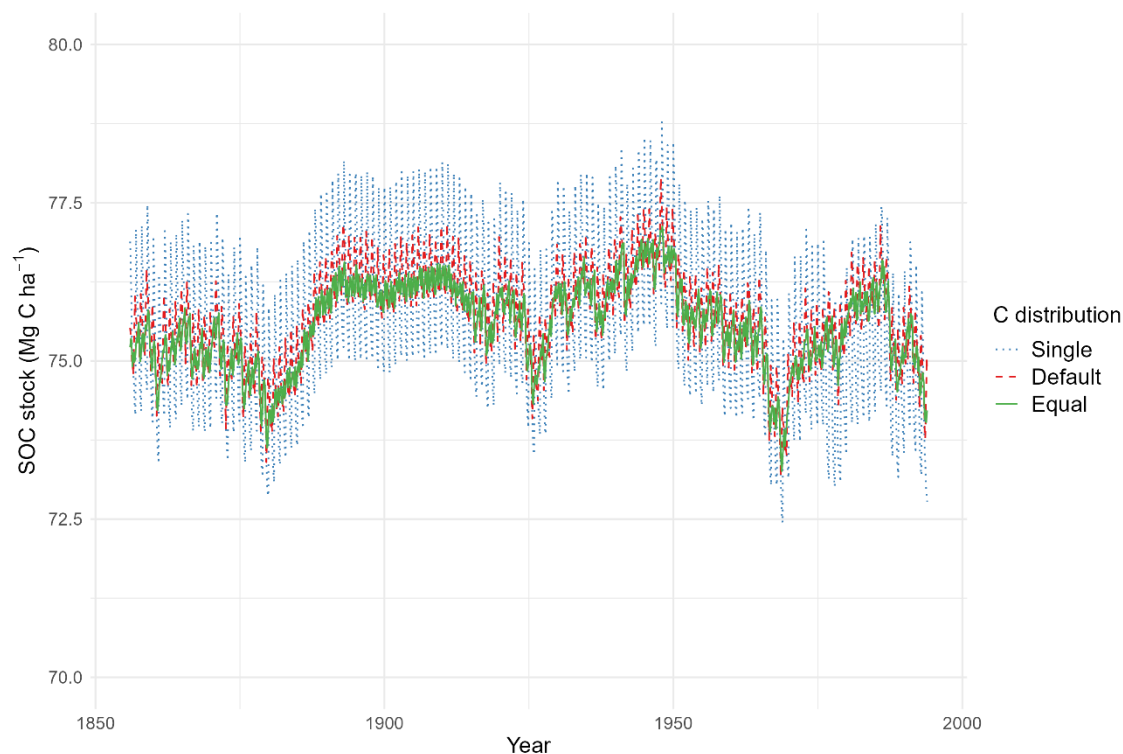


Figure 4.2 Long-term RothC model simulation using three different monthly C input distributions. The single approach total C input entered in January, the default approach was the land management file available for the Park Grass on the RothC model, and the equal approach was the annual sum C input divided equally between each month.

4.3.2 Rate modifier comparison

A major defining feature of SOC models is their decomposition rates, which are influenced by environmental rate modifiers. To evaluate the effects of implementing an SCF, rate modifiers from the RothC_{Rdef} and RothC_{Rmod} were compared to those from the standard RothC model during the spin-up phase. As the spin-up is based on LTA climate conditions, repeated monthly averages across all years of the spin-up. Consequently, only twelve unique decomposition rates were estimated, as the same set of monthly LTA values was used for every year. Figure 4.3 compares the monthly ξ rate modifiers from RothC_{Rdef} and RothC_{Rmod} to those from the original RothC model. RothC_{Rdef} showed poor agreement with the original RothC model (RMSE = 0.31), while RothC_{Rmod} exhibited strong agreement (RMSE < 0.01), demonstrating successful implementation of the SCF.

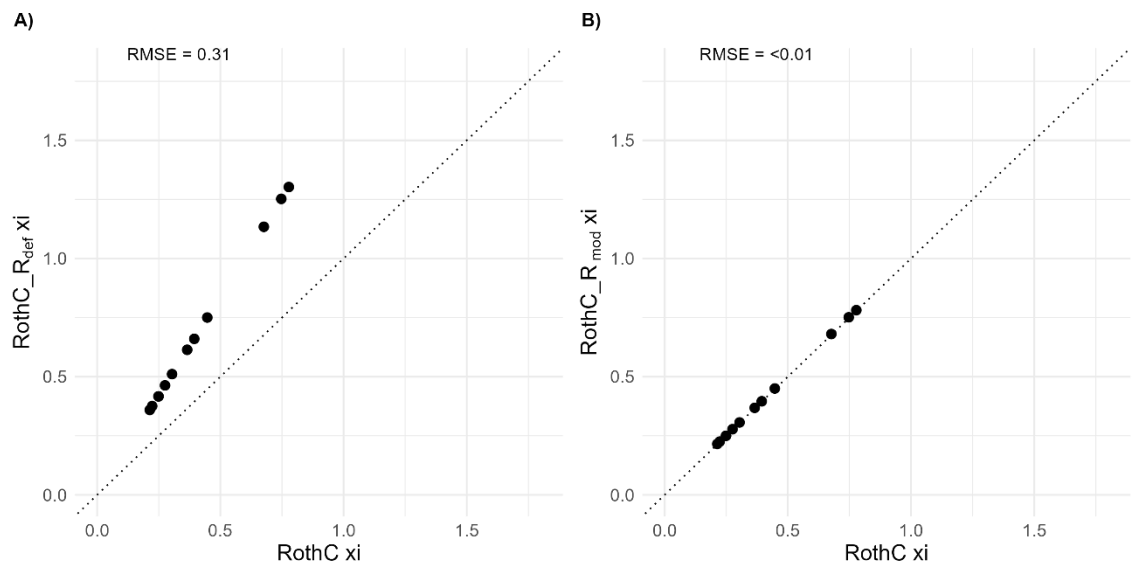


Figure 4.3 Monthly ξ rate modifiers during the model spin-up phase. The standard RothC model is used as the reference. A) Comparison of ξ values from RothC_R_def . B) Comparison of ξ values from RothC_R_mod . The black dotted line represents the 1:1 line (slope = 1), indicating perfect agreement.

To further assess model agreement under time-varying conditions, a 10-year period from 1960 to 1969 ($n=120$ months) was selected, beginning at the point where reliable meteorological data for evaporation estimates were available. Figure 4.4 presents a comparison of monthly rate modifiers for temperature (fT), moisture (fW) and total rate modifier (fT , fW and SCF) between RothC_R_mod and the original RothC model. Across all rate modifiers, the RMSE was consistently <0.01 , indicating very strong agreement between the two model structures over this period.

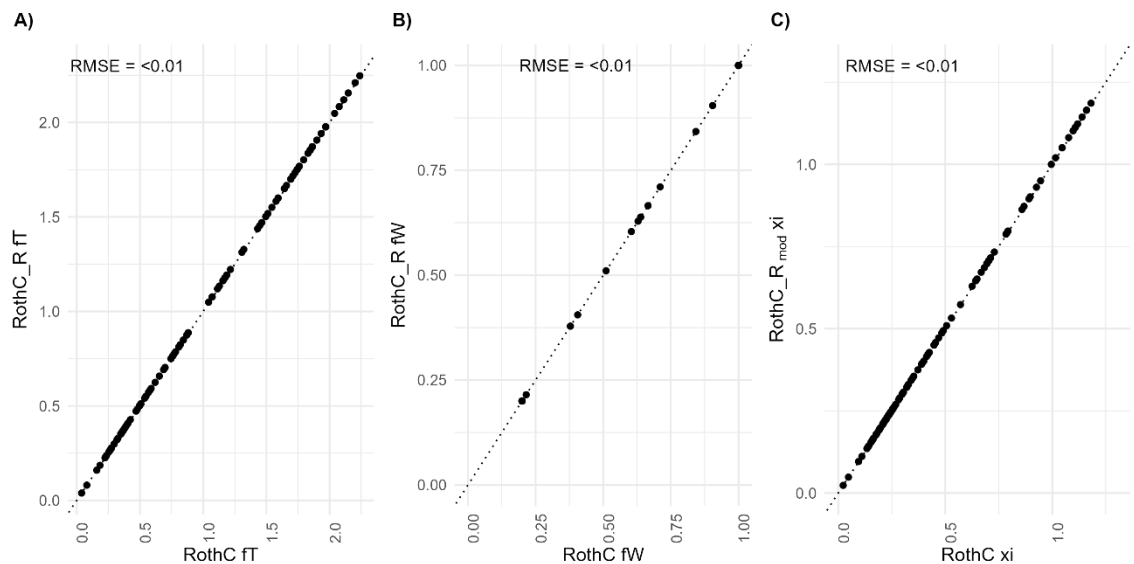


Figure 4.4 Comparison of monthly rate modifiers from RothC_R_mod to the standard RothC model over a 10-year period (1960-1969, $n=120$). A) Temperature rate modifiers (fT). B) Moisture rate modifiers (fW). C) Total rate modifier (ξ) calculated as the product of fT , fW and the soil cover factor. All graphs include the 1:1 reference line (slope = 1), indicating perfect agreement.

4.3.3 Model evaluation

As the equilibrium SOC stock from the RothC spin-up was not directly accessible, all models were extended for an additional 30 years using the same inputs as the spin-up phase, required to extract an approximate model equilibrium SOC value. The estimated equilibrium SOC stocks were 80.72, 50.70, and 79.94 Mg C ha⁻¹ for RothC, RothC_R_{def}, and RothC_R_{mod}, respectively. These results are summarised in Table 4.3, while Figure 4.5 presents the SOC estimates for each model. Due to the unavailability of the original RothC spin-up data, only projections post-spin-up could be visualised.

Table 4.3 Comparison of simulated equilibrium SOC stocks and deviation metrics for RothC_R_{def} and RothC_R_{mod}. RothC is used as the reference model for all difference calculations. All values are expressed as Mg C ha⁻¹.

Model	Equil. SOC stock	Avg. difference to RothC	Max difference	Min difference	RMSE	MAE
RothC	80.72	-	-	-	-	-
RothC_R _{def}	50.70	29.90	30.02	29.8	29.899	29.899
RothC_R _{mod}	79.94	0.65	0.78	0.54	0.65	0.647

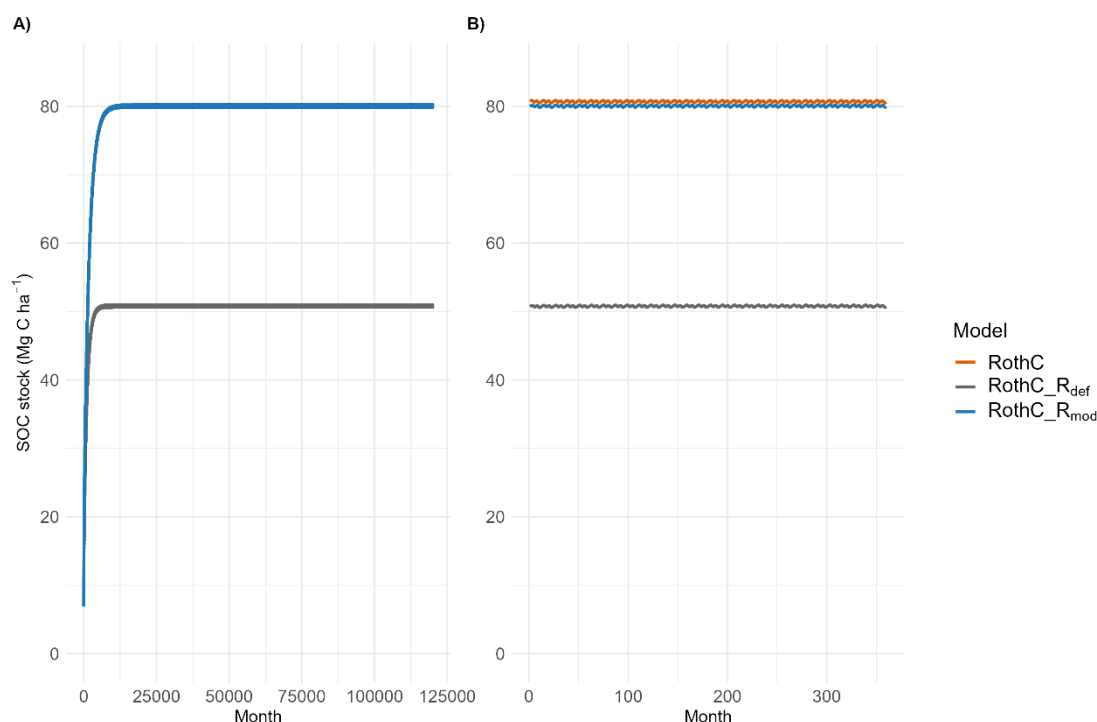


Figure 4.5 Soil organic carbon (SOC) stocks for the Park Grass site simulated by RothC, RothC_R_{def}, and RothC_R_{mod}. A) Model spin-up from 0 to 10,000 years. B) 30-year projected equilibrium run using identical model input data.

To further evaluate model differences, we tested their sensitivity to different initialisation starting points. Unlike the previous equilibrium comparison, the emphasis here was on the short-term (21-year) model differences arising from initial pool sizes rather than the long-term equilibrium conditions. The simulation was conducted over the period 1991–2011 using monthly meteorological data to isolate the effects of initial pool configuration on

model behaviour. Two approaches were applied: (i) each model (RothC, RothC_R_{def}, and RothC_R_{mod}) was initialised with pool sizes determined from an independent spin-up, and (ii) all models were prescribed an identical initial pool size determined by RothC. Table 4.4 presents the performance metrics under these two approaches, while Figure 4.6 illustrates the resulting simulation differences.

Table 4.4 Comparison of simulated equilibrium SOC stocks and deviation metrics for RothC_R_{def} and RothC_R_{mod} over the period 1991-2011. RothC is used as the reference model for all difference calculations. All values are expressed in Mg C ha⁻¹.

Model	Initial pool sizes	Initial value	Final value	Max diff.	Min diff.	Avg diff.	MAE	RMSE
RothC	RothC determined	80.72	77.52	-	-	-	-	-
RothC_R _{def}	RothC_R _{def} determined	50.70	48.35	30	28.9	29.46	29.457	29.458
RothC_R _{mod}	RothC_R _{mod} determined	79.94	76.84	0.8	0.4	0.63	0.63	0.635
RothC_R _{def}	RothC determined	80.72	67.61	9.9	0.1	6.45	6.447	6.922
RothC_R _{mod}	RothC determined	80.72	77.22	0.3	< -0.1	0.18	0.182	0.197

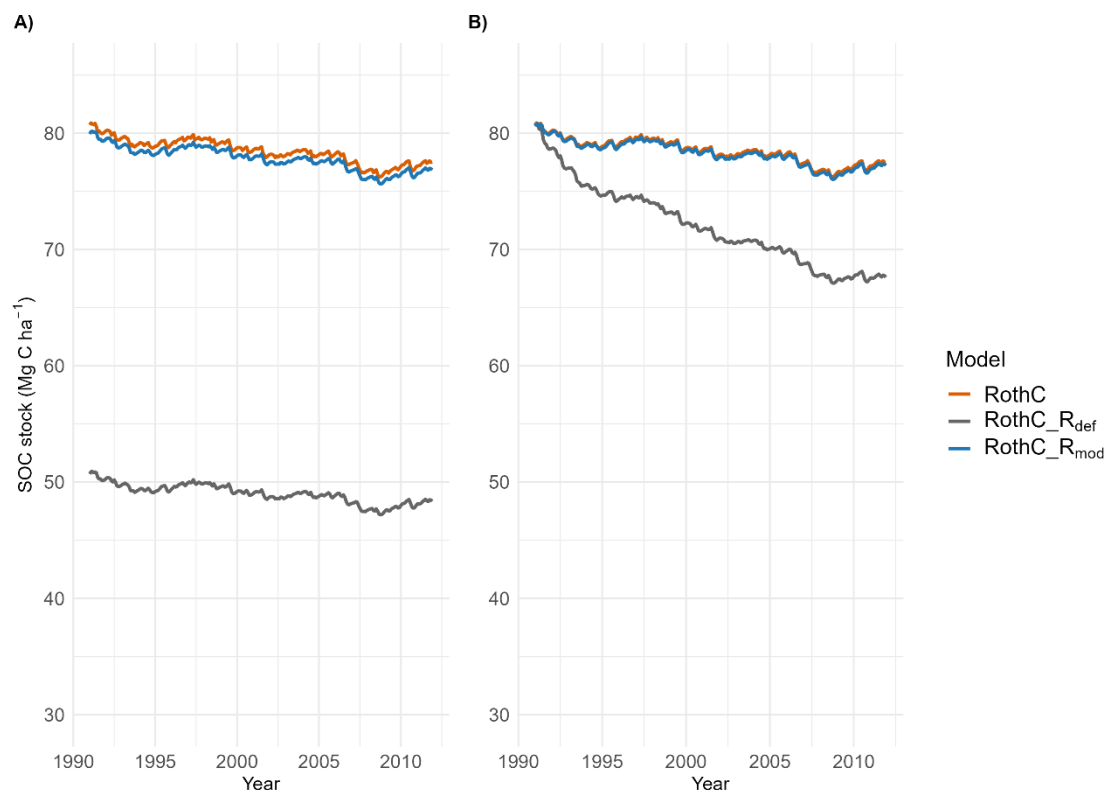


Figure 4.6 SOC stock trajectories over a 21-year simulation period under two initialisation methods: A) Each model used its own spin-up to define initial SOC pool sizes. B) All models were initialised using the RothC-derived pool sizes.

4.3.4 Evapotranspiration method comparison

Figure 4.7 compares monthly ET estimates derived from evaporation over water converted to ET using RothC's internal conversion factor (0.75) and the ET_{PM} method. The seasonal

distribution of ET is visualised using monthly boxplots. The ET_{PM} method consistently produced higher ET values than the evaporation-over-water derived estimates, highlighting the methodological influence on moisture dynamics in SOC simulations.

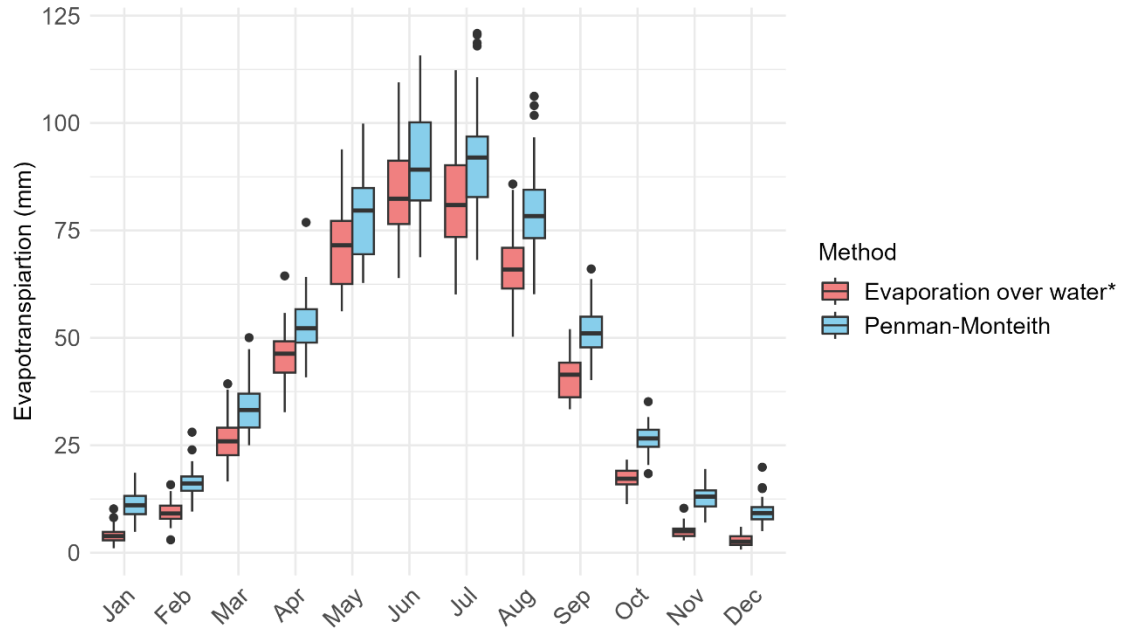


Figure 4.7 Comparison of monthly potential evapotranspiration (ET) estimates for the Park Grass site (1960-1993) using two methods: (1) evaporation over water, converted to ET using RothC's internal factor of 0.75, and (2) the Penman-Monteith method. Boxplots represent the monthly distribution of ET values. The RothC method reflects an adjusted approximation of ET rather than raw evaporation, and consistently yields lower values than Penman-Monteith estimates.

4.3.5 Park Grass simulation replication

Given that the $RothC_{R_{mod}}$ was found to replicate the RothC model under identical conditions faithfully, it was selected for use in the Park Grass simulation. Figure 4.8 presents simulated SOC stocks for each Park Grass plot 3d and 14d over the full period (1856-1993) using the three $RothC_{R_{mod}}$ variants described in Table 4.2. The variants differ in their approach to ET estimation and C input specification. To aid comparison with the original study, reference model outputs were extracted from Coleman *et al.* (1997) using the WebPlotDigitizer tool (Rohatgi, 2024). The reference lines are intended to serve as guidelines for visual comparison. The main differences between the simulated SOC stock values and those extracted from Coleman *et al.* (1997) arise from differences in model structure and inputs (e.g., $RothC_R$ versus RothC, annual versus monthly C inputs, difference in ET_{PM} and OPE). Minor discrepancies may also reflect extraction uncertainties, such as interpolation errors due to slight misalignment in time series or axis calibration.

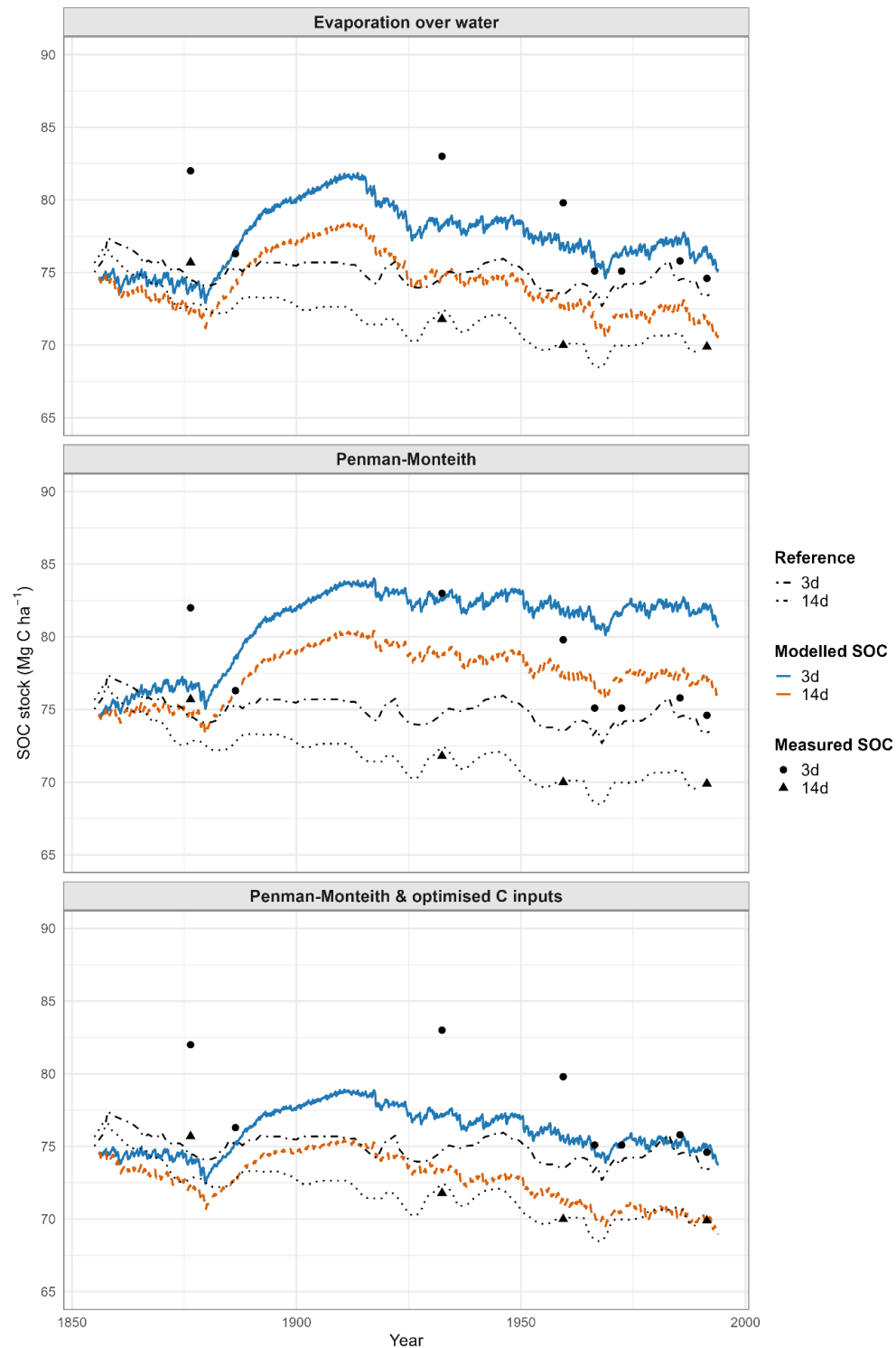


Figure 4.8 Simulated soil organic carbon (SOC) stocks for Park Grass plot 3d (blue) and 14d (orange) from 1856 to 1993 using three RothC_R model variants. The black dashed line and black dotted line represent the reference simulated SOC stock from Coleman *et al.*'s (1997) study extracted using WebPlotDigitizer. Top panel: Evaporation over water with C inputs from Coleman *et al.* (1997). Middle panel: Penman-Monteith evapotranspiration with C inputs from Coleman *et al.* (1997). Bottom panel: Penman-Monteith evapotranspiration with inverse modelled (fitted) C inputs. Each variant applies identical site parameters except for differences in evapotranspiration method and C input values.

Table 4.5 summarises the model performance, measured as the RMSE between modelled and observed SOC stocks. Variant 3, ET_{PM} and corresponding inverse modelled C inputs ($2.57\text{--}2.27 \text{ t C ha}^{-1} \text{ yr}^{-1}$) achieved the lowest RMSE, followed by Variant 1 (evaporation over

water with Coleman *et al.* (1997) C inputs (3–2.7 t C ha⁻¹ yr⁻¹), while Variant 2 (ET_{PM} with Coleman *et al.* (1997) C inputs (3–2.7 t C ha⁻¹ yr⁻¹) exhibited the poorest performance.

Table 4.5 Root mean square error (RMSE) between measured and modelled SOC stocks for Park Grass plot simulations using three RothC_R_{mod} variants. All values expressed in Mg C ha⁻¹.

Variant	Plot 3d	Plot 14d	Average
Evaporation over water	3.61	2.82	3.22
Penman-Monteith	5.12	6.27	5.70
Penman-Monteith & Inverse C inputs	3.8	2.04	2.92

4.4 Discussion

4.4.1 Carbon input distribution

Our findings suggest the RothC model is relatively insensitive to the method of C input distribution for long-term simulations. Currently, the default RothC_R functions are not configured to operate with monthly C inputs, which presents a limitation when comparing the models under variable monthly C input scenarios. However, this could be addressed with code modifications, possible within the SoilR implementation, to investigate the similarities and differences between models further. For now, we recommend equal C input distribution when performing comparisons of RothC and RothC_R, as this approach aligns most closely with SoilR's current handling of C inputs and, therefore, provides a more comparable basis.

It is also important to note that the C input distribution can influence specific results presented in this study. Specifically, the maximum and minimum differences between simulations are particularly sensitive to the distribution of C inputs, as this alters the peaks and troughs of predicted SOC stocks. However, the C inputs distribution would most likely have an insignificant impact on the overall SOC stock predictions.

4.4.2 Model comparison

A direct comparison of rate modifiers between models provides the most robust basis for a mathematical comparison, given that rate modifiers are both models' primary drivers of pool decomposition. The output of the models (e.g., estimated SOC stock values) further highlights the effects of the rate modifiers, provides a visual aid, and allows for additional performance indices to be calculated. We propose that a detailed model comparison must incorporate both rate modifiers and SOC stock values for a comprehensive model evaluation.

The RMSE metric evaluation is dependent on the context. In our xi-modifier analysis, a faithful model adaptation should successfully produce an RMSE as close to zero as possible, as the selected goal is to produce decomposition rates identical to the source model. Given this context, the RothC_R_{def} model performed quite poorly based on the selected performance metrics, creating a relatively high RMSE of 0.31 when compared to the RothC

model for the spin-up phase. For the SOC stock simulation, a successful model implementation should estimate SOC stocks within a high level of accuracy (e.g., 1 to 5% of the simulated SOC stock). The RothC_R_{def} model produces an average difference of 29.90 Mg C ha⁻¹ yr⁻¹ after the spin-up phase, indicating a 40% underestimation of SOC stocks. Overall, the RothC_R_{def} model performed poorly due to a consistently higher decomposition rate when SCF is not included, resulting in a systematic underestimation of predicted SOC stock values compared to the original RothC model.

In contrast, the RothC_R_{mod} exhibited rate modifiers nearly identical to those of RothC, yielding RMSE values of less than 0.01. This indicates a similar modification of decomposition rates under the same environmental conditions. The effect on SOC dynamics was minimal, with an average annual SOC stock difference of 0.63 Mg C ha⁻¹ yr⁻¹, equivalent to an underestimation of ~0.8%. Based on these performance metrics, RothC_R_{mod} most closely replicated RothC behaviour, both in terms of modifier outputs and simulated SOC stocks. This consistency provides confidence in using RothC_R_{mod} as an effective alternative to the original RothC model.

The alignment between RothC_R_{mod} and the original RothC model can be further improved by initialising RothC_R_{mod} using the final SOC pool sizes obtained from the RothC spin-up phase. Although the RothC Windows interface does not allow extraction of all annual pool sizes during spin-up, it does provide the final pool sizes. When these RothC-derived pools are used to initialise RothC_R_{mod}, the average SOC stock difference decreases to just 0.18 Mg C ha⁻¹ yr⁻¹, corresponding to a negligible underestimation of 0.24%. This finding suggests that, in some cases, it may be beneficial to perform the spin-up using the RothC model and then switch to RothC_R_{mod} for forward simulations. This approach offers dual advantage of maintaining consistency with RothC while leveraging the flexibility and transparency of the generalised model framework.

While the RothC and RothC_R_{mod} exhibit no significant differences, it is essential to recognise that they are not identical systems. The discrepancies between the rate modifiers and outputs from RothC and RothC_R_{mod} are minimal, making it challenging to pinpoint precisely where the differences occur. We assume the differences are likely due to the structure of SoilR, reflecting a general model framework and requiring annual C inputs and/or different rounding mechanisms between the underlying software architecture, contributing to a slightly higher decomposition rate experienced by the RothC_R_{mod}. However, a significant advantage of the RothC_R implementation is the ease and flexibility of use and that it is open-source software, which supports greater transparency in model development and facilitates community refinement and enhancement.

Comparative studies between RothC and RothC_R are limited in the published literature, although Lefebvre *et al.* (2020) and Riggers *et al.* (2019) do provide some detailed insights. Lefebvre *et al.* (2020) amended RothC_R by incorporating a SCF to represent periods of soil cover and bare months typical in sugarcane systems in Brazil. They also examined equilibrium values derived from spin-up runs across various soil texture groups, with slight differences occurring between their amended RothC_R and the RothC model. However, this approach may overlook potential short-term variations, if any. Our study observed minimal differences between RothC_R_{mod} and RothC during short- and long-term simulations. Furthermore, these differences can be further reduced if the RothC_R_{mod} model is initialised with RothC pool sizes.

Unlike Lefebvre *et al.* (2020), Riggers *et al.* (2019) did not report specific code modifications but evaluated multiple SOC models implemented in SoilR against their respective parent models, including a RothC_R adaptation. They observed high agreement between their RothC_R and the original RothC model, reporting an R^2 of 0.9989. This high level of agreement collaborates with our findings, as RothC_R_{mod} similarly achieved low MAE and RMSE values, confirming its reliability as a faithful emulation of RothC for simulating SOC stock dynamics in permanent temperate grasslands. However, such a high level of agreement is difficult to achieve without accounting for the SCF, highlighting the importance of documenting code amendments, as the RothC_R_{def} is not a faithful adaptation of RothC unless you are only focusing on permanently bare soils.

The modification of SCF also varies depending on the type of ecosystem. The RothC_R model operates with an annual SCF, whereas the original RothC model applies a monthly SCF. Lefebvre *et al.* (2020) accounted for this difference by adjusting the SCF based on the ratio of fallow to covered months, deriving an annual SCF suited to their study. For grassland or other land-use systems that are not permanently covered by vegetation, an average SCF (SCF_{avg}) is required. This can be expressed as:

$$SCF_{avg} = \frac{(0.6 \times M_{covered}) + (1.0 \times M_{bare})}{12} \quad (4.9)$$

where SCF_{avg} is calculated by weighting the covered reduction coefficient (0.6) by the number of covered months ($M_{covered}$) and the bare coefficient (1.0) by the number of bare months (M_{bare}). Therefore, within the RothC_R model, it is essential to treat SCF as a dynamic, tailored coefficient to accurately represent the original RothC model's monthly SCF approach. A similar approach would be necessary to incorporate into Equation 4.4, as bare or vegetated surfaces also impact it. Furthermore, this approach requires further validation to evaluate the differences between RothC and RothC_R.

Model spin-up runs can be problematic due to sensitivity to initial parameterisations and input data (Nemo *et al.*, 2017). Alternative approaches, such as fractionation methods (Zimmermann *et al.*, 2007) and pedo-transfer function (PTF) methods (Weihermüller *et al.*, 2013), have been proposed to obtain the initial SOC pool values. These methods typically rely on soil texture as a proxy for determining individual pool sizes. However, initialising unverified RothC model implementations with these alternative spin-up approaches is likely to introduce substantial errors within the model simulations. Our results (Table 4.4) indicate that after 21 years of simulation, the RothC_{R_{def}} model initialised with RothC-derived pool sizes resulted in an increase of 19.26 Mg C ha⁻¹ than when initialised with values determined by RothC_{R_{def}}. This finding highlights the critical importance of long-term model validation, as short-term simulations may fail to capture slow SOC dynamics and potential discrepancies arising from incorrect initialisations. Comprehensive, time-appropriate validation is essential to ensure the reliability of SOC modelling approaches.

4.4.3 Park Grass replication

To validate the RothC_{R_{mod}} model, we replicated the findings of Coleman *et al.* (1997), a study initially used to calibrate and validate the RothC model. Although we aimed to mirror Coleman *et al.* (1997), a replicate simulation was not possible due to data uncertainties. Weather data is an important model input and driver of the RothC model (Coleman *et al.*, 2024). The weather inputs from the Coleman *et al.* (1997) study were not provided; hence, we obtained meteorological measurements from the Rothamsted weather station via the e-RA database. The e-RA database provides daily meteorological records for the Rothamsted weather station from 1853, which we used to calculate monthly average climatic inputs.

While the climatic inputs sourced from the e-RA database provide a close approximation, the absence of the original climate data used by Coleman *et al.* (1997) makes it impossible to assess the exact degree of similarity. This highlights a broader challenge in SOC modelling, the replicability of model results, which can significantly affect the comparability and accuracy of model outputs across studies.

One known difference lies in the treatment of evaporation; Coleman *et al.* (1997) used measured OPE, which was subsequently converted to ET equivalent using RothC's internal conversion. In contrast, this study employed either evaporation over water converted to ET using the RothC internal factor of 0.75 or direct estimates from ET_{PM}. Without access to the OPE measurements used in the original study, it is not possible to determine how closely our estimates align with those of Coleman *et al.* (1997). Notably, we observed differences between the two ET estimation methods. On average, the ET_{PM} method produced higher ET values than evaporation over water ET equivalent. These higher ET values led to lower

values of the moisture rate modifier, which in turn reduced decomposition rates and resulted in higher SOC stock estimates.

The simulations of the Park Grass plots 3d and 14d all performed well, producing satisfactory RMSE ranging from 2.04 to 6.27 Mg C ha⁻¹. The Park Grass simulation using evaporation over water produced an average RMSE of 3.22 Mg C ha⁻¹, while ET_{PM} variation produced an average RMSE of 5.7 Mg C ha⁻¹. Considering the difference between monthly ET estimates between the methods, this difference did not propagate significantly throughout the SOC stock estimates. When the ET_{PM} variant was adjusted using optimised C inputs estimated via inverse modelling, it produced the lowest average RMSE of 2.92 Mg C ha⁻¹. However, this is to be expected when supplying a site simulation with the desirable amount of C inputs to achieve a known SOC stock measurement.

Another important aspect is the difference between the optimised C inputs between studies. Coleman *et al.* (1997) found a C input of 3 t C ha⁻¹ yr⁻¹ and 2.7 t C ha⁻¹ yr⁻¹ to be optimum in fitting the modelled SOC stock values to measured SOC stock values. In our study, when using ET_{PM}, we found 2.57 t C ha⁻¹ yr⁻¹ and 2.27 t C ha⁻¹ yr⁻¹ to be the best fit. However, Coleman *et al.* (1997) emphasised that the inversely estimated C inputs do not necessarily represent real or accurate C inputs. Instead, the difference between C inputs likely demonstrates the difference in decomposition rates derived from the evaporation data inputs.

For example, in Coleman *et al.*'s (1997) study and our evaporation over water simulation, the model is supplied with 3 t C ha⁻¹ for plot 3d to achieve the measured SOC stock value. This may indicate a higher rate of decomposition, which is offset by a higher C input estimate. For the model variant using ET_{PM} and inverse C inputs, plot 3d is supplied with 2.57 t C ha⁻¹, indicating that rate modifiers derived from ET_{PM} produce lower decomposition rates. As a result of the lower decomposition rates, the model requires a lower C input estimate to achieve the desired SOC stock measurement.

Another potential difference in model inputs stems from handling missing meteorological data. Like many long-term weather stations, the Rothamsted weather station has missing variables for days, months and years. We substituted missing monthly values with long-term averages for that associated month. However, it is unknown if Coleman *et al.* (1997) employed the same substitution, which could further contribute to the input differences between our study.

Despite the noted differences in model inputs, our replication of the Park Grass simulation for plots 3d and 14d using RothC_R_{mod} displays a very similar result to the findings from Coleman *et al.* (1997) using the RothC model. Since Coleman *et al.* (1997) did not provide model performance metrics for the Park Grass plots, we cannot directly compare model

performances. A more rigorous evaluation of the performance metrics of RothC_R_{mod} would involve directly comparing them against the performance metrics of Coleman *et al.* (1997). Nevertheless, our findings demonstrate that RothC_R_{mod} can achieve a high degree of similarity to the RothC model under analogous conditions. This increases our confidence in the RothC_R_{mod} being utilised to simulate SOC stocks in grasslands.

4.4.4 Issues and limitations

Coleman *et al.* (1997) and Smith *et al.* (1997) were among the earliest attempts at validating the RothC model, comparing it against other SOC models and a wide range of long-term experiments encompassing various ecosystems, management practices, and soil types. In recent years, however, model validation processes have been criticised, with recommendations for a more robust and in-depth approach (Garcia *et al.*, 2023; LeNoë *et al.*, 2023).

Garcia *et al.* (2023) outlined criteria for appropriate model validation as follows: 1) there is a clear distinction between the calibration and validation data; 2) validation data is not used for model initialisation; 3) authors provide metrics of model performance from an appropriate statistical analysis; and 4) validation data are directly measured, not the output from a model or interpolation. LeNoë *et al.* (2023) recommend independent diachronic validation (e.g., SOC change over a specific period) of SOC models at all scales, using sites and networks that provide time series of SOC stocks at plot, national, and regional scales.

Considering the recommendations from Garcia *et al.* (2023) and LeNoë *et al.* (2023), our model validation does not fully adhere to all criteria. There is not a clear distinction between the calibration and validation data. Still, the RothC model was developed and explicitly parameterised for modelling SOC in arable topsoils from the Rothamsted long-term field experiments (Coleman *et al.*, 2024). The Park Grass experiments are close to these arable experiments and likely share similar macro-environmental conditions (e.g., climate, soil formation). Due to this proximity and shared conditions, the Park Grass simulations may benefit from the empirically derived relationships used to parameterise the RothC model.

Another issue with our simulation is the calculation of C inputs. Coleman *et al.* (1997) calculated the C inputs by running the RothC model inversely. To run the RothC model in this way, total SOC stock and site settings (e.g., climatic and edaphic conditions) are required. This approach means that our study was not an independent validation, as it relied on inputs that were not directly measured but estimated through a model. Using models to generate inputs that favour the desired output often leads to overfitting, as the model does not represent the underlying biogeochemical processes generating this C input (Famiglietti *et al.*, 2021). This lack of representation can obscure the model's true performance and reduce its reliability.

Many of the limitations in model validation discussed previously stem from the original experimental design. Improving our approach requires moving away from the methodology outlined in Coleman *et al.* (1997), which would hinder our simulation replication. One of the primary limitations is the absence of validation attempts for RothC_R_{mod} across diverse ecosystem types, regions, and scales. However, expanding RothC_R_{mod} to different ecosystem types in different regions is beyond the scope of our research, which focuses primarily on mineral grassland soils in temperate climates. Nevertheless, one could argue that since the rate modifiers are the most defining characteristic of SOC models, and the RothC and RothC_R_{mod} modifiers show excellent agreement with our performance metrics, this agreement would be consistent under any ecosystem once the SCF is adjusted correctly. We consider the comparison between rate modifiers to be a validation process, as this alignment increases model applicability.

A further limitation is the MS Windows user interface of RothC, which restricts access to certain outputs and complicates data handling. For instance, obtaining the entire monthly SOC stock outputs from the 10,000-year model spin-up is not possible using the current interface. Additionally, other key parameters, such as specific pool decomposition rates, are hard-coded, limiting flexibility for scenario testing, model calibration, modification, and sensitivity analysis. Accessing other model output parameters, such as the rate modifiers, is cumbersome. These values are provided in the output report via a text file and must be manually transferred to another environment for statistical analysis. These additional steps introduce inefficiencies and complicate long-term and large-scale analysis by requiring repetitive manual tasks prone to human error.

Such limitations in the RothC's interface reduce its accessibility for extensive or automated analyses. This constraint highlights the importance of models for efficient and seamless data export, statistical analysis and integration with other programs, which are essential for scaling up model applications and improving workflow efficiency in SOC modelling studies.

4.5 Conclusions

The RothC_R_{mod} model, implemented within a generalised modelling framework, demonstrates behaviour closely aligned with the original RothC model while significantly improving usability, transparency, and flexibility. Importantly, this work illustrates the value of a modular framework such as SoilR, which allows researchers to implement, modify, and evaluate SOC models consistently and transparently. This framework-based approach enables not only improved model usability but also facilitates direct model intercomparison, calibration to empirical datasets, and adaptation to site-specific conditions or novel environment modifiers.

Increased usability has positive implications for both research and policy. By moving away from hard-coded, black-box systems and toward transparent, code-accessible model structures, researchers can more readily calibrate models to local data and adapt them for specific applications. Many processes within RothC_R_{mod} can be automated, potentially serving as an efficient and powerful tool for various stakeholders.

Our comparison between RothC_R_{mod} and RothC validates this implementation for simulating SOC dynamics in permanent mineral grasslands within temperate regions. However, the broader significance lies in demonstrating how generalised frameworks enable reproducible, transferable SOC modelling outputs. We emphasise the importance of ensuring that any model implementation remains faithful to the structure and assumptions of the parent model, and that all code amendments are fully documented to ensure reproducibility.

While the slight difference observed between RothC_R_{mod} and RothC ($<1 \text{ Mg C ha}^{-1}$) is justified by the gains in usability and flexibility, the real value is in the ability to replicate, test, and compare models within a common framework. This trade-off supports the broader objective of advancing SOC modelling through transparent and interoperable tools that can be adapted to diverse environmental and management contexts.

Chapter 5: Balancing complexity: a case study of the RothC_R model input sensitivity

Abstract

The RothC model is widely applied in SOC simulations across plot, regional and global scales. However, it lacks internal sub-models to estimate key inputs such as evapotranspiration (ET) and carbon (C) inputs, which must be derived externally using empirical or auxiliary models. While RothC performs reliably under data-rich conditions, particularly at research farms, its application at broader spatial scales is often limited by the availability of the required input data. To address these constraints, this study builds on the SoilR-based modelling framework developed and evaluated in earlier chapters, which was found to faithfully replicate the original RothC model but with the benefit of increased transparency, flexibility, and potential for automation. Here, we utilise this framework to conduct sensitivity analyses that would be difficult or infeasible with the original RothC model. We provide additional insights into the model using one-at-a-time (OAT) sensitivity analysis, global sensitivity analysis of extreme climate conditions, and a model input ensemble approach.

The OAT analysis revealed that temperature was the most influential driver, with a strong and nearly linear sensitivity response. Rainfall and ET exhibited moderate effects but in opposite directions due to their combined influence on the RothC moisture modifier. SOC stocks responded linearly to changes in C input and were relatively insensitive to clay content except in low-clay conditions. Simulations of extreme wet and dry years produced minimal changes in SOC stocks, likely due to the unrealistic assumption of static C inputs during extreme climatic events and lack of model adaptations to reflect pool-specific temperature sensitivities and conditions such as waterlogging.

The model input ensemble tested eleven combinations of ET and C input estimation methods against a benchmark simulation. In the unmanaged plot, all combinations yielded root mean square error (RMSE) values below 10 Mg C ha⁻¹, whereas in the managed plot, only five combinations achieved values below this threshold. Among the ET methods, the maximum RMSE difference observed was 2.35 Mg C ha⁻¹ in plot 3d and 2.87 Mg C ha⁻¹ in plot 14d. C input method had a greater influence with maximum RMSE differences of 6.24 Mg C ha⁻¹ and 20.63 Mg C ha⁻¹ for plots 3d and 14d, respectively. The appropriate combination of C and ET methods depends on the availability of data. For data-rich contexts, the Penman-Monteith ET and Poeplau-J methodology pairing is recommended for unmanaged systems, and Penman-Monteith ET with the Miami model is recommended for managed systems. Under data-limited conditions, the Thornthwaite ET and Miami model combination

achieved good performance for plots, representing a practical balance between feasibility and model performance in large-scale SOC assessment.

5.1 Introduction

The RothC model has been extensively applied in SOC simulations across plot, regional and global scales (Coleman *et al.*, 1997; Falloon and Smith, 2002; Gottschalk *et al.*, 2012). Despite its wide application and validation, RothC outputs remain sensitive to input data quality, model structure, and scale of implementation (Maas and Lal, 2023; Riggers *et al.*, 2019; Qin *et al.*, 2016). These limitations highlight the importance of understanding how the RothC model behaves under varying data input and methodological choices (e.g., Maas and Lal, 2023; Riggers *et al.*, 2019).

The RothC model is known to require relatively few data inputs (Campbell and Paustian, 2015; Sierra *et al.*, 2012), which is partly responsible for its widespread use. Its primary inputs include climate data (e.g., temperature, rainfall and evapotranspiration (ET)), soil properties (clay content), and carbon (C) inputs from plant residues and manure (Coleman *et al.*, 2024). However, RothC lacks internal sub-models to estimate ET and C inputs (Coleman *et al.*, 2024), and these values must therefore be derived externally, often using auxiliary models or empirical approaches. RothC's performance is highly sensitive to how ET and C inputs are estimated, as divergent estimation methods can lead to markedly different SOC predictions, even under identical soil and climate conditions (e.g., Maas and Lal, 2023; Qingsong *et al.*, 2023; Riggers *et al.*, 2019).

While previous RothC studies have investigated RothC across different climates, land uses, and management types (Afzali *et al.*, 2019; Paramesh *et al.*, 2022; van Wesemael *et al.*, 2010), a number have incorporated additional sub-models to expand its scope or improve model performance (e.g., Doblas-Rodrigo *et al.*, 2023; Farina *et al.*, 2013; Jebari *et al.*, 2021; Shirato and Yokozawa, 2005). Other efforts have examined the model's sensitivity to parameterisation (Janik *et al.*, 2002; Paul *et al.*, 2003; Wüst-Galley *et al.*, 2021) or the model's response to different model input methods (Maas and Lal, 2023; Qingsong *et al.*, 2023). However, to our knowledge, no study has explicitly evaluated how RothC responds across a gradient of input complexity, particularly in the transition from data-rich (e.g., research farms) to data-limited (e.g., commercial farms) environments.

This gap is important as many RothC applications are evaluated at data-rich locations but are subsequently deployed elsewhere under the assumption that model performance will generalise. Yet, in many application settings, the availability of detailed input data is often constrained, potentially undermining the model's reliability. To substantiate this, we review numerous RothC grassland studies to assess the diversity in ET and C input estimation methods across various spatial and environmental contexts. This synthesis (Appendix B.1,

Table 5B.1) reveals substantial variation in both ET methods and C input methods employed, often dictated by the availability of data or ease of implementation.

To evaluate the impact of different inputs, we classified ET and C estimation methods from identified in this synthesis into three categories based on data requirements and process representation: simple, intermediate, and complex. Evapotranspiration methods can be broadly categorised by data complexity and similarity in underlying assumptions. The simplest methods include Thornthwaite (1948) and Thornthwaite and Mather (1955), which rely on average monthly temperatures and latitude and are based on empirical relationships to estimate ET. Intermediate methods include those of Priestly and Taylor (1972), Hargreaves and Samani (1985), Hargreaves (1994), Prentice *et al.* (1993), and Sitch *et al.* (2003), which rely on daily or monthly temperature, solar radiation, and empirical coefficients calibrated for different climates. Penman-Monteith (Monteith, 1965) uses complex methods that integrate the surface energy balance, canopy resistance, and aerodynamic principles, and requires daily temperature, solar radiation, wind speed, humidity, and vapour pressure to estimate ET.

Similarly, the C input estimation methods identified in this synthesis were also classified according to their methodological complexity into three categories: simple, intermediate, and complex. Simple methods derive C inputs based on empirical relationships, including the Miami model or those outlined by the Intergovernmental Panel on Climate Change (e.g., C inputs derived from DM yields and applying generic adjustment coefficients for arable systems) (IPCC, 2006, 2019). The former estimates NPP and, ultimately, C inputs based on annual temperature and precipitation (Lieth, 1973). Intermediate methods quantify C input from recorded or national averages of plant biomass, root-to-shoot ratios (R:S), and assume that only a portion is available for SOC turnover, such as the methodologies proposed by Bolinder *et al.* (2007), Bielek and Jurcova (2010), and Poeplau (2016). Complex methods for estimating C inputs are data- and process-intensive, involving either inverse modelling approaches (e.g., RothC run in inverse mode) or process-based frameworks such as the Global Livestock Environmental Assessment Model (GLEAM) and the CENTURY model. While GLEAM simulates biophysical processes within livestock and manure management systems, CENTURY explicitly represents plant growth, litter production, and their interactions with management and climate (Coleman *et al.*, 2024; Dondini *et al.*, 2023; Parton, 1996a).

The variation of model inputs reflects necessary adaptations to deal with data limitations, climate conditions, and research application needs. Plot-scale simulations often occur in data-rich environments, such as long-term experiments, which can employ complex methods, whereas regional and national studies typically rely on simpler approaches that

reflect data limitations. Although it is often assumed that more complex inputs yield more accurate SOC estimates (FAO, 2019), recent studies have shown that simpler methods can perform equally well, or better, in data-limited environments (e.g., Davoudabadi *et al.*, 2024; Maas and Lal, 2023; Vázquez-Amábile *et al.*, 2025). This underscores the need to evaluate how RothC performs across gradients of input complexity, to identify satisfactory trade-offs between model performance and data complexity.

Understanding RothC's sensitivity to different inputs depends on both the method employed and the relative importance or influence of the input as a driver of SOC. While local sensitivity analysis (SA) can identify the influence of individual drivers, ET is not independent in RothC because it interacts with temperature and rainfall through the environmental modifier (ξ). As ξ reflects a nonlinear combination of climate variables, isolating ET in a local SA may obscure its influence. To address this, we also conduct a global SA to evaluate RothC's behaviour under more extreme climate conditions, where temperature, rainfall, and ET vary simultaneously.

Unlike previous SA efforts that focus primarily on calibration (e.g., Janik *et al.*, 2002; Paul *et al.*, 2003) or on comparing input methods (e.g., Maas and Lal, 2023; Qingsong *et al.*, 2023), here we investigate how RothC performs against the complexity of data inputs. To our knowledge, no study has explicitly evaluated RothC's performance with regard to data granularity. To achieve this, we will operate the RothC model with optimum data inputs and manually degrade the inputs by supplying modelling efforts with simpler model-derived estimates, allowing us to evaluate how different levels of input complexity influence model performance under varying data conditions. Our goal is to identify the optimal combinations of model inputs that produce the most satisfactory results while minimising data requirements.

Specifically, we aim to: (i) assess the sensitivity of RothC to its primary input drivers (e.g., climate, management and soil); (ii) evaluate the behaviour of RothC's ξ under more extreme scenarios that capture variations in temperature, rainfall, and ET; (iii) examine how different ET and C input estimation methods influence model outputs; and (iv) identify input configurations that achieve satisfactory performance under data-limited conditions.

5.2 Data and methods

5.2.1 Site description

The RothC sensitivity analysis (SA) was conducted using data from the Park Grass experiment, the oldest continuous permanent grassland trial, located at Rothamsted, Harpenden, England (51°48' N, 0°22' W; elevation 133m) (MacDonald *et al.*, 2018; Rothamsted Research, 2006; Silvertown *et al.*, 2006). The site has a temperate climate, with

silty clay loam soils that are moderately well-drained (Silvertown *et al.*, 2006). Further site details are provided in Section 4.2.2.

Sub-plots 3d and 14d were selected for this study due to their prior use in RothC simulations by Coleman *et al.* (1997) and the findings from Chapter 4. These plots serve as optimal benchmark sites for the model simulations, exhibiting high agreement between observed and modelled SOC stocks, as evidenced by low root-mean-square-error (RMSE) (see Section 4.3.4). Additionally, the availability of the detailed management and meteorological data from the electronic Rothamsted archive (e-RA) (see Perryman *et al.*, 2018) supports the evaluation of different model input methods for estimating C inputs and ET. The two plots also differ in management, plot 3d receives no external amendments. In contrast, plot 14d is being actively managed with Nitrogen, Phosphorus, Potassium, Sodium sulphate and Magnesium sulphate spread at rates of 96 kg, 17kg, 225 kg, 15kg, and 10kg, respectively (MacDonald *et al.*, 2018).

A 25-year time period (1965-1989) was selected as the optimal timeframe for evaluating the multi-model ensemble of C and ET estimation methods. This interval corresponds to the most consistent management conditions within the baseline RothC simulations throughout the Park Grass experiment. In 1965, nearly all Park Grass plots were subdivided into four sections to investigate the influence of lime application. Plot 14d underwent further subdivision in 1989. Furthermore, all meteorological data from the Rothamsted weather station recorded before 1955 should be treated with caution, as there was much uncertainty about the sensitivity of the equipment (Penman, 1948). Therefore, this period represents a phase of relatively uniform management and reliable meteorological records, providing consistent C input and ET estimates across both plots and allowing for a more robust comparison of input methods.

5.2.2 Model description

The SoilR framework (Sierra *et al.*, 2012) was used to implement the RothC model within the R environment (R Core Team, 2024). SoilR provides a flexible matrix-based modelling framework that enables the construction of multi-model ensembles to evaluate alternative input-estimation methods (e.g., Riggers *et al.*, 2019). This implementation, hereafter referred to as RothC_R, was demonstrated to be a faithful adaptation of the RothC model (see Chapter 4). A detailed description of the RothC model is provided in Section 4.2.1, and code amendments are outlined in Section 4.2.4.

5.2.3 Estimation methods for model input ensemble

Estimation methods for the model ensemble were selected based on their complexity, reflecting a gradient from simple to complex approaches for both ET and C input estimation

methods. Three ET estimation methods were chosen to represent increasing complexity and data requirements: Thornthwaite (1948), Hargreaves (1994) and Penman-Monteith (Monteith, 1965). The Penman-Monteith (Monteith, 1965) approach is widely regarded as the most robust and data-intensive method and is the recommended approach by the FAO (Allen *et al.*, 1998). Hargreaves (1994) serves as an intermediate method, suitable where Penman-Monteith is impractical due to data limitations and is the FAO-recommended alternative (Allen *et al.*, 1998). Thornthwaite (1948), a temperature-based empirical method, represents the simplest approach and is frequently applied in RothC grassland studies.

Similarly, C input estimation methods were selected to reflect increasing levels of complexity, including the Miami Model, Poeplau's (2016) methodology, and the RothC inverse approach. The Miami model is one of the simpler approaches utilised in large-scale RothC studies and is empirical (e.g., Geremew *et al.*, 2024; Peralta *et al.*, 2022). In contrast, Poeplau's (2016) method provides an intermediate approach that incorporates site-specific information, using recorded dry matter (DM) yields alongside empirical assumptions, and has been applied successfully in several grassland sites across Europe (e.g., Jebari *et al.*, 2021; Poeplau, 2016). The RothC inverse approach represents the most complex method, as it requires detailed site-specific soil, climate, and management data, together with measured SOC stocks, to estimate C inputs.

The benchmark simulation for Park Grass plots 3d and 14d employed Penman-Monteith and the RothC (original) inverse-derived C inputs. This configuration, previously validated in Chapter 4, demonstrated strong agreement between measured and modelled SOC stocks and represents a data-rich scenario. For the analysis, the benchmark was systematically degraded by replacing more complex input methods with simpler alternatives, enabling direct comparison across input configurations. This approach provides a structured basis for evaluating RothC performance under contrasting data-rich to poor environments.

5.2.4 Evapotranspiration methods

All the data required to calculate ET using Thornthwaite (1948), Hargreaves (1994) and Penman-Monteith (Monteith, 1965) methods were obtained from the Rothamsted meteorological records via the e-RA database (Perryman *et al.*, 2018).

Thornthwaite

The Thornthwaite (1948) ET method can be expressed as:

$$ET_{THO} = 16 \times \left(\frac{10 \times T}{I} \right)^a \quad (5.1)$$

where,

ET_{THO}: Thornthwaite ET in mm per month
T: mean monthly temperature in °C (if T < 0, ET_{THO} = 0)
I: Annual heat index, calculated as:

$$I = \sum_{i=1}^{12} \left(\frac{T_i}{5}\right)^{1.514} \quad (5.2)$$

where, T_i is the mean temperature of the month i in °C.

α is an exponent determined by I:

$$\alpha = (6.75 \times 10^{-7})I^3 - (7.71 \times 10^{-5})I^2 + (1.79 \times 10^{-2})I + 0.49239 \quad (5.3)$$

The ET_{THO} was calculated using the R package Standardized Precipitation Evapotranspiration Index (SPEI, Beguería *et al.*, 2014).

Hargreaves

The Hargreaves (1994) equation is expressed as:

$$ET_{HAR} = 0.0023 \times (T_{mean} + 17.8) \times (T_{max} - T_{min})^{0.5} \times R_a \quad (5.4)$$

where,

ET_{HAR}: Hargreaves ET in mm per month

T_{mean}: Mean daily air temperature

T_{max}: Maximum daily air temperature

T_{min}: Minimum daily air temperature

R_a: Extraterrestrial radiation (MJ/m²/day) is calculated based on astronomical equations using latitude, elevation, and time of year.

To calculate ET_{HAR}, we utilised the R package 'FAO56' (Ahani and Mousavi Nadoushani, 2023), which follows equations from the FAO guidelines (Allen *et al.*, 1998).

Penman-Monteith

The Penman-Monteith (Monteith, 1965) is expressed as:

$$ET_{PEN} = \frac{0.408\Delta(R_n - G) + \gamma \frac{900}{T + 273} u_2 (e_s - e_a)}{\Delta + \gamma(1 + 0.34u_2)} \quad (5.5)$$

where,

ET_{PEN}: Penman-Monteith ET in mm per month

R_n: Net radiation at crop surface (MJ/m²/day)

G: Soil heat flux density (MJ/m²/day)

u₂: Wind speed at 2 meters height (m/s)

e_s: Saturation vapour pressure at air temperature (kPa)

e_a: Actual vapour pressure (kPa)

Δ: Slope of the saturation vapour pressure curve (kPa/°C)

γ: Psychrometric constant (kPa/°C)

T: Mean air temperature (°C)

To calculate Penman-Monteith (PEN), the R package 'FAO56' (Ahani and Mousavi Nadoushani, 2023) was employed, and it implemented equations from Allen *et al.* (1998). Calculations of ET methods are outlined in Appendix B.3.

5.2.5 Carbon inputs methods

Miami model

The Miami Model (Lieth, 1973) estimates NPP using empirical functions based on mean annual temperature and annual precipitation, which were fitted to global NPP observations from the 1970s. The Miami model estimates NPP (NPP_{Miami}) for a particular location using a minimum temperature or precipitation function:

$$NPP_{Miami} = \min(NPP_T, NPP_P) \quad (5.6)$$

where,

$$\begin{aligned} NPP_T &= 3000(1 + \exp(1.315 - .119 \times \bar{T}))^{-1} \\ NPP_P &= 3000(1 - \exp(-0.000664 \times \bar{P})) \end{aligned} \quad (5.7)$$

Here, $\bar{T}$ is long-term annual mean temperature (°C), and $\bar{P}$ is long-term annual precipitation (mm). The estimated NPP (in $\text{g m}^{-2} \text{ yr}^{-1}$) is converted to C inputs in $\text{t C ha}^{-1} \text{ yr}^{-1}$ as follows:

$$C_{input}_{Miami} = NPP_{Miami} \times 0.01 \times 0.45 \times 0.72 \quad (5.8)$$

where 0.01 converts g m^{-2} to t ha^{-1} , 0.45 converts dry biomass to C (Kätterer *et al.*, 2011), and 0.72 represents the fraction of NPP entering the soil for a grassland system (Peralta *et al.*, 2022). Grieser *et al.* (2006) provide further details on the Miami model equations. Long-term average temperature and rainfall data from 1965 to 1989 were used to calculate the C input.

Poeplau methodology

The Poeplau (2016) methodology uses the following equations and assumptions to quantify total C inputs:

$$ANPP = \frac{HB}{0.7} \times 0.45 \quad (5.9)$$

where ANPP is aboveground net primary production ($\text{Mg C ha}^{-1} \text{ yr}^{-1}$), and HB is harvested biomass ($\text{Mg DM ha}^{-1} \text{ yr}^{-1}$). It assumes HB accounts for 70% of total ANPP and contains a C concentration of 45% (Kätterer *et al.*, 2011). Aboveground carbon inputs (AC_{in}) were calculated with the following function:

$$AC_{in} = \frac{ANPP \times 0.3}{2} + FC_{in} \quad (5.10)$$

where 0.3 is part of the ANPP that is not harvested. It is further assumed that only 50% of the fraction is available for the formation of soil organic matter. The FC_{in} is the total fertiliser-derived C input.

The total belowground net primary production (BNPP; $Mg\ C\ ha^{-1}\ yr^{-1}$) is calculated as:

$$BNPP = ANPP \times R:S \quad (5.11)$$

The R:S is dependent on species composition and management practices. We selected two different R:S methods. Poeplau (2016) derived an average R:S from fertilised and unfertilised plots of 5.9 ± 1.9 and 2.4 ± 1.5 , respectively. Additionally, Jebari *et al.* (2021) described an equation to estimate the R:S based on levels of nitrogen (N) application ($kg\ N\ ha^{-1}$):

$$R:S = 4.7375e^{-0.0043 \times N_{input}} \quad (5.12)$$

The C inputs derived from BNPP (BC_{in}) were calculated as follows:

$$BC_{in} = \frac{BNPP}{2} \quad (5.13)$$

We determined the fraction of total BNPP that is distributed to a certain sampling depth (d), using the following function from Poeplau (2016):

$$BNPP_d = \frac{d \times (d_{50} + d_r)}{d_r \times (d_{50} + d)} \quad (5.14)$$

where d_r is the maximum rooting depth, and d_{50} is the depth to which 50% of the total BNPP is distributed. Finally, the total C input (TC_{in} ; $Mg\ C\ ha^{-1}\ yr^{-1}$) to a certain depth (d) was calculated as:

$$TC_{ind} = BC_{in_d} + AC_{in} \quad (5.15)$$

For more information, see Poeplau (2016). Calculations of Miami and Poeplau C input methods are outlined in Appendix B.3.

RothC inverse modelling

We applied the original RothC model in inverse mode to estimate the annual C input required to match the observed SOC stocks under specific climate, soil, and management conditions. Carbon inputs were calculated using digitised SOC stock values from plots 3d and 14d, along with observed weather and Penman-Monteith derived ET inputs. The estimated C inputs were $2.57\ t\ C\ ha^{-1}\ yr^{-1}$ for plot 3d and $2.27\ t\ C\ ha^{-1}\ yr^{-1}$ for plot 14d. Section 4.2.3 provides further details on these values and the process.

5.2.6 Sensitivity analysis

Local Sensitivity Analysis

A one-at-a-time (OAT) local SA was conducted on the main inputs to the RothC model, including C inputs, climatic variables (temperature, precipitation, ET), and clay percent. The Park Grass plot 3d simulation was selected as the baseline. For this analysis, temperature was altered by $\pm 0.5^{\circ}\text{C}$, $\pm 1.0^{\circ}\text{C}$ and $\pm 1.5^{\circ}\text{C}$. Rainfall, ET and C inputs were adjusted by $\pm 5\%$, $\pm 10\%$, and $\pm 15\%$. Clay content was modified in increments of 5% and 10%. Climatic perturbations were applied to monthly inputs to preserve seasonality. While the selected ranges may not be realistic, the primary goal here was to evaluate the model's response to changes in inputs. All simulations were initialised with identical SOC pool sizes, and only one driver was altered at a time, ensuring that the results were attributed solely to the parameter of interest.

Global Sensitivity Analysis

A global sensitivity analysis was conducted for climate-related drivers, using the Park Grass plot 3d simulation as a reference. Four climatic scenarios were designed to evaluate model responses under co-varying climate stressors. Scenario 1: a 1.5°C increase in temperature and a 15% increase in rainfall and ET values; Scenario 2: a 1.0°C decrease in temperature and a 10% decrease in rainfall and ET values; Scenario 3: an extreme wet scenario; and Scenario 4: an extreme dry scenario. Scenarios 1 and 2 apply uniform perturbations, imposing fixed absolute changes to temperature and proportional adjustments to rainfall and ET across all months. The focus here was not on the realism of the scenarios, but on evaluating the model responses to an altered climate.

Scenarios 3 and 4 simulate seasonal climatic extremes based on actual weather observations. A 30-year monthly mean baseline (1961-1990) for temperature, rainfall and evaporation was obtained from the e-RA database. These values were compared to recent extreme years, with 2012 being a wet year and 2022 being a dry year, selected to derive monthly adjustment factors. These factors were then applied to modify the whole simulation period, replicating the seasonal patterns of those extreme conditions.

While the extreme wet and dry scenarios are not intended to represent future climate trajectories, they serve to illustrate the model behaviour under repeated years of climatic stress. All simulations were initialised with the same SOC stock, and all other parameters were held constant to isolate the effects of climate drivers. Monthly adjustment values used for Scenarios 3 and 4 are provided in Appendix B.2.

Model input sensitivity

To evaluate the model's sensitivity to ET and C inputs, we conducted a multi-model ensemble by testing different combinations of estimation methods. This sensitivity analysis

closely mirrors the RothC_R model configuration described in Section 4.2.6, with minor amendments to accommodate the specific input combinations evaluated. A 25-year simulation period (1965-1989) was selected, aligning with consistent site management practices and high-quality data availability. All simulations were initialised with the same SOC pool sizes, derived from the corresponding benchmark simulations for Park Grass plots 3d and 14d.

When operating the model with the ET_{THO} , ET_{HAR} , and ET_{PEN} methods, the evaporation coefficient (pE) was set to 1.0 (Sierra *et al.*, 2012). The model operation varied for the C input methodology. The RothC inverse and Miami model C input methods were a constant single value applied annually throughout the model simulation. In contrast, the Poeplau (2016) methodology recommends dynamic annual C inputs, which the RothC_R structure does not support by default without further code amendments. To address this, we used a five-year mean C input estimates (e.g., 1965-1969, 1970-1974, etc), allowing for some temporal variability without increasing model complexity (additional code, etc).

To differentiate between different model input combinations, a consistent naming convention was adopted. Simulations were labelled using the first three letters of the ET method capitalised, followed by the C input method name in lowercase. For example, a model using Thornthwaite ET and Miami-derived C inputs was designated as THO.miami. Two variants of the Poeplau method were included: one using R:S ratios from fertilised and unfertilised plots as reported in Poeplau (2016), denoted as poeplau_P. The other uses R:S ratios from nitrogen application rates following the methodology by Jebari *et al.* (2021), denoted as poeplau_J. The model combinations and naming conventions are summarised in Figure 5.1.

		Evapotranspiration methods		
		Thornthwaite (THO)	Hargreaves (HAR)	Penman-Monteith (PEN)
C input methods	Miami model	THO.miami	HAR.miami	PEN.miami
	Poeplau (R:S = Poeplau (2016))	THO.poeplau_P	HAR.poeplau_P	PEN.poeplau_P
	Poeplau (R:S = Jebari <i>et al.</i> (2021))	THO.poeplau_J	HAR.poeplau_J	PEN.poeplau_J
	RothC inverse	THO.rothc	HAR.rothc	<u>PEN.rothc</u>

Increasing complexity (red arrow pointing right)

Increasing applicability (purple arrow pointing left)

Figure 5.1 Matrix of a combination of methods for modelling evapotranspiration and carbon inputs. The methods in the top left are the simplest, while the methods in the bottom right are the most complex and data demanding. PEN.rothc is underlined as it represents the benchmark simulation.

5.2.7 Statistical analysis

The influence of individual input drivers on the model outputs was quantified using the sensitivity index (S_i) reported by Janik *et al.* (2002). The S_i expresses the relative change in total SOC for a relative change in the selected parameter value; therefore, it is dimensionless. The S_i can be described as:

$$S_i = ((C_2 - C_1)/C_1)/((P_2 - P_1)/P_1) \quad (5.16)$$

where,

P_1 is the initial value of variable P ;

P_2 is the altered value of variable P ;

C_1 is the predicted SOC stock before altering the variable P ;

C_2 is the predicted SOC stock after altering the variable P .

The S_i ranges from -1 to +1, where values close to +1 indicate a strong positive sensitivity and values close to -1 indicate a strong negative sensitivity. Values close to zero suggest low or negligible sensitivity to the driver in question. To evaluate the model performance in the multi-input ensemble, the RMSE was used, as detailed in Section 4.2.7. The interpretation of RMSE performance is context-dependent; however, in similar SOC simulation studies, an RMSE <5 Mg C ha⁻¹ indicates excellent agreement, 5-10 is considered good, 11-20 moderate/reasonable agreement, and values >20 reflect poor model performance (e.g., Barančíková *et al.*, 2023; Doblas Rodrigo *et al.*, 2022; Falloon and Smith, 2002; Jebari *et al.*, 2021).

5.3 Results

5.3.1 OAT results

The OAT SA alteration of climatic and C inputs drivers revealed a range of responses, as shown in Table 5.1. Temperature increases consistently reduced modelled SOC stocks, while decreases led to SOC gains. Rainfall exhibited a similar trend, where higher rainfall levels reduced SOC. In contrast, ET (Penman) displayed the opposite behaviour. Higher rates of ET led to increased SOC values, while lower ET values reduced modelled SOC stock. As expected, increasing C inputs led to proportional increases in modelled SOC stocks, whereas reductions in C inputs led to declines. The S_i ranged from -0.83 to +0.56 across all climatic and C input drivers, indicating moderate to high sensitivity. Temperature exhibited the strongest negative sensitivity (S_i : -0.76 to -0.83), followed by rainfall (S_i : -0.43 to -0.51). ET showed moderate positive sensitivity (+0.41 to +0.56), and C inputs displayed a consistent moderate positive S_i of +0.56 across all perturbations. These patterns are displayed in Figure 5.2, with modelled SOC stocks and S_i shown for each parameter.

Table 5.1 One-at-a-time sensitivity analysis of RothC modelled SOC stocks in response to fixed changes ($\pm 0.5^{\circ}\text{C}$, $\pm 1.0^{\circ}\text{C}$, $\pm 1.5^{\circ}\text{C}$) in temperature and proportional changes ($\pm 5\%$, $\pm 10\%$, $\pm 15\%$) in rainfall, evapotranspiration, and carbon (C) inputs. Final SOC stock and stock difference (diff.) are expressed in Mg C ha^{-1} . The sensitivity index (S_i) represents the dimensionless ratio of the relative change in SOC to the relative change in the corresponding input parameter.

Parameter	Change	Final SOC stock estimate	SOC stock diff.	Difference (%)	S_i
Temperature	+0.5°C	70.95	-2.89	3.92	-0.78
Temperature	+1.0°C	68.15	-5.69	7.71	-0.77
Temperature	+1.5°C	65.44	-8.40	11.38	-0.76
Temperature	-0.5°C	76.83	2.98	4.04	-0.81
Temperature	-1.0°C	79.90	6.06	8.21	-0.82
Temperature	-1.5°C	83.07	9.23	12.49	-0.83
Rainfall	+5%	72.01	-1.84	2.49	-0.5
Rainfall	+10%	70.38	-3.47	4.69	-0.47
Rainfall	+15%	69.05	-4.79	6.49	-0.43
Rainfall	-5%	75.71	1.87	2.53	-0.51
Rainfall	-10%	77.14	3.3	4.46	-0.45
Rainfall	-15%	78.76	4.91	6.65	-0.44
Evapotranspiration	+5%	75.79	1.94	2.63	0.53
Evapotranspiration	+10%	77.11	3.27	4.42	0.44
Evapotranspiration	+15%	78.33	4.49	6.08	0.41
Evapotranspiration	-5%	71.79	-2.05	2.78	0.56
Evapotranspiration	-10%	69.75	-4.09	5.54	0.55
Evapotranspiration	-15%	67.85	-5.99	8.12	0.54
C input	+5%	75.92	2.08	2.82	0.56
C input	+10%	78	4.16	5.64	0.56
C input	+15%	80.08	6.24	8.45	0.56
C input	-5%	71.76	-2.08	2.82	0.56
C input	-10%	69.68	-4.16	5.64	0.56
C input	-15%	67.6	-6.24	8.45	0.56

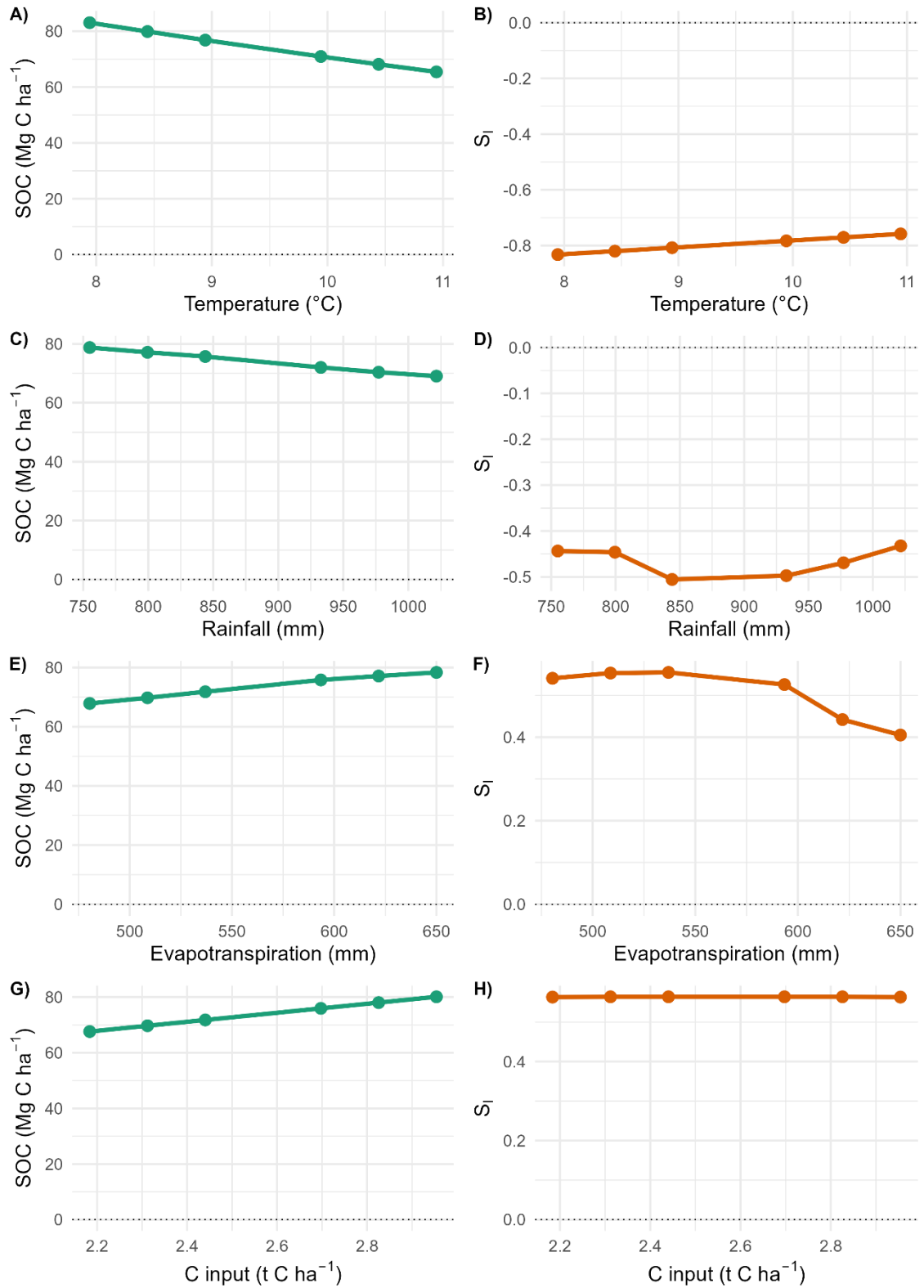


Figure 5.2 One-at-a-time sensitivity analysis of the RothC model illustrating the effect of individual parameter perturbations on simulated soil organic carbon (SOC) stocks. Each row represents a different input variable (A-B) temperature, (C-D) rainfall, (E-F) evapotranspiration, and (G-H) carbon (C) inputs. Left column graphs display the final SOC stock (Mg C ha⁻¹), while right column graphs display the corresponding sensitivity index (S_i). Temperature perturbations were applied as fixed offsets ($\pm 0.5^\circ\text{C}$, $\pm 1.0^\circ\text{C}$, $\pm 1.5^\circ\text{C}$), while rainfall, ET, and C inputs were adjusted proportionally ($\pm 5\%$, $\pm 10\%$, $\pm 15\%$). Note that the sensitivity index axis varies to represent the values for the different inputs.

The OAT simulations of clay content are summarised in Table 5.2. As expected, increasing clay content resulted in higher modelled SOC stocks. However, sensitivity indices revealed that clay was a relatively insensitive parameter compared to climatic or C input drivers, with the S_i ranging from 0.017 to 0.157 (Figure 5.3). The highest sensitivity occurred with substantial reductions from the baseline clay content (23.4%), particularly at 0% clay. Beyond this, an incremental increase in clay yielded diminishing S_i responses, indicating a nonlinear effect.

Table 5.2 One-at-a-time sensitivity analysis of the effect of clay content on soil organic carbon (SOC) stocks modelled with RothC. The initial clay content was 23.4%, with incremental increases and decreases applied to evaluate changes in SOC stock. Final SOC stock and SOC stock difference (diff.) are expressed as Mg C ha^{-1} . Sensitivity index was calculated as the relative change in SOC stocks divided by the relative change in the clay parameter.

Clay content (%)	Final SOC stock (Mg C ha^{-1})	SOC stock diff. (Mg C ha^{-1})	Difference (%)	S_i
23.4	73.84			
0	62.22	-11.63	-15.74	0.157
5	65.53	-8.31	-11.26	0.143
10	68.39	-5.46	-7.39	0.129
15	70.91	-2.93	-3.97	0.111
20	72.88	-0.97	-1.31	0.09
25	74.22	0.38	0.52	0.075
30	75.12	1.28	1.73	0.061
35	75.67	1.82	2.47	0.05
40	76.00	2.16	2.93	0.041
45	76.23	2.39	3.23	0.035
50	76.38	2.54	3.44	0.03
60	76.56	2.72	3.69	0.024
70	76.72	2.87	3.89	0.02
80	76.93	3.09	4.19	0.017
90	77.29	3.45	4.67	0.016
100	77.9	4.06	5.49	0.017

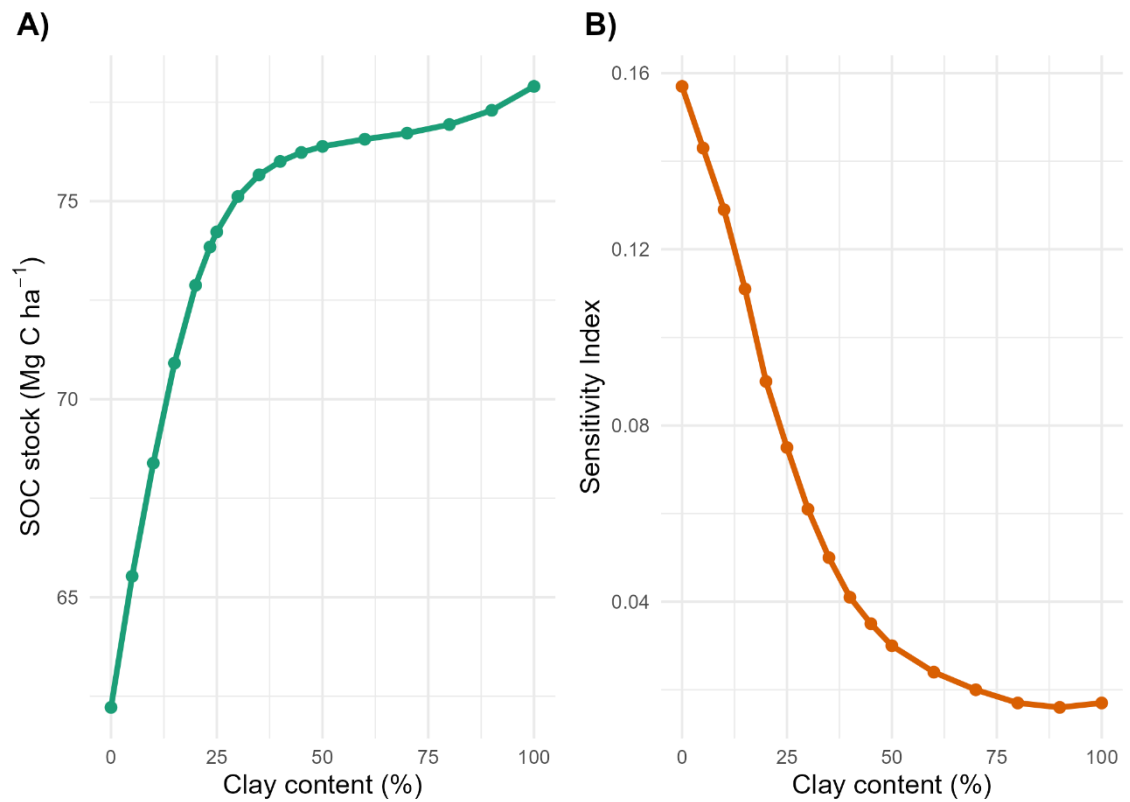


Figure 5.3 One-at-a-time sensitivity analysis of modelled soil organic carbon (SOC) stock in response to changes in clay inputs (Graph A). The corresponding sensitivity index is calculated as the relative change in SOC stocks divided by the relative change in the clay parameter (Graph B).

5.3.2 Global Sensitivity Analysis

The global SA of climatic drivers demonstrated the effects of simultaneous changes in temperature, rainfall and ET on modelled SOC stocks (Table 5.3; Figure 5.4). Scenario 1, which imposed a 1.5 °C increase in temperature and a 15% increase in rainfall and ET values, led to the greatest decline in SOC stocks, equivalent to a reduction of 10.84%. In contrast, Scenario 2, -1.0 °C temperature decrease and a 10% reduction in rainfall and ET, yielded the highest SOC stock of 79.48 Mg C ha⁻¹, representing a 7.64% increase. The wet year scenario (Scenario 3), based on 2012 conditions, produced a final SOC stock of 69.91 Mg C ha⁻¹, corresponding to a 5.33% decrease. The dry year scenario (Scenario 4), reflecting 2022 conditions, led to a more moderate decline, with SOC decreasing by 2.01% to 72.36 Mg C ha⁻¹.

Table 5.3 Final simulated soil organic carbon (SOC) stocks and SOC stock differences relative to the baseline simulation under different climate scenarios. Scenario 1 applied a +1.5°C increase in temperature and a 15% increase in rainfall and ET. Scenario 2 applied a -1.0°C temperature decrease and a 10% decrease in rainfall and ET. Scenario 3 replicated the monthly conditions of a wet year (2012), and Scenario 4 simulated a dry year (2022). All values are expressed in Mg C ha⁻¹.

Scenario	Final SOC stock	SOC stock diff.	Difference (%)
Baseline	73.84		
Scenario 1 (Increase)	65.84	-8.00	-10.84
Scenario 2 (Decrease)	79.48	5.64	7.64
Scenario 3 (Wet)	69.91	-3.93	-5.33
Scenario 4 (Dry)	72.36	-1.48	-2.01

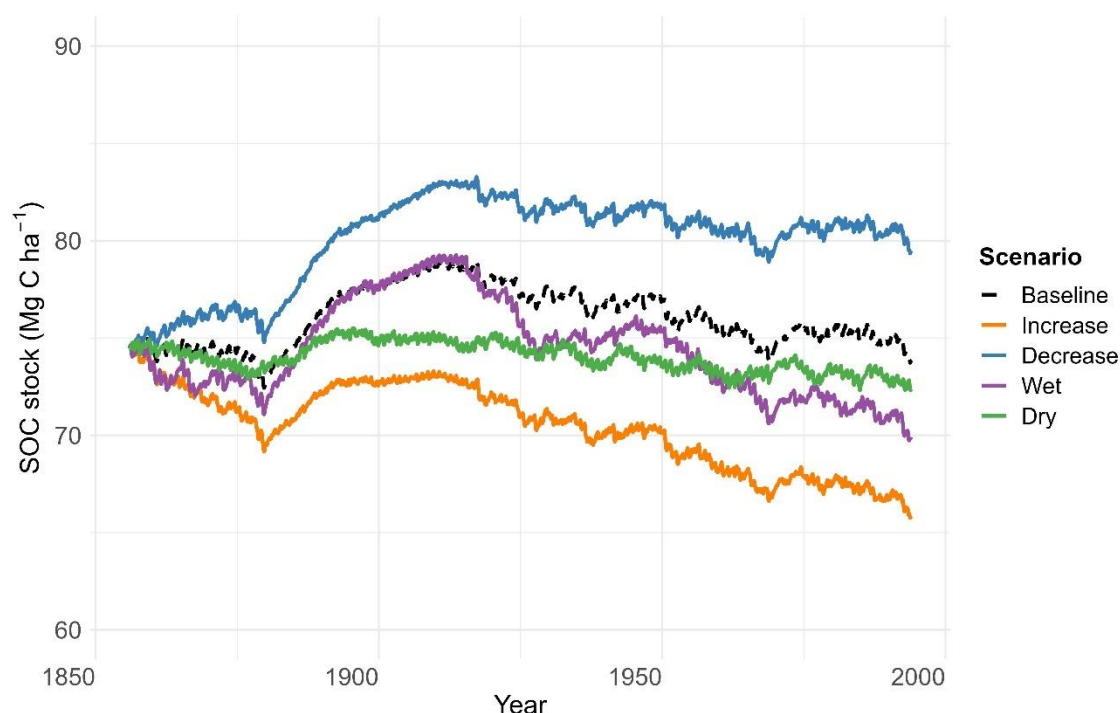


Figure 5.4 Simulated soil organic carbon (SOC) stock trajectories under four climate perturbation scenarios. Scenario 1 reflects increased temperature (+1.5 °C), rainfall, and ET (+15%). Scenario 2 applies a uniform decrease in temperature (-1.0 °C), rainfall, and ET (-10%). Scenarios 3 and 4 replicate historical wet (2012) and dry (2022) years using empirically derived monthly adjustments for Park Grass plot 3d from 1856 to 1993.

5.3.3 Model input sensitivity

The ET estimates derived from the ET_{THO}, ET_{HAR}, and ET_{PEN} methods exhibited systematic seasonal trends as outlined in Figure 5.5. ET_{HAR} values on average were the highest and peaked during May to July, whereas ET_{THO} produced consistently higher ET estimates from September to December. ET_{PEN} generally provided intermediate values across the years.

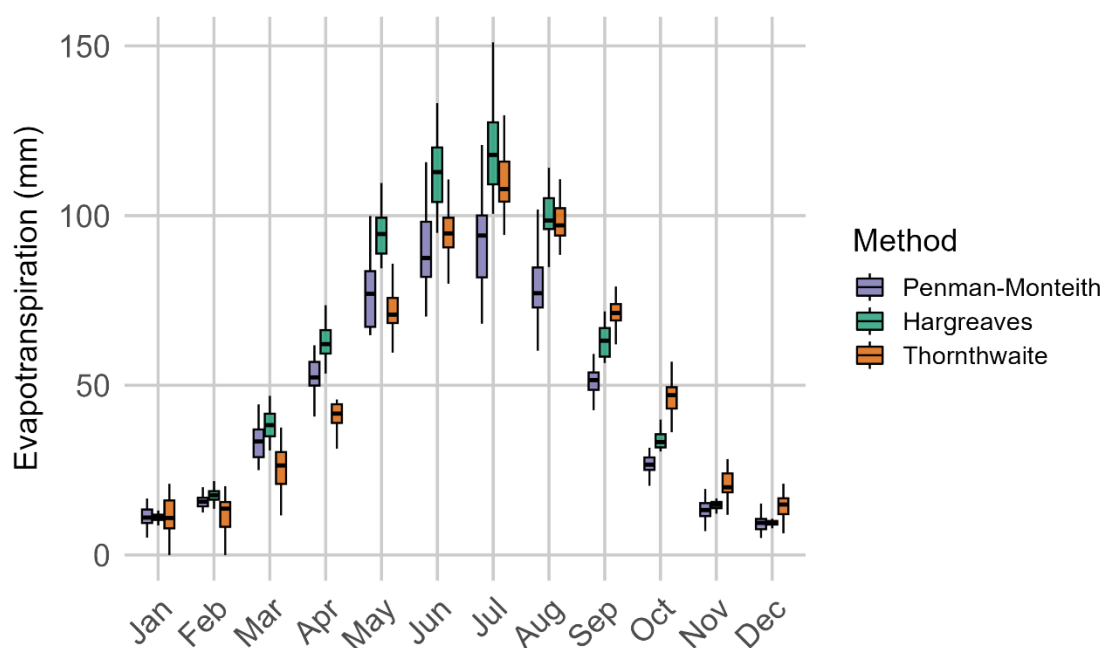


Figure 5.5 Monthly evapotranspiration (ET) distributions estimated with the Penman-Monteith, Hargreaves, and Thornthwaite methods. Boxplots represent ET variability from 1960 to 1993, highlighting the systematic differences between methods.

The influence of these ET methods on RothC_R xi modifier is shown in Figure 5.6, which illustrates broadly overlapping distributions with only small differences between methods. Despite their modest size, these differences are sufficient to impact the simulated SOC stocks over time. ET_{HAR} yielded the lowest xi rate modifier values, indicating the lowest rates of decomposition. In contrast, ET_{PEN} resulted in the highest values, producing the highest rates of decomposition.

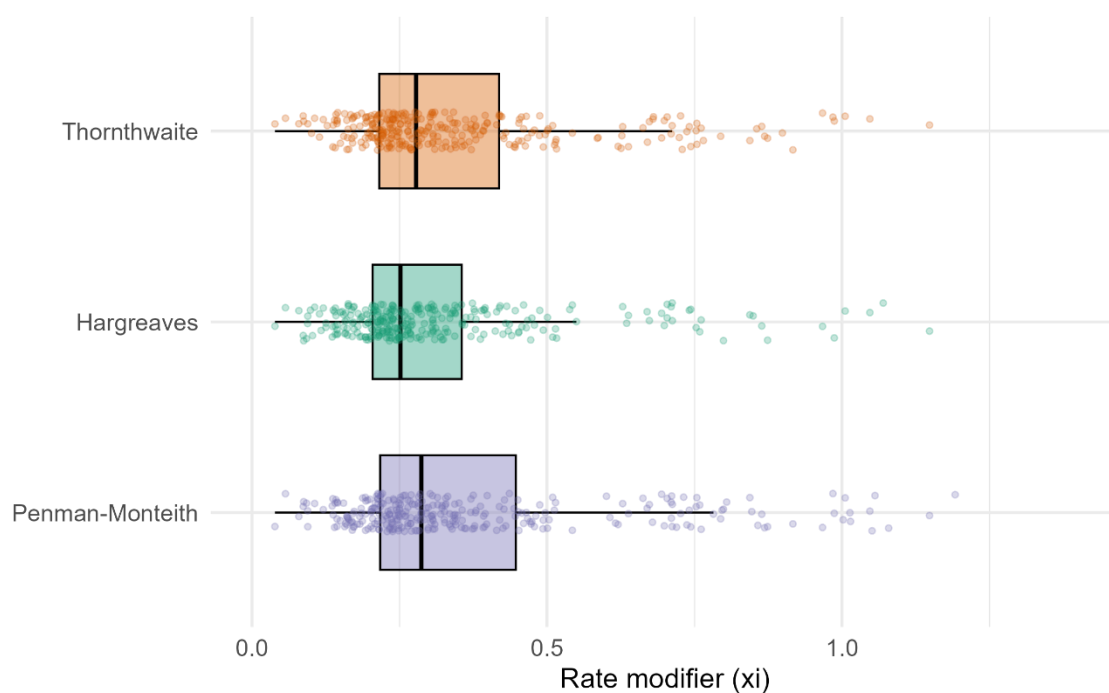


Figure 5.6 Distribution of the RothC_R environmental rate modifiers for three different evapotranspiration methods: Thornthwaite, Hargreaves and Penman-Monteith.

The C input estimates differed substantially across methods, as shown in Table 5.4, reflecting the methodological variation in how C inputs were derived. Figure 5.7 further illustrates the variability in recorded DM yields and the corresponding annual C inputs, calculated using Poeplau's (2016) method with two different R:S ratios.

Table 5.4 Carbon inputs ($\text{t C ha}^{-1} \text{ yr}^{-1}$) into the RothC_R model based on selection estimation methods.

	Miami	Avg. Poeplau_P	Avg. Poeplau_J	RothC
Plot 3d	3.87	3.79	3.01	2.57
Plot 14d	3.87	4.79	6.03	2.27

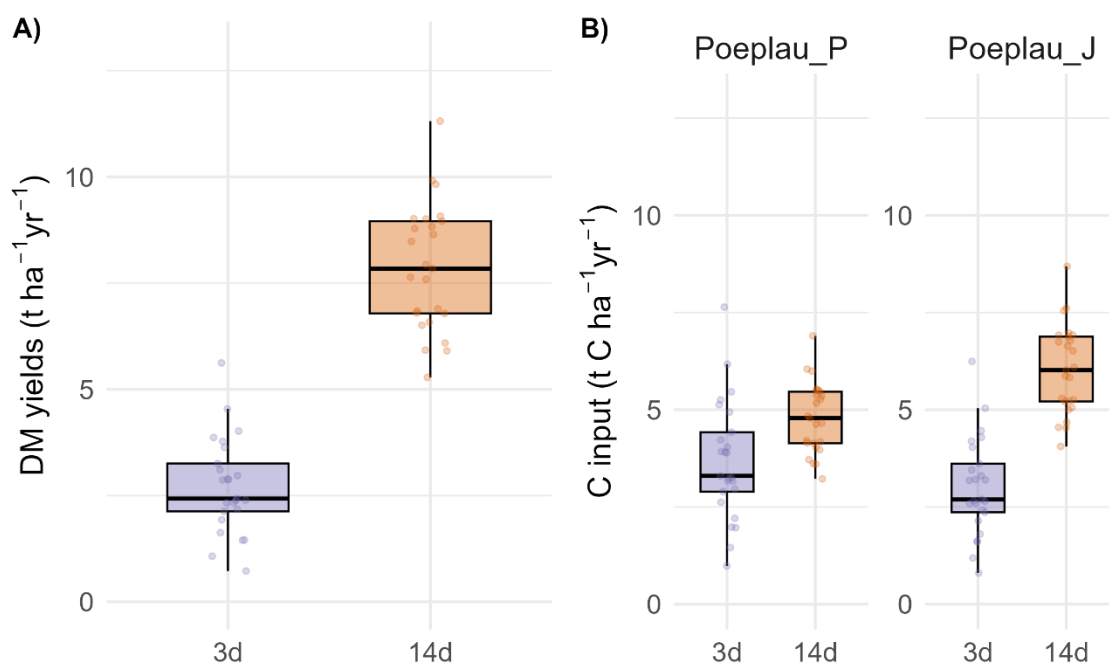


Figure 5.7 Boxplots comparing (Graph A) dry matter (DM) yields ($\text{t ha}^{-1} \text{ yr}^{-1}$) recorded from Park Grass plots 3d and 14d. Graph B demonstrates the annual C inputs ($\text{t C ha}^{-1} \text{ yr}^{-1}$) derived from the DM yields based on Poeplau's (2016) methodology using two different root-to-shoot ratios.

The influence of different combinations of ET and C input methods on the RothC-R model produced a wide range of simulated SOC stocks, ranging from 71.00 to 97.74 Mg C ha^{-1} . SOC trajectories for plot 3d are shown in Figure 5.8, and for plot 14d in Figure 5.9.

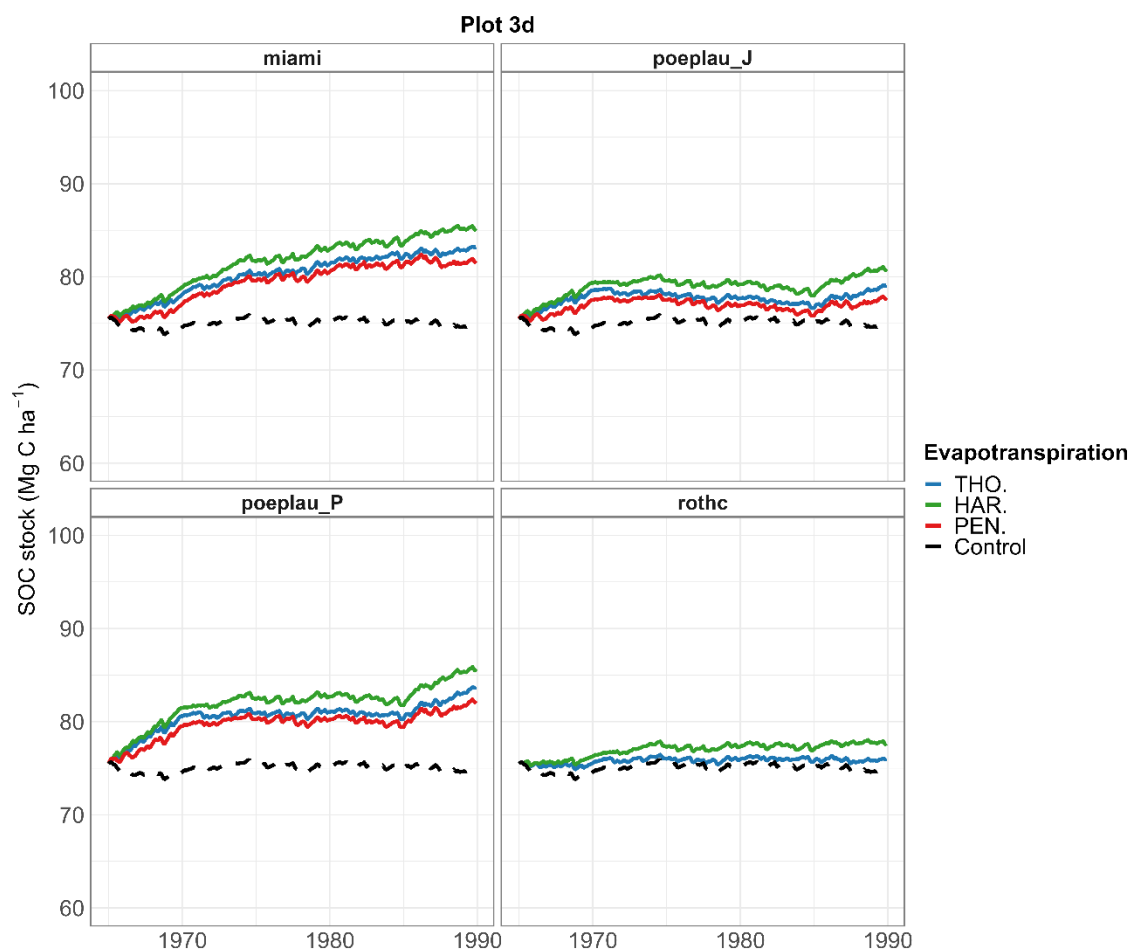


Figure 5.8 Effect of different combinations of evapotranspiration and carbon input modelling methods on SOC stock estimates for Park Grass plots 3d. Each sub-graph represents a carbon input method, with each coloured line representing the corresponding evapotranspiration method (Thorntwaite; THO, Hargreaves; HAR, Penman-Monteith; PEN). The baseline is the black dashed line, and the model combination is PEN.rothc.

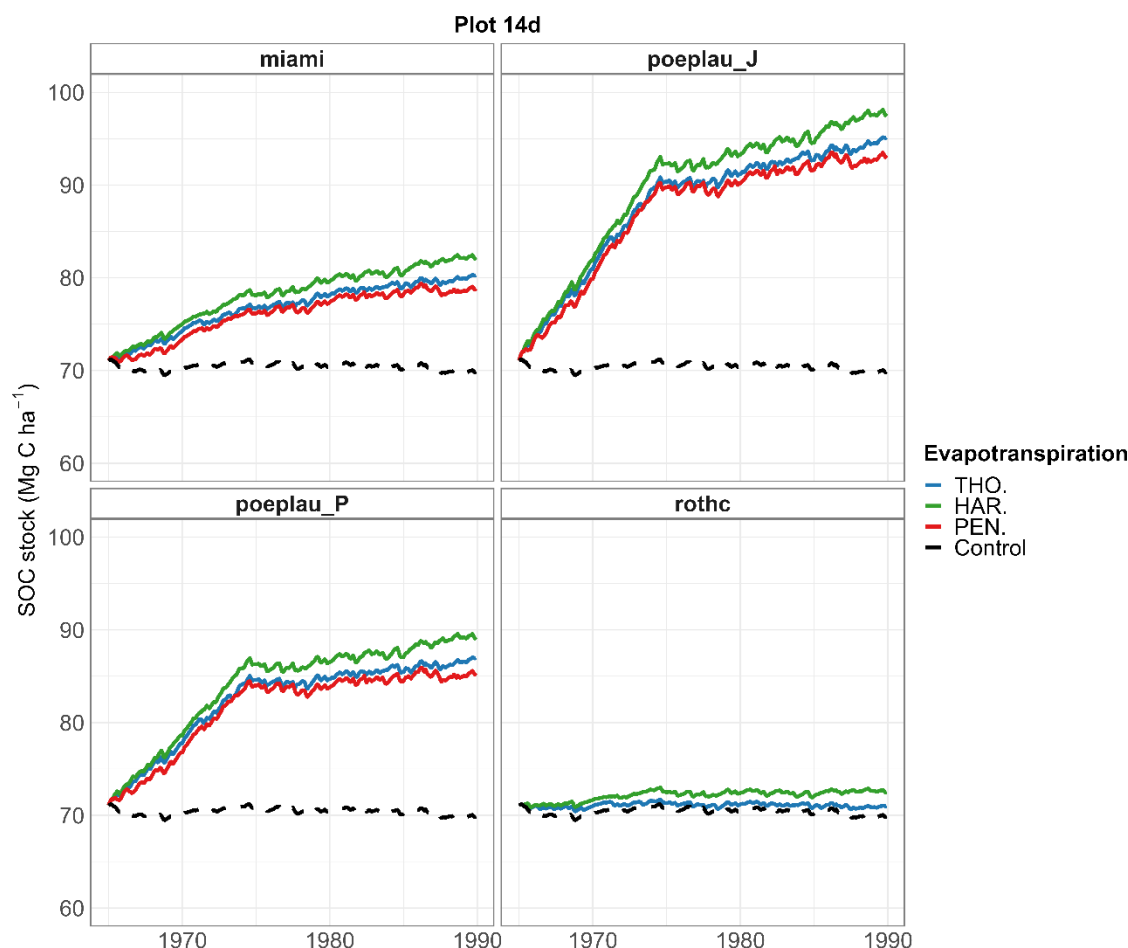


Figure 5.9 Effect of different combinations of evapotranspiration and carbon input modelling methods on SOC stock estimates for Park Grass plots 14d. Each sub-graph represents a carbon input method, and each coloured line represents the corresponding evapotranspiration method (Thorntwaite; THO, Hargreaves; HAR, Penman-Monteith; PEN). The baseline is the black dashed line, and the model combination is PEN.rothc.

Root mean square error values varied significantly across plots and model input combinations, ranging from 0.79 to 20.63 Mg C ha⁻¹, indicating differing degrees of model performance. Figure 5.11 ranks the RMSE values from smallest to largest for each model combination. For plot 3d, eight model combinations resulted in RMSE values below 5 Mg C ha⁻¹, indicating excellent agreement, while the remaining three combinations produced RMSE values between 5 and 10 Mg C ha⁻¹, signifying good agreement. In contrast, for plot 14d, only two model combination results in values below 5 Mg C ha⁻¹, with three additional combinations falling between 5 and 10 Mg C ha⁻¹. The remaining model combinations for plot 14d produced moderate to poor RMSE values ranging from 12.80 to 20.63 Mg C ha⁻¹. Additionally, detailed results of those model input combinations are provided in Appendix B.4.

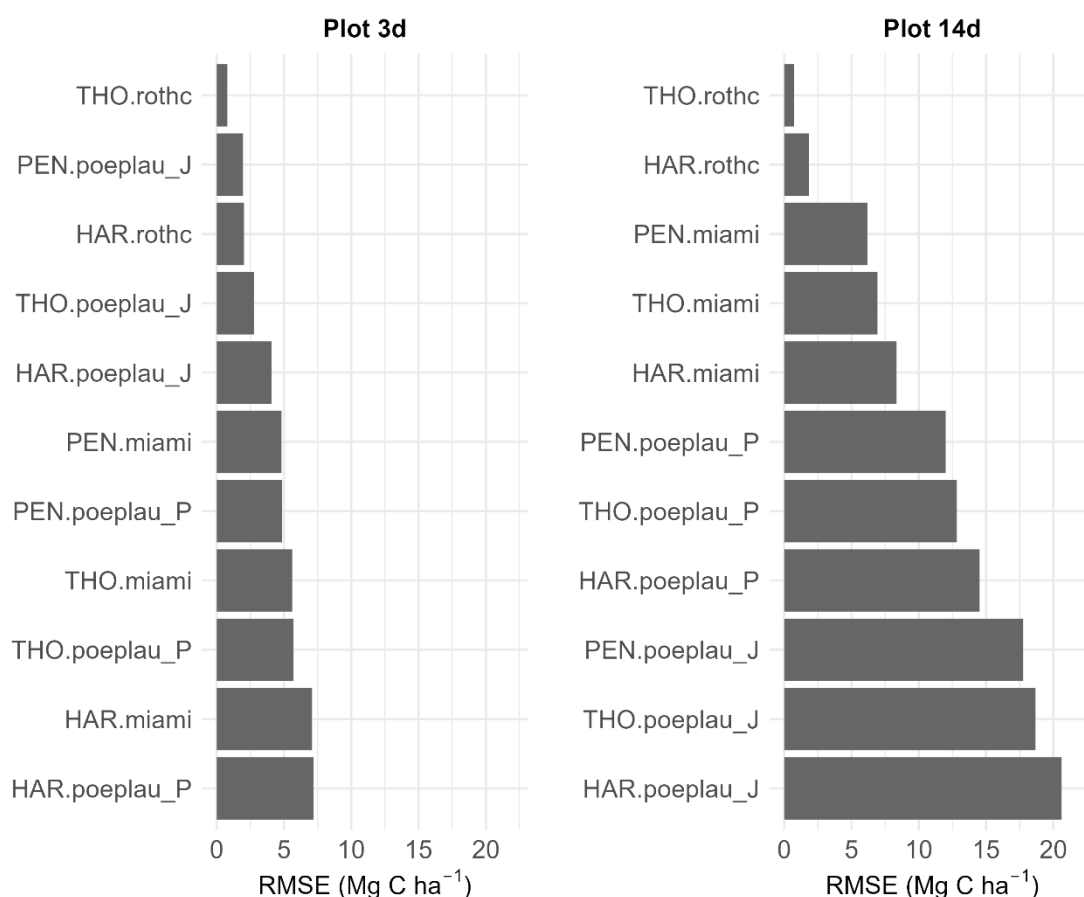


Figure 5.10 Different combinations of modelling methods for evapotranspiration and carbon inputs ranked by RMSE (Mg C ha⁻¹) from smallest to largest for the Park Grass plot 3d and 14d simulations.

5.4 Discussion

5.4.1 OAT analysis

The OAT SA conducted in this study provided a structured evaluation of the RothC_R model's responsiveness to independent perturbations in key drivers: temperature, rainfall, ET, C input and clay content. By applying controlled perturbations and quantifying responses using the S_i , this analysis explores the individual contribution of each driver to simulated SOC stock dynamics.

Temperature perturbations (± 0.5 - 1.5°C) demonstrated a strong, nearly linear influence on simulated SOC stocks. SOC consistently decreased under warmer temperature perturbations and increased under colder perturbations, with a slight asymmetry observed. Increases in SOC were slightly greater under colder perturbations than under equivalent warmer conditions. This behaviour reflects the non-linear sensitivity of decomposition processes in the RothC. Similar findings were reported by Janik *et al.* (2002), who identified temperature as the most sensitive driver of SOC turnover. These results underscore the importance of accurately capturing temperature variability in SOC modelling.

Rainfall and ET are both components of the RothC moisture modifier and exhibited an inverted relationship in their influence on SOC stocks. Rainfall perturbations ($\pm 15\%$) led to moderate and relatively linear changes in SOC stocks. Increased rainfall consistently reduced SOC, while decreased rainfall enhanced SOC stocks. The S_I values remained relatively stable across perturbations, indicating a near-horizontal relationship between rainfall changes and SOC dynamics within the test range.

By contrast, ET perturbations produced a positive linear response in SOC stocks, with higher ET increasing SOC and lower ET reducing it. However, similarly, the S_I values displayed a near-horizontal relationship between ET changes and SOC dynamics within the test range. Both rainfall and ET S_I values peaked at $\pm 5\%$ perturbations and then declined, suggesting that the model becomes slightly less sensitive to further perturbations. These responses reflect the non-linear interactions within the moisture modifier. Moreover, given that the impact of temperature is 'independent', in that it has a specific temperature modifier, within RothC, unlike precipitation and evaporation, which are combined within the moisture modifier. Consequently, the model exhibits greater sensitivity to temperature drivers than to moisture-related drivers, as the effects of precipitation and evaporation can partially offset one another within the moisture modifier, thereby reducing overall model sensitivity.

Carbon input perturbations revealed a symmetric and linear response in both SOC stocks and S_I values. Increases and decreases in C input led to proportional changes in SOC, and the completely flat horizontal S_I trend confirms this driver operates under a direct and linear influence without evidence of diminishing returns over the simulation period.

Clay content, in contrast, showed low sensitivity, particularly at higher values, indicating a clay saturation effect within the model. The model was most responsive to changes in low-clay conditions, where small perturbations had relatively larger impacts on SOC stocks. After a certain threshold ($\sim 40\%$ clay content), the influence of clay content diminishes. These results align with those of Janik *et al.* (2002), who also reported high model sensitivity to clay in sandy soils but negligible sensitivity at higher clay contents.

It is important to recognise that this analysis was based on a single site, Park Grass plot 3d, which may limit generalisability to other environments, soil types and management systems. Additionally, the S_I values are sensitive to the baseline value used in the analysis. For comparative purposes, S_I values computed using alternative clay baseline values are provided in Appendix B.4. Despite these limitations, the OAT SA yielded key insights into the RothC model dynamics. The main findings including: 1) temperature is the most sensitive driver; 2) rainfall and ET exert inverse but moderate effects on SOC stocks due to their combined role in the moisture modifier; 3) C input influences SOC stocks linearly and

proportionally, indicating it's a predictability as a driver; and 4) Clay content has limited influence at high levels but may be critical in low-clay soils.

5.4.2 Global analysis

The global SA simulated the impact of extreme climatic scenarios on modelled SOC stocks modelled with RothC. Overall, these scenarios resulted in only minor deviations from the baseline simulation, particularly in the extreme wet and dry scenarios, a finding that is likely a byproduct of how model inputs were handled in the simulations.

A key limitation of our approach is the assumption of constant, uniform C inputs throughout the simulation period. Extreme climatic events significantly impact plant growth and, consequently, C inputs. For instance, Barker *et al.* (2024) documented severe reductions in grassland productivity during the 2022 summer drought in the UK, attributing yield losses to high temperatures and limited soil moisture. Similarly, Finn *et al.* (2018) conducted a controlled drought experiment in Ireland and Switzerland, reporting yield reductions of up to 87% in both monocultures and mixed-species swards. These findings strongly suggest that vegetation-derived C inputs are highly climate sensitive and should be dynamically adjusted in models when simulating extreme climate events.

However, accurately quantifying C inputs under such variable conditions remains uncertain. Even under normal conditions, estimating C inputs derived from plant residues remains a challenging task. As a result, applying static C inputs under these scenarios likely masked the true sensitivity of SOC dynamics, limiting the interpretability of our results.

In addition to input limitations, the limitations of the RothC model must be acknowledged. The model is not intended for application in waterlogged soils (Coleman *et al.*, 2024) and has been shown to perform poorly in semi-arid or arid environments (Farina *et al.*, 2013; Giongo *et al.*, 2020). Several modifications have been proposed to address these shortcomings. For example, Lobe *et al.* (2005) demonstrated that RothC simulations in semi-arid South Africa estimated unrealistically low C inputs due to consistently high ET values, which drove the moisture modifier to its minimum threshold. In response, Farina *et al.* (2013) adapted RothC for arid regions by adjusting the bare soil moisture deficit limitation and lowering the minimum default moisture modifier value to below 0.2, allowing greater flexibility in simulating SOC under dry conditions.

Similarly, Shirato and Yokozawa (2005) developed a modified RothC model to simulate SOC stocks in Japanese paddy fields. Their approach introduced submergence factors to differentiate between waterlogged and non-waterlogged periods. Applying RothC_R to simulate SOC stocks under extreme wet years, where prolonged saturation is likely, would

require similar adjustments. Without such modifications, the model's output may misrepresent soil C dynamics under both extreme wet and dry conditions.

A further limitation arises from RothC's uniform application of environmental rate modifiers across all conceptual SOC pools. Georgiou *et al.* (2024), using global soil datasets, found that the temperature sensitivity of particulate organic carbon is, on average, 28% higher than that of mineral-associated organic matter, with differences reaching 53% in cooler climates. This suggests that applying a single temperature modifier across all pools oversimplifies the responses of SOC. Yan *et al.* (2017) further demonstrated that SOC decomposition rates were 59% to 282% higher in the topsoil than in the subsoil in two regions of China. They also noted that more recalcitrant C pools at depth might respond more sensitively to warming. Together, these studies emphasise the need for pool-specific and depth-specific decomposition rate modifiers to improve model realism under extreme climate or climate change scenarios.

To address these limitations comprehensively, future RothC modelling under extreme climatic conditions would require: 1) dynamic, climate-sensitive C input estimation; 2) modifications to the default model to account for waterlogged and dry climatic conditions; and 3) heterogeneous decomposition rate functions for different conceptual SOC pools and soil depths to account for the effects of elevated temperatures. Such modifications would significantly increase model complexity and are beyond the scope of our research. As such, results from the extreme wet and dry simulations presented here should be interpreted with caution and not assumed to reflect actual SOC stock trends.

Nevertheless, our findings align broadly with previous RothC findings based on European grasslands under projected climate change, although the scenarios tested here represent more extreme wet and dry conditions. For example, Xu *et al.* (2011a) simulated SOC dynamics under projected climate change at eight Irish grassland sites and reported SOC stock losses of 2-6% over 40 years. Similarly, Smith *et al.* (2005) estimated that climate change would result in a 6-9% reduction in mean SOC stocks across European grasslands by 2080. These studies suggest that climate change can lead to moderate SOC declines. Yet, they may underestimate the impact of extreme events unless models are further adapted to capture C input variability and altered decomposition processes under such conditions.

5.4.3 Model input analysis

In this study, the model input SA focused on varying only ET and C input estimation methods, as these are externally derived inputs in RothC. The performance of each model input combination was evaluated against the baseline simulation using the RMSE metric calculated across the entire 25-year simulation period. The results revealed contrasting patterns between plots and estimation methods. For the unmanaged plot 3d, all eleven

model input combinations yielded RMSE values $<10 \text{ Mg C ha}^{-1}$, indicating good agreement with the benchmark. In contrast, only five model input combinations for the managed plot 14d produced RMSE values below this threshold. Among ET methods, the maximum RMSE difference observed was $2.35 \text{ Mg C ha}^{-1}$ in plot 3d and $2.87 \text{ Mg C ha}^{-1}$ in plot 14d. In comparison, the selected C input methods yielded substantially broader RMSE ranges: $6.24 \text{ Mg C ha}^{-1}$ for plot 3d and $20.63 \text{ Mg C ha}^{-1}$ for plot 14d. These findings confirm that C input estimation exerted a greater influence on SOC stock predictions than the ET method, particularly under managed conditions.

Literature on RothC sensitivity to different ET estimation methods is limited, restricting direct comparison. However, Maas and Lal (2023) tested three ET approaches, Thornthwaite and Mather (1955), Droogers and Allen (2002), and Tegos *et al.* (2017), and reported a maximum RMSE difference of 7.4 Mg C ha^{-1} , suggesting that their ET methods introduced greater variability than those used here.

Our analysis revealed a counterintuitive result: the simplest ET method, ET_{THO} , produced SOC predictions comparable to those from the most complex and data-intensive ET_{PEN} when identical C inputs were used. Similarly, Maas and Lal (2023) found that their simplest ET model (Thornthwaite and Mather, 1955) proved to be the closest match to the observation data and resulted in the most similar SOC stock estimates to the benchmark simulation. These findings suggest that RothC does not require sophisticated ET estimates to achieve reliable simulations, although this behaviour may also reflect an internal bias. In our analysis, the mean annual ET estimates were 554mm, 681mm, and 619mm for ET_{PEN} , ET_{HAR} , and ET_{THO} , respectively, with model performance declining as annual ET increased. Consistent with Maas and Lal (2023), our results indicate that RothC is highly sensitive to wet biases in ET models.

In contrast, the choice of C input method had a more substantial and variable influence on model performance. The inverse RothC-derived C input consistently yielded the most accurate results, with all associated RMSE values falling below $2.02 \text{ Mg C ha}^{-1}$. This outcome is expected, as the inverse method estimates C inputs based on the known outputs (e.g., observed SOC stocks), effectively conditioning the inputs on the outputs and minimising model error. This finding is consistent with previous studies that used inverse modelling techniques with the RothC model and similarly reported very low RMSE values (Afzali *et al.*, 2019; Geremew *et al.*, 2024). For instance, Afzali *et al.* (2019) and Geremew *et al.* (2024) operated the RothC model inversely to determine the quantity of C entering the soil to maintain the specific SOC stock measured in the experiment. Afzali *et al.* (2019) reported an RMSE of $0.014 \text{ Mg C ha}^{-1}$ for their evaluation of rangeland sites in Bandbast rangelands in southern Iran, while Geremew *et al.* (2024) reported RMSE values of 0.013 and 0.074 Mg C

ha⁻¹ for two different soil sampling campaigns in northwestern Ethiopia. Liu *et al.* (2011) did not use the RothC model with inverse C inputs but employed a C input estimation method that utilised an optimised root-to-shoot ratio (R:S) achieved by inverse modelling techniques and reported high model accuracy.

By contrast, C inputs derived from Poeplau's (2016) methodology showed considerable variability. The average RMSE for the Poeplau methods was 4.42 Mg C ha⁻¹ in plot 3d, but increased significantly to 16.07 Mg C ha⁻¹ in plot 14d. However, RMSE values revealed from Poeplau's methodology are consistent with similar methods in the literature (Barančíková *et al.*, 2023; Doblas-Rodrigo *et al.*, 2022; Jebari *et al.*, 2021).

Barančíková *et al.* (2023) estimated carbon inputs using DM yields and manure applications following Bielek and Jurcova (2010) and simulated SOC dynamics at a long-term grassland site in Suchy Vrch, Slovakia. Across eight measured SOC values under various fertilisation strategies, RMSE ranged from 8 to 15 Mg C ha⁻¹, indicating good to moderate agreement between modelled and observed SOC stocks. Doblas-Rodrigo *et al.* (2022) estimated C inputs from average DM yields and R:S ratios based on Bolinder *et al.* (2002) and applied the RothC model to simulate SOC stocks across 21 grassland sites in northern Spain. The model achieved an average RMSE of 9.31 Mg C ha⁻¹, indicating reasonable predictive performance across diverse sites. Jebari *et al.* (2021) applied Poeplau's (2016) C input methodology using N-dependent R:S ratios to simulate SOC stocks for four European temperate moist grasslands, reporting an average RMSE of 11.36 Mg C ha⁻¹. Incorporating additional sub-models for ruminant excreta, plant residue traits, and moisture dynamics reduced the RMSE substantially to 2.77 Mg C ha⁻¹, highlighting the value of site-specific refinements.

Carbon input estimates based on the Miami model were identical due to the plots' uniform weather. As this method does not account for management differences, it yielded relatively consistent RMSE values of 5.83 Mg C ha⁻¹ (plot 3d) and 7.15 Mg C ha⁻¹ (plot 14d). While this consistency may benefit broad-scale applications, it may underperform under site-specific or intensively managed conditions. Each C input method presents distinct trade-offs. Net primary production-based approaches like the Miami Model offer simplicity and broad applicability but ignore site-specific conditions. Yield-based and empirical methods can incorporate management variability but often rely on scarce or uncertain data, especially for belowground inputs, which are influenced by fertilisation and local environmental conditions (Heikkinen *et al.*, 2014; Wiesmeier *et al.*, 2016). While RothC lacks an internal C input sub-model, this may be advantageous for flexible applications. Models with integrated plant growth models are often limited to specific land uses, restricting the application of certain models (Smith *et al.*, 1997).

Furthermore, some models require belowground C inputs from root turnover or rhizodeposition, which tend to be unavailable. Moreover, the RothC model works with the total C inputs (aboveground plus belowground), making it less dependent on detailed partitioning and enhancing its practical usability across systems (Smith *et al.*, 1997). One noteworthy trend observed in our analysis was that the benchmark model configuration (PEN.rothc) produced the lowest SOC stock estimates among all combinations. This suggests that RothC simulations at Park Grass may inherently favour lower ET and C input values. This bias may warrant future investigation of alternative approaches, especially methods that might lead to lower SOC stock predictions.

5.4.4 Selection of appropriate approaches

The selection of suitable C and ET input methods for the RothC is highly dependent on data availability. In this section, we first evaluate the most effective combinations under conditions without data constraints, followed by recommendations for data-limited contexts.

No data limitations

For the unmanaged grassland plot 3d, all model input combinations performed well (RMSE <10 Mg C ha⁻¹). Based on our results, we recommend the combination of ET_{PEN} and poeplau_J for unmanaged grasslands, which resulted in an RMSE of 1.96 Mg C ha⁻¹. Although this was not the absolute lowest RMSE recorded, this combination avoids overfitting or generalised approaches such as inverse modelling, which may mask underlying processes of SOC dynamics. However, caution is warranted. The apparent success of the PEN.poeplau_J combination may be partially coincidental. The estimated C input from Poeplau_J method for plot 3d (3.01 t C ha⁻¹ yr⁻¹) was similar to the benchmark inverse estimate of 2.57 t C ha⁻¹ yr⁻¹, possibly explaining the lower RMSE. If this method were consistently robust, we would expect a similar level of agreement in the managed grassland plot (14d), which was not observed.

In plot 14d, which represents a managed grassland, model performance was more variable. Based on our results, we recommend the combination of ET_{PEN} and Miami model-derived C inputs, as this combination was the third-best-performing configuration and avoided reliance on inverse estimates. This is unexpected, as the Miami model is the simplest C input method used in this study. However, the Poeplau methodology may offer improved performance if site-specific data, such as R:S ratios, d_r , or d_{50} , were available. In their absence, we relied on default literature values, which may not be appropriate for Park Grass (Poeplau, 2016).

With Data limitations

RothC is frequently applied in regional and global SOC modelling due to its moderate data requirements (e.g., Morais *et al.*, 2019; van Wesemael *et al.*, 2010). However, even these requirements can be too data-intensive for grassland systems at larger spatial scales. For instance, Morais *et al.* (2019) implemented RothC globally using a single grassland class, compared to 28 arable and 16 forestry classes, due to limitations in land-use and management sources. Similarly, van Wesemael *et al.* (2010) simulated national grassland SOC stocks without country-specific data on permanent grasslands, resulting in the use of assumed values for input parameters.

These examples underscore the persistent challenge of data scarcity for grasslands in large-scale modelling efforts. While the model input combinations recommended earlier (e.g., ET_{PEN} and Poeplau's (2016) methodology) may offer improved accuracy, they are often impractical at regional or national scales due to data availability constraints. In such contexts, it is essential to prioritise methods that minimise data demands. For data-limited applications, we recommend the combination of ET_{THO} and Miami model-derived C inputs. The THO.miami combination yielded satisfactory RMSE values for both plots 3d and 14d and may represent a viable compromise between performance and feasibility for larger-scale assessments.

5.4.5 Limitations

A key limitation of our model input ensemble is the relatively short simulation period. We conducted simulations over 25 years, which is likely insufficient to fully assess the long-term sensitivity of the RothC model to different ET and C input combinations. Some plot 14d SOC simulations under different model input configurations had not yet reached equilibrium, implying longer simulations (e.g., 50-100 years) may reveal more pronounced differences between scenarios, particularly if the baseline simulation is near equilibrium. However, extending the simulation period is constrained by the limited availability of long-term datasets with consistent management practices and uniform plot configurations, which are necessary for reliable model benchmarking.

This temporal limitation is especially relevant for the C inputs derived from the Miami model, our recommended approach, as its SOC projections appear to be increasing. Extended simulations may shift modelled SOC trajectories sufficiently to alter RMSE rankings and reverse current interpretations of method performance. Moreover, all simulations were initialised with identical SOC pool sizes, estimates where lower C inputs may appear more similar, as there was not enough time available to accumulate SOC stock differences over the period of 25 years.

Geographical representativeness is another constraint. The analysis was confined to a single experimental site, limiting the generalisability of our findings across diverse grassland types, management regimes and climatic zones. Sensitivity patterns identified here may differ in other environments.

Lastly there was parameter uncertainty, especially in the Poeplau (2016) C input methodology. We applied the Poeplau (2016) method using generic literature values (e.g., R:S ratio, d_r , d_{50}) rather than site-specific measurements. Authors have acknowledged that generic C input methods can be improved if adapted to local conditions. For example, Heikkinen *et al.* (2014) estimated C inputs by following Bolinder *et al.* (2007) using measured above- and belowground biomass with an appropriate root turnover time specific to the area of interest. They found that applying a coarser, literature-derived turnover rate increased modelled SOC stocks by approximately 15%, resulting in poorer agreement between simulated and observed values. This highlights the need for locally refined input data to improve model performance and reduce uncertainty.

5.5 Conclusions

This study evaluated the sensitivity of the RothC_R model to variation in key input drivers, including climate variables (temperature, rainfall, ET), C inputs, and clay content. Through a combination of OAT and global sensitivity analyses, as well as a model input ensemble incorporating multiple estimation methodologies, we examined how the selection and complexity of external inputs affect modelled SOC stocks.

The OAT sensitivity analysis revealed that RothC_R is most sensitive to changes in temperature, with a near-linear and asymmetric response. Colder temperatures increased modelled SOC more strongly than warming reduced it. Rainfall and ET exhibited opposing and non-linear patterns, with ET having a notably positive influence on modelled SOC accumulation. In contrast, clay content showed limited sensitivity except in low-clay conditions. Carbon inputs displayed a linear, symmetric effect on modelled SOC, reinforcing the need for reliable C input estimates.

Global sensitivity analysis further demonstrated that coordinated changes in climate variables (temperature, rainfall, ET) can significantly affect modelled SOC stocks. Notably, extreme wet and dry year scenarios derived from empirical meteorological records highlighted RothC_R's limited ability to simulate SOC dynamics under extreme climate conditions. These results reflect known limitations of RothC's environmental modifier, particularly their simplified representation of soil moisture dynamics and the absence of an explicit treatment of waterlogging.

The model input ensemble exhibited considerable variability in simulated SOC stocks. The maximum RMSE difference observed was 2.87 Mg C ha⁻¹ for ET methods, and 20.63 Mg C ha⁻¹ for C input methods. While more complex input combinations (e.g., ET_{PEN} or RothC inverse-derived C inputs) generally produced better agreement with the benchmark simulation, several combinations of simple and intermediate approaches performed nearly as well. Notably, the simplest model input combination of THO.miami yielded acceptable RMSE values across both plots and is highly applicable in data-limited environments. This study highlights that simpler methodologies can yield estimated SOC stock results similar or in some cases more accurate than complex methodologies.

Our findings suggest several practical and methodological implications. First, the RothC model's performance is highly sensitive to input configurations, suggesting that even if the model has been validated for a specific ecosystem, substituting or altering input estimation methods may compromise its performance. Second, in data-limited contexts, simple input derivation methods such as those based on empirical models can offer acceptable performance and may be preferable due to their practicality and lower data demands. Lastly, the current RothC implementation assumes uniform rate modifiers across all SOC pools and soil depths, which may limit its capacity to accurately simulate SOC dynamics under future climate extremes.

Chapter 6: Application of a general modelling framework to estimate carbon stocks in mineral grasslands under temperate climatic conditions at field and farm scale

Abstract

Accurate estimation of SOC stocks is essential for informing and improving national GHG emissions inventories. Ireland currently utilises Tier 1 methodologies to estimate SOC stocks for grasslands, relying on default land-use factors and assumptions around organic matter inputs. These values do not consider the site-specific environmental context or management information, limiting their ability to represent local variability in SOC dynamics. To meet new and evolving regulatory requirements and improve reporting accuracy, many countries are adopting more sophisticated, geographically refined, Tier 3-based approaches. However, significant challenges remain in employing Tier 3-based approaches in grasslands, particularly in terms of consistency and comparability, as well as the ability to transfer methods across scales and to new locations. To address this, we employ a generalised modular framework that incorporates a Tier 3-based model to derive estimates of SOC stocks in mineral grasslands across Ireland at field and farm scale, referred to as the Mineral Grassland (MG) Model.

The MG Model consists of various modules, including a climate module, a C input model, and the RothC model implemented in R, through the SoilR package. The MG Model requires minimal data inputs, namely latitude, longitude, clay (as %), known SOC stock measurement (Mg C ha^{-1}) and sampling depth, allowing for broad applicability across data-limited sites. Critically, as the MG model employs available, standardised datasets, within a common model framework, locations can be directly compared to one another.

We evaluated the approach against data from 28 mineral grassland sites obtained from an existing soil carbon database, SoilC (Kiely *et al.*, 2009). Although the overall performance was found to be poor, indicated by the root mean square error (RMSE) of $22.7 \text{ Mg C ha}^{-1}$, the MG showed good performance for SOC stocks ranging between 73 and 105 Mg C ha^{-1} . The MG model, in its current configuration, underestimates in high SOC stock soils, especially those with low clay content.

Despite these limitations, the MG model provides a potential framework for Tier 3-compatible SOC estimation, aiming to address the challenges of consistency, transparency and comparability. Furthermore, use of the generalised modelling framework, outlined in Chapter 3, supports a multi-model ensemble approach, demonstrated here with the incorporation of the Introductory Carbon Balance Model. Refinements of the model can be achieved through improved carbon input estimates, calibration using more extensive field

datasets, and incorporation of additional validated SOC models. These enhancements could substantially improve model accuracy and support the development and implementation of the MG model as a national tool to inform emissions policy.

6.1 Introduction

Soil organic carbon (SOC) plays a crucial role in maintaining soil health, influencing key physicochemical properties such as nutrient cycling, providing a buffering capacity against pollutants, and regulating water (Adeniyi *et al.*, 2024; Wiesmeier *et al.*, 2019). Beyond its agronomic importance, SOC sequestration is increasingly recognised as a cost-effective strategy to support climate change mitigation. Global estimates suggest that agricultural soils have a SOC sequestration potential of approximately 2-3 Gt C yr⁻¹ within the top one metre of soil, potentially offsetting 20-35% of current anthropogenic GHG emissions (Minasny *et al.*, 2017). The IPCC's Sixth Assessment Report estimated that enhanced soil carbon management in grasslands alone could deliver a technical mitigation potential of 1.0 Gt CO₂ yr⁻¹ or 0.273 Gt C (range: 0.2-2.6 Gt CO₂ yr⁻¹ or 0.055-0.710 Gt C yr⁻¹) (Nabuurs *et al.*, 2022). Enhancing SOC to increase the mitigation potential of soil would contribute to efforts aimed at closing the global emissions mitigation gap (Goglio *et al.*, 2015; Paustian *et al.*, 2019b). In addition to its climate benefits, increasing and maintaining SOC stocks improves ecosystem resilience and enhances soil structure, fertility, and biological functioning (Smith *et al.*, 2020; Stockmann *et al.*, 2015). Understanding the spatial variability of SOC is essential for sustainable agriculture and enabling landowners to make more informed, site-specific management decisions that promote SOC sequestration or storage and ultimately soil health (Adeniyi *et al.*, 2024).

Ireland has committed to achieving climate neutrality by 2050, a target embedded in national legislation through the Climate Action and Low Carbon Development (Amendment) Act 2021. However, the agricultural sector, which accounted for 36.2% of national GHG emissions in 2023 (EPA Ireland, 2025), faces significant challenges in delivering emissions reductions while maintaining food security. A key research and policy priority in meeting Ireland's climate reporting obligations is the improvement of emissions and removals estimates for agriculture and land use, consistent with methodological advances in international and EU frameworks (IPCC, 2019; Regulation (EU) 2024/3012). Currently, Ireland reports GHG emissions in grassland using a Tier 1 methodology that relies on global default emission factors (EPA Ireland, 2025). However, this approach lacks the capacity to reflect site-specific variability in soil properties, climate conditions and land management practices, limiting its accuracy and policy relevance (Bellassen *et al.*, 2022).

To improve the accuracy of SOC stock estimates both within Ireland and comparable temperate agroecosystems, a transition towards higher-tier reporting approaches is

essential. The transition from Tier 1 to Tier 3 reporting is consistent with the 2019 Refinements to the 2006 IPCC Guidelines (IPCC, 2019) and is further supported by emerging EU regulatory frameworks including the carbon removals and carbon farming framework (Regulation (EU) 2024/3012) and the revised land use, land use change and forestry (LULUCF) Regulation (Regulation (EU) 2023/839), both of which prioritise the adoption of Tier 3 methods for estimating carbon emissions and removals in key land-use categories by 2030.

Previous attempts at higher-tier SOC modelling efforts conducted in Ireland have primarily focused on single-site studies (e.g., Dondini *et al.*, 2009; Khalil, 2014; Necpálová *et al.*, 2014; van Groenigen *et al.*, 2011), limiting their applicability to broader spatial assessments and the ability to compare between sites. A likely reason for this emphasis on a limited number of sites is due to the limited availability of input data required by many of the Tier 3 models (e.g., Flattery *et al.*, 2018; Necpálová *et al.*, 2014; Saunders *et al.*, 2022), coupled with operational limitations associated with SOC models (Sierra *et al.*, 2012). We selected the RothC model (see Section 2.6) because it remains a popular choice for Tier 3 methodologies to estimate GHG emissions and removals in different countries, e.g., Australia's FullCam model, Japan's modified RothC, Switzerland (Smith *et al.*, 2020) and was identified as a suitable SOC model for Ireland by Byrne and Kiely (2009).

RothC has been validated using long-term experimental data across various ecosystems, climate conditions, and management practices (Campbell and Paustian, 2015; Sierra *et al.*, 2012; Smith *et al.*, 1997, 2020) and requires fewer and more readily obtained data inputs than other Tier 3 models. Furthermore, the initialisation parameters and factors that alter the decomposition rates are empirically derived from the Rothamsted long-term experimental plots (Qingsong *et al.*, 2023). Ireland's relative proximity to the Rothamsted experimental site and similarity of climate and management practices suggest that the model could be reliably transferred to Ireland (e.g., Byrne and Kiely, 2009; Dondini *et al.*, 2009; Jebari *et al.*, 2021; van Groenigen *et al.*, 2011).

A generalised model framework is essential to ensure consistency in SOC stock estimation across different ecosystems and allow for standardised comparisons at multiple spatial scales, including local, regional and national levels to support both site-specific assessments and broader policy applications (Peralta *et al.*, 2022). We propose to employ the general model framework within a simple, modular, generic, multi-point SOC stock model designed to operate at the field or farm scale that can estimate SOC stock across an array of sites within Ireland, assuming only limited data is available. Our proposed approach represents a hybrid configuration that will support integration of site-specific (e.g., point source) data when available with available climatic gridded (e.g., spatial) datasets.

For this model to be applicable, it must meet the following criteria: 1) the model must operate at the field or farm scale; 2) it must be able to operate with limited data inputs; and 3) it must be adaptable to modifications for future improvements. Developing SOC modelling frameworks capable of accurately estimating SOC stock at a field or farm scale is critical for improving national and regional estimates, ultimately enhancing global SOC inventories (Saunders *et al.*, 2022; Vitharana *et al.*, 2019). Furthermore, a hybrid configuration will enable model applications to more accurately reflect local conditions.

The RothC model requires C inputs and evapotranspiration (ET) estimates from external sources or auxiliary models. As demonstrated in Chapter 5, we employed a multi-model ensemble to evaluate how varying levels of data granularity (e.g., specific to general) influence the performance of the RothC_R model. Our results indicated that the accuracy of the RothC simulations is particularly sensitive to the selection of ET and C input estimates, corroborating findings by previous studies (e.g., Maas and Lal, 2023; Riggers *et al.*, 2019; Wiesmeier *et al.*, 2016). While it is often assumed that complex high-resolution data inputs can improve model accuracy (FAO, 2019), our ensemble analysis in Chapter 5 revealed that in data-limited environments, such complexity can decrease model accuracy when relying on default parameters. Consequently, we adopted a simplified input configuration using the Miami Model of Net Primary Production (NPP) (Lieth, 1973) and the Thornthwaite (1948) method for ET derivation. As discussed in Section 5.4.4, this configuration was identified as the most satisfactory approach when compared to more complex methodologies, providing an appropriate balance between model performance and data availability.

Our research objectives for this chapter are: i) identify environmental factors influencing SOC stock variability across mineral grassland sites; ii) evaluate the performance of the RothC model in estimating SOC stocks for Irish grasslands; iii) determine key drivers of the SOC stock estimates in the RothC model; iv) demonstrate the applicability of our approach to generate SOC stock estimates at farm-scale, and; v) demonstrate the modular design that facilitates multi-model ensembles and intercomparison studies.

6.2 Materials and methods

6.2.1 Model configuration

We developed the Mineral Grassland (MG) model, a modular approach designed to provide uniform SOC stock estimates under minimal data availability for use at both farm and field scales. The MG model, which relies on the model framework evaluated in previous chapters, requires the following inputs: latitude, longitude, clay percentage, sampling depth (cm) and known SOC stock. The MG model consists of three components: 1) the Climate module, 2) the C input model, and 3) the RothC model implementation.

Climate Module

The climate module is the initial component of the MG model, providing essential meteorological inputs. It uses 1×1km resolution daily gridded datasets based on the Irish Transverse Mercator (TM65) projection, developed by Met Éireann through interpolation of long-term in situ observations. These datasets include daily rainfall and temperature, which are available online (Met Éireann, n.d.). Gridded datasets from Met Éireann, originally as CSV files, were converted to Network Common Data Forms (NetCDF) formats to facilitate efficient multi-dimensional data processing and spatial querying.

The NetCDF datasets were accessed and processed using the 'climate4R' package (Iturbide *et al.*, 2019), which extracts site-specific climate data by matching user-supplied latitude and longitude coordinates to their corresponding 1×1km grid cells. The package also supports the temporal aggregation of daily records into monthly mean temperatures and monthly total precipitation (Iturbide *et al.*, 2019), which are required as input to the MG model. Monthly mean temperature is used to calculate monthly potential ET via the Thornthwaite method (Thornthwaite, 1948), as implemented in the 'SPEI' R package (Beguería *et al.*, 2014). The C input model requires annual temperature and rainfall values, which are computed from the aggregated monthly values within Climate4R.

For this investigation, we utilised climate data spanning the period 1961 to 2020. A 10-year period from 1961 to 1970 was selected as the baseline for model spin-up, during which the model reaches equilibrium in SOC pool sizes. Although the World Meteorological Organization (WMO) typically defines climate as the average of 30-year periods (WMO, 2017), this shorter interval was selected due to inconsistencies in meteorological records prior to 1961, and because more recent data may not reflect historical climate conditions relevant to long-term SOC dynamics.

Carbon input model

The C input model of the MG model utilises the Miami model (Lieth, 1973), a simple conceptual model that estimates NPP based on annual mean temperature and total precipitation (Grieser *et al.*, 2006). The Miami Model is described in detail in Section 5.2.5. It estimates NPP as grams of dry matter (DM) per square meter per year ($\text{g DM m}^{-2} \text{ year}^{-1}$).

The Miami model offers a climate-based estimate of potential NPP; however, when used directly as a proxy for C inputs, it can significantly overestimate C inputs because not all NPP contributes to SOC formation. To address this limitation, previous studies utilising RothC with C inputs from the Miami Model incorporated a C input adjustment coefficient for specific land uses (Peralta *et al.*, 2022).

We adopted the methodology approach proposed by Peralta *et al.* (2022). We applied the same adjustment coefficient, of 0.72, which reflects the proportion of NPP assumed to enter

the soil C pool under grassland systems. This coefficient was applied uniformly across all grassland types in our model, consistent with the assumptions made by Peralta *et al.* (2022), with no distinction made between management or grassland classification. The DM yield is multiplied by the typical C content of dry biomass (45%, Kätterer *et al.*, 2011) to convert it to g C m² yr⁻¹. This value is then converted to tonne C ha⁻¹ yr⁻¹, as it is the required unit for the RothC_R model.

RothC model

The RothC model, implemented in R (RothC_R) via the SoilR package (Sierra *et al.*, 2012), has previously been shown to faithfully replicate the results of the original Windows RothC model (see Chapter 4). A detailed description of the RothC model structure is provided in Section 4.2.1. Within the MG model, the RothC_R model constitutes the final module and simulates SOC stocks based on climatic drivers, C inputs and soil properties. The climatic drivers consist of temperature, rainfall and ET, which are supplied by the Climate module. It also requires C inputs supplied by the C input model. Additionally, the RothC_R model requires clay content (as %), measured SOC stock value (Mg C ha⁻¹), and sampling depth (as cm), which are supplied by the user. Equally, clay values could be obtained for a location from national soil maps, assuming they are available and are sufficiently detailed for use at the farm or field level. A schematic overview of the MG model is provided in Figure 6.1.

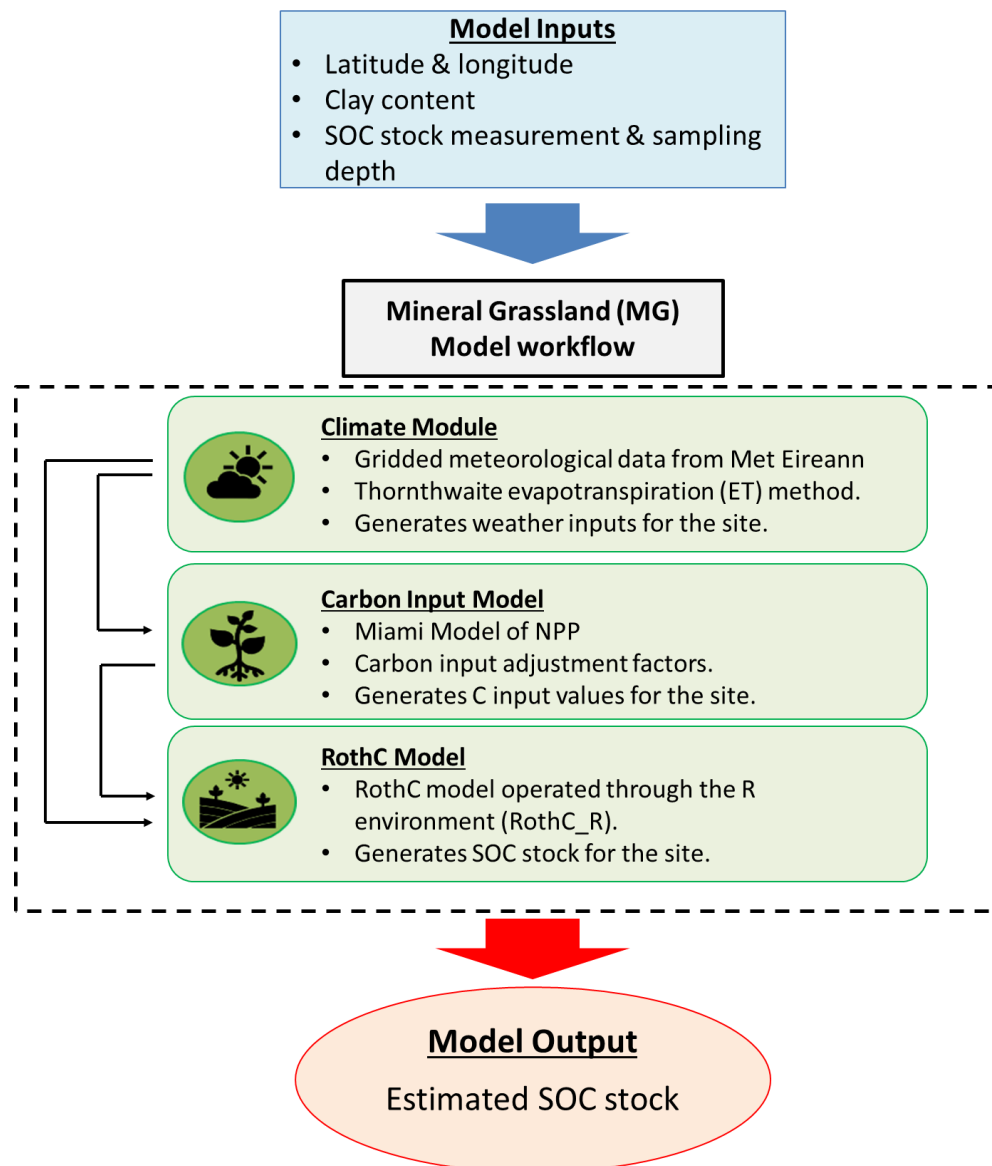


Figure 6.1 Workflow of the Mineral Grassland (MG) Model used to estimate soil organic carbon (SOC) stocks under data-limited conditions. The model is composed of three modular components: climate, carbon input, and SOC simulation, which integrate site-level inputs to produce monthly climatic variables, estimated carbon inputs, and SOC stock estimates.

6.2.2 Site selection

Two different datasets were employed to demonstrate the flexibility of the MG modelling approach in estimating SOC stocks across different spatial scales. The first dataset facilitates landscape-scale estimation, while the second enables farm-scale estimation. The site(s) within each category are described separately below.

6.2.2.1 Landscape scale

For the landscape site selection, we utilised the SoilC database reported by Kiely *et al.* (2009). SoilC is a soils database, reporting SOC stocks measured to a depth of 50cm for 71 sites across Ireland; it also contains information on land use at sampled sites. The sampling campaign for the SoilC project was undertaken between May 2006 and February 2007. Each

site was sampled for soil carbon concentration, bulk density (BD), soil texture and nutrient stock by fixed depth intervals (e.g., 0-5cm, 5-10cm) rather than by soil horizons. This ensured consistency in sampling methods and laboratory analysis.

The SoilC database was the most appropriate database for this study for a number of reasons: 1) It is land-use oriented, making it straightforward to identify the grassland sites, which removes additional uncertainty of using landcover data to identify grassland sites at the time the measurement were made; 2) The database was designed to support SOC modelling work which was not achieved due to time constraints of the original project; and, 3) it is readily accessible, allowing future replication and modifications. From the 71 sites, we identified and selected 28 geographically distributed grassland sites on mineral soils. The location of these grasslands is shown in Figure 6.2.

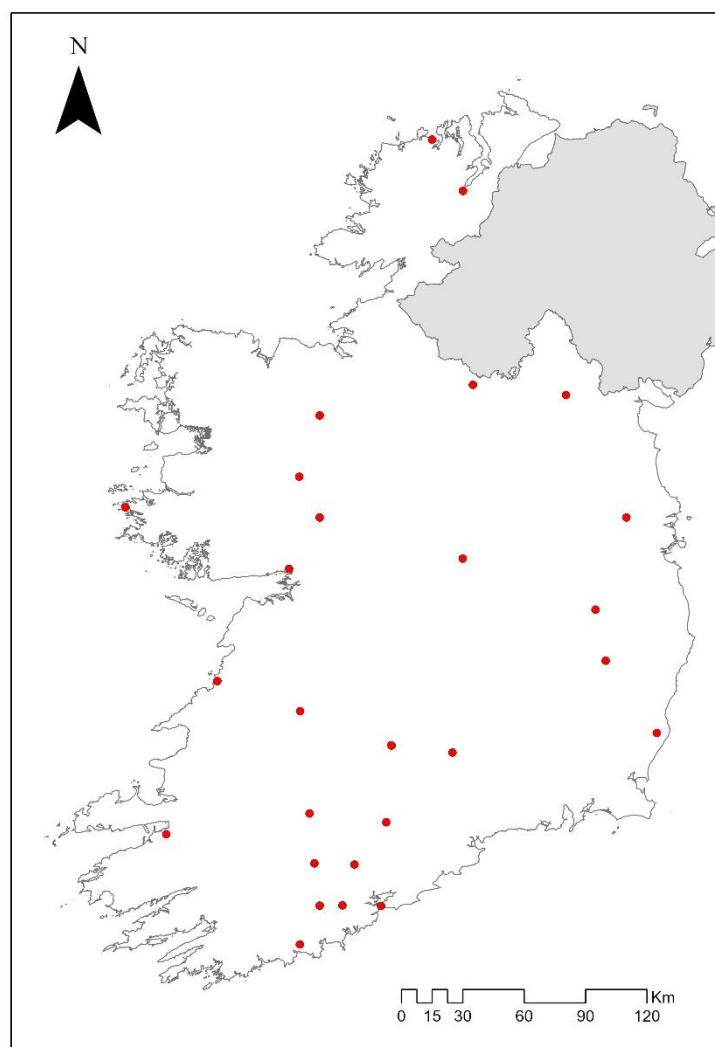


Figure 6.2 Location map of the 28 mineral grassland sites selected from the SoilC database (Kiely *et al.*, 2009).

The SoilC database includes SOC content (as %) for the following depths: 0-10cm, 10-25cm and 25-50cm, while BD is recorded in 5cm increments. It also contains additional

information, including general attributes, soil texture, chemical properties, and nutrient stocks, facilitating further analysis. The following environmental variables were explored as drivers of SOC stock variability: latitude, longitude, temperature (as °C), rainfall, elevation (m), actual BD (kg m^{-3}), carbon as % (%C), organic matter (OM, as %), carbon to nitrogen (C/N) ratio, pH, silt (as %), total sand (fine plus coarse sand, as %) and clay (as %). Further details regarding the soil sampling, preparation and analysis are described in Kiely *et al.* (2009). The database is publicly available online at: <https://eparesearch.epa.ie/safer/iso19115/displayISO19115.jsp?isoID=107>.

Although the IPCC guidelines recommend a SOC sampling depth of 0–30 cm (IPCC, 2019), extrapolating from the 25–50 cm layer to estimate the remaining 5 cm introduces uncertainty. Therefore, the 0–25 cm interval was selected as the most accurate representation of topsoil SOC for this analysis. All soil variables were harmonised to this depth using a mass-weighted averaging method, where layer values were weighted by the product of layer thickness and BD, to ensure consistency across chemical, physical, and textural properties. Soil organic carbon stock was calculated separately for the 0–10 cm and 10–25 cm layers using depth-specific BD and carbon concentration (%C) and then summed to derive total SOC to 25 cm. An overview of the site-level mass-weighted environmental and edaphic variables is presented in Table 6.1, and the dataset conversion is detailed in Appendix C.1.

Table 6.1 Description of the characteristics of mineral grassland sites in the SoilC database (Kiely *et al.*, 2009). Soil variables represent the weighted averages for the 0-25cm depth interval.

Site	County	Soil type		Elevation	Clay (%)	Sand (%)	Silt (%)	Bulk density (g cm ³)	C/N Ratio	Organic matter (%)	pH	Carbon (%)	SOC stock (Mg C ha ⁻¹)
68	Wexford	Gley		39	36.6	19.2	44.2	1.2	9.6	3.5	7.5	1.8	58.3
126	Carlow	Shallow Earth	Brown	120	6	69.9	24.1	1.1	11.2	6.3	6.9	4	111.9
180	Tipperary	Grey Podzolic	Brown	100	19.5	47.1	33.3	1	7.6	4.9	5.2	2.7	80.6
268	Kildare	Grey Podzolic	Brown	132	17.9	53.7	28.4	1	8.2	4.9	5.1	2.5	74.6
355	Cork	Brown Podzolic		58	7.5	40	52.6	1	9.1	6	5.6	3.4	77.9
358	Cork	Brown Podzolic		35	19	53.1	28	0.9	8.1	5.9	6	3.2	77.9
446	Kerry	Brown Podzolic		40	0.5	81.7	17.8	1	15.7	6.8	5	4.3	113.4
485	Cork	Grey Podzolic	Brown	105	32.4	28.2	39.4	0.8	10.1	9.9	5.8	5.2	121.7
633	Clare	Brown Podzolic		8	29	30.9	40.2	0.8	8.3	7.1	5	4.4	113.9
740	Galway	Shallow Earth	Brown	48	16.9	49.4	33.8	1	9.2	5.7	7.6	3.1	82.1
773	Offaly	Grey Podzolic	Brown	58	21.2	32.7	46.1	0.8	9.1	7.3	7.1	3.9	99
862	Galway	Grey Podzolic	Brown	63	9.9	52.8	37.3	0.9	12.9	7.8	7.1	4.6	108.7
876	Meath	Grey Podzolic	Brown	104	24.1	30.4	45.5	0.9	7.7	5.1	5.8	2.8	66.7
879	Galway	Sand		18	2.5	95.5	2	1	5	2.4	7.9	0.8	22.1
962	Mayo	Grey Podzolic	Brown	79	14.9	47.7	37.4	0.8	10.5	7.8	5.7	4.4	106.7
1102	Mayo	Podzol		96	3.8	69.6	26.6	0.6	18.7	15.2	5.6	6.7	141.4
1158	Monaghan	Acid Brown Earth		125	21.2	47.5	31.3	0.8	9.5	8.5	5.7	4.7	105.4
1176	Cavan	Gley		60	12.2	56.9	31	0.9	9.6	5.5	5.5	3.1	78.3
1319	Donegal	Grey Podzolic	Brown	44	9.4	54.8	35.7	1.1	9.5	4.9	6.2	2.5	72.8
1347	Donegal	Shallow Earth	Brown	16	14.9	49.3	35.7	1	8.8	6	6.6	3	81.3

3001	Tipperary	Gley	98	40.3	20.1	39.6	0.9	7.8	7.3	6.3	3.9	105.4
3002	Tipperary	Gley	102	22.3	44.2	33.5	1	8.2	10	6.7	5	127.5
3003	Cork	Acid Brown Earth	51	17.3	53.5	29.2	1.1	8.5	6.1	5.6	3.4	94.4
3004	Limerick	Grey Brown Podzolic	15	19.9	48.6	31.5	1.1	7.9	6.3	5.2	3.1	87.4
3005	Cork	Brown Podzolic	104	20.8	42.8	36.4	0.9	7.9	7.7	6.3	4	96.7
3006	Cork	Gley	187	12.9	46.7	40.4	1	13.9	8	6.3	4.3	103.8
3007	Cork	Brown Podzolic	69	17.5	53.9	28.5	1	8.1	7.3	6	3.8	95.5
3008	Cork	Grey Brown Podzolic	79	27.6	35.4	37	1.1	8.4	6.1	5.9	3	85.6

6.2.2.2 Farm level data

The Teagasc Johnstown Castle (JC) research farm is located in the southeast of Ireland, in County Wexford. The JC dairy enterprise comprises 140 Holstein Friesian cows plus heifers, run on a total grassland area of 73 ha, with 54 ha in the grazing platform (e.g., area adjacent to milking parlour) (Teagasc, 2023). The herd is split into two distinct systems: autumn-calving and spring-calving. However, herd numbers and the area under active management for the dairy herd can vary slightly from year to year due to experimental field trials. Current research initiatives at JC include studies of alternative dietary strategies, methane mitigation, and multi-species swards.

The soils at JC are derived from complex glacial drift deposits, resulting in considerable spatial heterogeneity across the farm. The predominant parent material is a fine loamy till, occasionally overlain by stratified sand. Soils are classified into three main textural groups: fine loamy, sandy, and coarse loamy over fine loamy, which are subdivided by drainage status (well, imperfect, poor). A soil campaign was conducted at JC with samples collected and analysed by soil horizons (Anon, 2008).

To derive representative soil properties values for modelling, results from individual horizons were harmonised to the IPCC (2019) recommended 0-30cm depth interval. In the absence of bulk density data for each horizon, depth-weighted averaging was applied. Each horizon's contribution was weighted according to its thickness, allowing for proportional representation of properties within the topsoil profile. While mass-weighted averaging would provide a more accurate estimate, BD values are not available at the measurement sites. Table 6.2 presents the dominant soil classification, drainage characteristics and depth-weighted averages for total sand, silt and clay (as %) for 0-30cm. The spatial distribution of soil types and drainage classes is illustrated in Figure 6.3.

Table 6.2 Soil groups, classifications and drainage categories for dairy enterprise on the Johnstown Castle estate. Each classification and drainage combination was given a unique map unit. The total sand, silt and clay was the weighted average for the 0-30cm depth interval.

Map Unit	Soil group	Classification	Drainage category	Sand (%)	Silt (%)	Clay (%)
A1	Fine loamy soils	Brown earth	Moderate	50.1	31.7	18.2
A2	Fine loamy soils	Gley	Imperfect	43.6	38.4	18
A3	Fine loamy soils	Gley	Poor	46.9	38.5	14.6
B1	Sandy soils	Brown podzolic	Well to excessively	93	4	3
B2	Sandy soils	Brown podzolic	Moderate well	93	4	3
C1	Coarse loamy over fine loamy	Brown earth	Well drained	63.7	24	12.3
C2	Coarse loamy over fine loamy	Brown Earth	Moderate to imperfect	48.7	34.3	17
C3	Coarse loamy over fine loamy	Gley	Poor	80	11	9

The JC Dairy enterprise has limited measured SOC stock data available. Paddocks 10 and 11, commonly referred to as the ‘tower fields’ due to the presence of an eddy covariance flux tower, have SOC measurements from 2006 to 2021. Byrne and Kiely (2009) reported a combined SOC stock of 78.72 Mg C ha⁻¹ to a depth of 20cm for these fields based on samples collected in 2006. More recent measurements conducted in early 2021 estimated SOC stocks of 122.98 Mg C ha⁻¹ and 113.62 Mg C ha⁻¹ for paddocks 10 and 11 at 0-30cm, respectively. However, these recent estimates assumed that the BD measured for the 0-10cm layer remained constant throughout the 10-30cm depth interval, potentially leading to over- or under-estimation of total SOC stock.

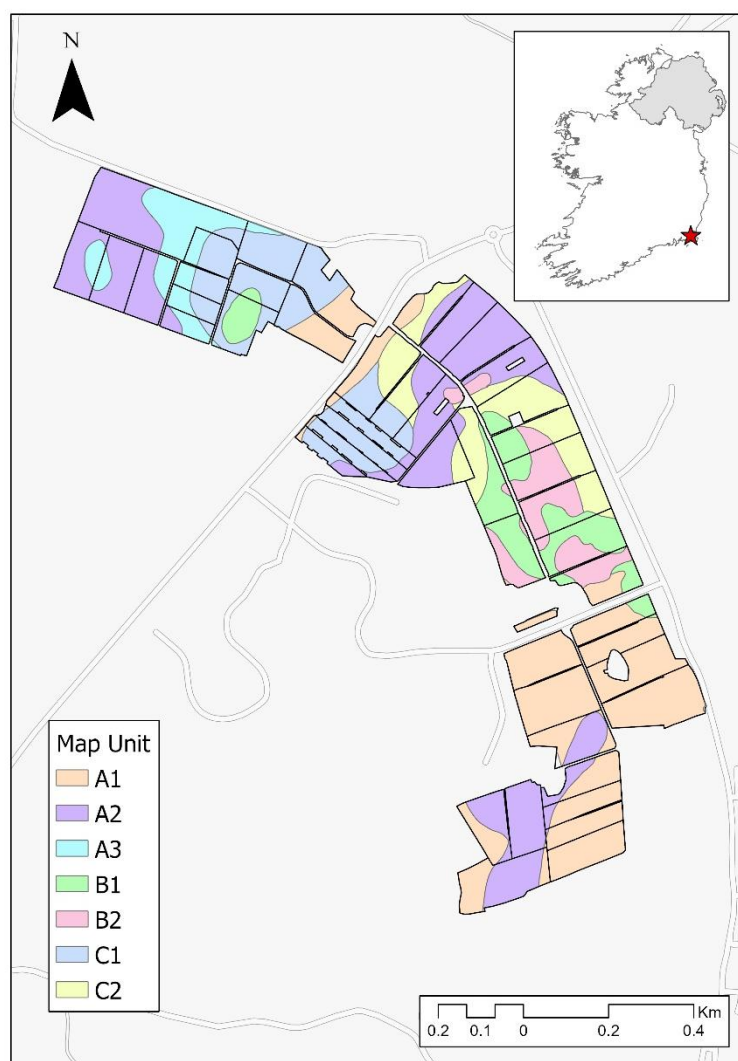


Figure 6.3 The spatial distribution of soil classification on the Johnstown Castle dairy enterprise for the selected paddocks (Anon, 2008). The map units are outlined in Table 6.2.

To facilitate comparison across depths, SOC stocks were rescaled to between 0-20cm and 0-30cm. Assuming uniform SOC density with depth, the 2006 SOC stock estimate of 78.82 Mg C ha⁻¹ at 0-20cm scales rises to 118.08 Mg C ha⁻¹ at 0-30cm. Conversely, the 2021 SOC measurements of 122.98 Mg C ha⁻¹ and 113.62 Mg C ha⁻¹ at 0-30 cm for Paddocks 10 and 11 correspond to 81.99 Mg C ha⁻¹ and 75.75 Mg C ha⁻¹, respectively, when scaled to 0-20 cm. Assuming all measurements are representative of SOC stocks at or near steady-state conditions, the average SOC stock for the tower fields is estimated at 78.8 Mg C ha⁻¹ for 0-20 cm and 118.2 Mg C ha⁻¹ for 0-30 cm.

The MG Model, as implemented here, does not incorporate site-level management detail. While RothC accounts for the influence of farm management by making adjustments to the C inputs, the MG model employs the Miami model to estimate C inputs based solely on climate. Given the close proximity of paddocks within the JC Dairy Enterprise, both climate and, by extension, C input estimates were assumed to be homogeneous across all selected

paddocks. The study area was subdivided into eight map units, each defined by unique combinations of soil texture and drainage class (e.g., A1, B1, C3). A mosaic-tile modelling approach was implemented, in which each map unit was treated as an independent simulation 'tile'. SOC stock estimates (Mg C ha^{-1}) were generated for each tile using the MG model and subsequently upscaled according to the areal extent of each unit. This enabled the model to capture spatial heterogeneity across the JC dairy platform.

6.2.3 Model operation

The MG model operates within the R environment (R Core Team, 2024) and requires site parameters to be provided via comma-separated values (CSV) files or other compatible formats, enabling automated and standardised SOC stock estimation across all sites or paddocks. However, RothC modelling approaches vary depending on study objectives, scale, and land use. This section outlines the configuration and implementation of the RothC_R model as applied within the MG model.

The inert organic matter (IOM) pool is first estimated using the Falloon *et al.* (1998) pedotransfer function (PTF), which relates known SOC stock values to estimate the size of the IOM pool:

$$IOM = 0.049 \times SOC^{1.139} \quad (6.1)$$

The IOM pool is considered completely inert and does not undergo decomposition. For all SoilC sites, known SOC stock values were obtained from Table 6.1. For the paddocks located within JC, we assumed a SOC stock value of 118 Mg C ha^{-1} , based on the average of $118.2 \text{ Mg C ha}^{-1}$ to a depth of 0-30cm.

To initialise the four active RothC pools (decomposable plant material, DPM; resistant plant material, RPM; microbial biomass, BIO; humified organic matter, HUM), a 500-year spin-up phase is performed. This simulates long-term equilibrium by starting all pools at zero and applying constant average climatic and C inputs until stability is reached. For the model spin-up, 10-year monthly averages of temperature, precipitation and ET were employed over the 1961-1970 period, together with a long-term average (LTA) for annual average C input derived from the Miami model for the same reference period (1961-1970). The DPM/RPM ratio was fixed at 1.44, the default value for most agricultural crops and improved grasslands (Coleman *et al.*, 2024).

Following spin-up, the model enters the simulation phase, covering the period from 1971 to 2020, using monthly average meteorological data (temperature, rainfall and ET). As the RothC_R model is designed to operate with constant annual C inputs, it cannot incorporate temporally varying inputs (e.g., monthly or yearly) without additional amendments. Therefore, a compromise was adopted using a 5-year average C input (e.g., 1971-1975,

1976-1980), while continuing to apply monthly meteorological data. Although the RothC model includes a separate input vector for farmyard manure (FYM), we excluded FYM from simulations. This decision reflects both the Miami model's tendency to overestimate total C inputs and the absence of explicit management data within the SoilC database. The MG model script is provided in Appendix C.2.

6.2.4 Model validation

The SoilC database has only a single SOC stock measurement per site. As a result, the recommended validation approach based on repeated, independent measurements validation is not feasible, as it requires temporal SOC data collected over time at the same location (LeNoë *et al.*, 2023). Consequently, we employed a space-for-time validation approach, in which model simulations are compared against a SOC observation from a series of sites across the landscape. In this approach, variation among sites is driven by differences in climate, land-use and land-use history, and soil types, and provides the basis for evaluating the model performance.

6.2.5 Statistical analysis

The normality of the data was assessed visually (e.g., via Q-Q plots and histograms) and using the Shapiro-Wilk test at the 5% significance level to inform the selection of appropriate statistical methods. The environmental drivers of SOC stocks did not follow a normal distribution; therefore, the Spearman rho correlation test was used to evaluate the strength and direction of monotonic relationships. Although the model input variables met the normality assumptions, Spearman's rho was also employed for consistency across variable sets. Categorical variables were excluded from analysis due to insufficient sample sizes, which could compromise statistical reliability.

Model performance was assessed using root-mean-square-error (RMSE) and normalised RMSE (NRMSE). RMSE quantifies the absolute difference between modelled and measured SOC stock values and is described in Section 4.2.7. NRMSE provides a relative measure of model accuracy by expressing RMSE as a percentage of the mean observed SOC stock. This standardisation facilitates comparison across models and datasets. The NRMSE was calculated as follows:

$$NRMSE (\%) = \left(\frac{RMSE}{Mean\ Observed\ SOC} \right) \times 100 \quad (6.2)$$

A lower NRMSE (%) indicates better model performance.

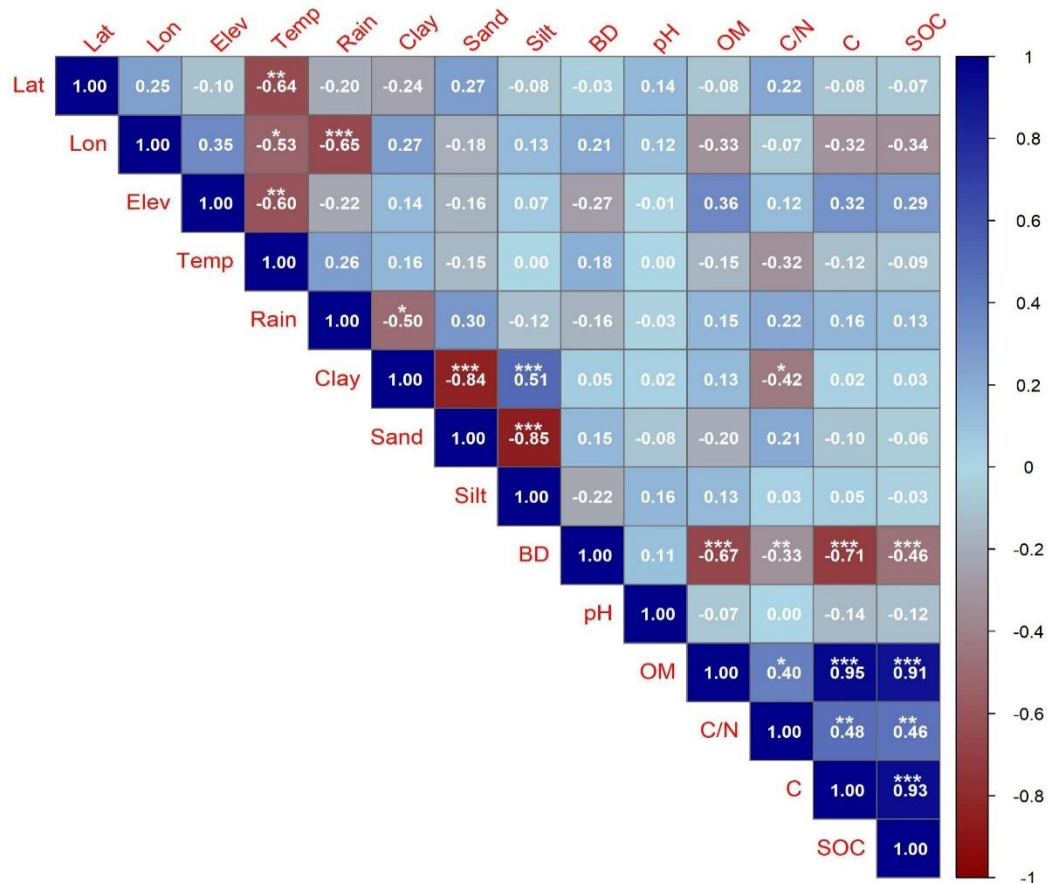
6.3 Results

6.3.1 Environmental drivers of SOC stocks: Measured

The Spearman Rho correlations between environmental variables for the selected SoilC sites are presented in Table 6.3. Several statistically significant relationships were identified with varying strengths. The significant SOC stock relationships included a strong positive correlation between %C and SOC ($\rho = 0.93$, $p < 0.001$), OM and SOC ($\rho = 0.91$, $p < 0.001$), a moderate positive correlation between C/N ratio and SOC ($\rho = 0.46$, $p < 0.05$), and a moderate negative correlation between BD and SOC ($\rho = -0.46$, $p < 0.001$).

Additionally, measured SOC stock values were imported to ArcGIS to visually assess for regional or gradient trends (Figure 6.4). However, no clear spatial patterns or gradients were observed. This lack of spatial coherence is most likely an artefact of the restricted sample size ($n = 28$). Detecting regional relationships would likely require a substantially larger number of sites.

Table 6.3 Spearman correlation matrix of environmental variables for the selected SoilC sites. The colour gradient represents correlation strength, with blue indicating positive and red indicating negative correlations. Asterisks denote levels of significance levels: $p < 0.05$ (*), $p < 0.01$ (**), and $p < 0.001$ (***). The environmental variables are latitude (Lat), longitude (Lon), elevation (Elev, m), Temperature (Temp, °C), Rainfall (Rain, mm), clay (%), sand (%), silt, bulk density (BD, kg m^{-3}), pH, organic matter (OM, as %), C/N ratio (C/N), carbon (C %) and soil organic carbon stock (SOC, Mg C ha^{-1}).



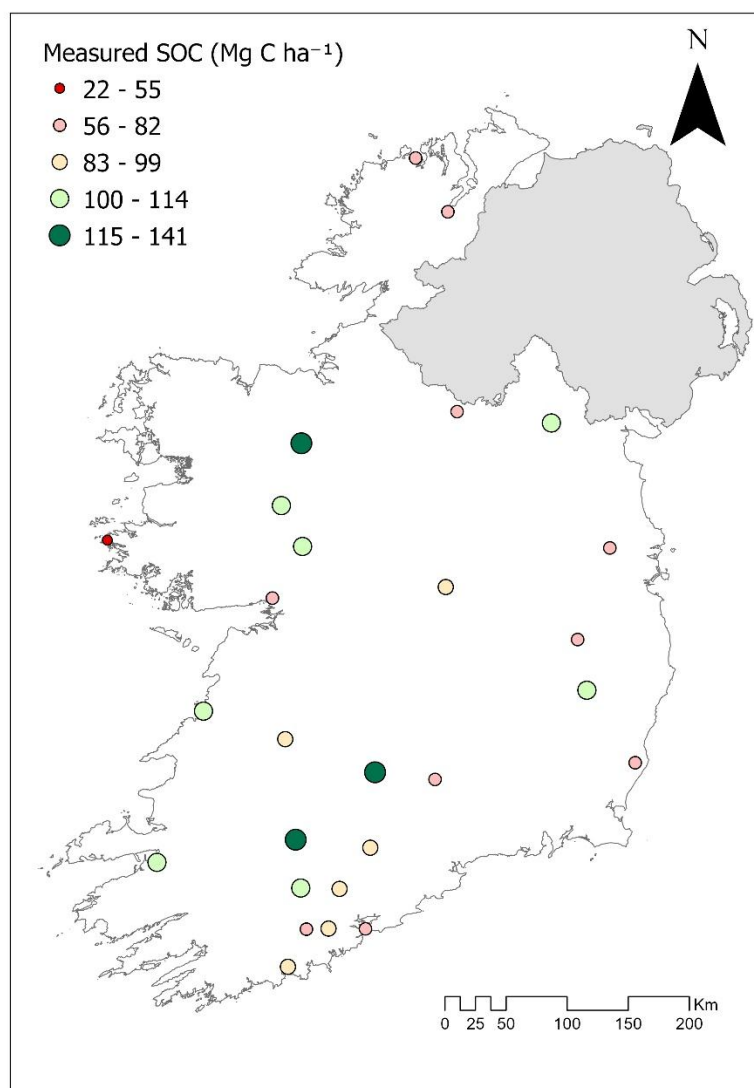


Figure 6.4 Spatial distribution of measured soil organic carbon (SOC) stocks (Mg C ha⁻¹) for the selected SoilC sites. SOC values are grouped using the Natural Breaks classification method to highlight inherent groupings.

6.3.2 Model performance

Table 6.4 summarises the MG model outputs across the 28 mineral grassland sites from the SoilC database. This includes long-term averages (LTA; 1961 to 2007) for climatic variables, average C input and estimated SOC stock for 2007 to coincide with the SoilC measurements.

Table 6.4 Outputs of the Mineral Grassland (MG) model for the 28 mineral grassland sites in the SoilC database. Climatic and C input variables are long-term annual averages (1961-2007), while the estimated SOC stock corresponds to the modelled SOC value for February 2007.

	Temperature	Rainfall	ET	C input	Estimated stock	SOC
	(°C)	(mm)	(mm)	(t C ha ⁻¹)	(Mg C ha ⁻¹)	
Mean	9.7	1086.8	622.9	4.4	88.5	
Min	8.8	1306.5	608.1	3.9	58.8	
Max	10.5	850.3	637.3	4.9	107	
Standard deviation	0.5	130.5	8.1	0.3	16.2	

Figure 6.5 presents box plots illustrating the variability of key MG model inputs and outputs, which include LTA annual temperature, LTA rainfall, LTA ET, estimated C input, estimated IOM pool size, and recorded clay content. The distributions highlight the differences in the variability in model parameters across the selected SoilC sites.

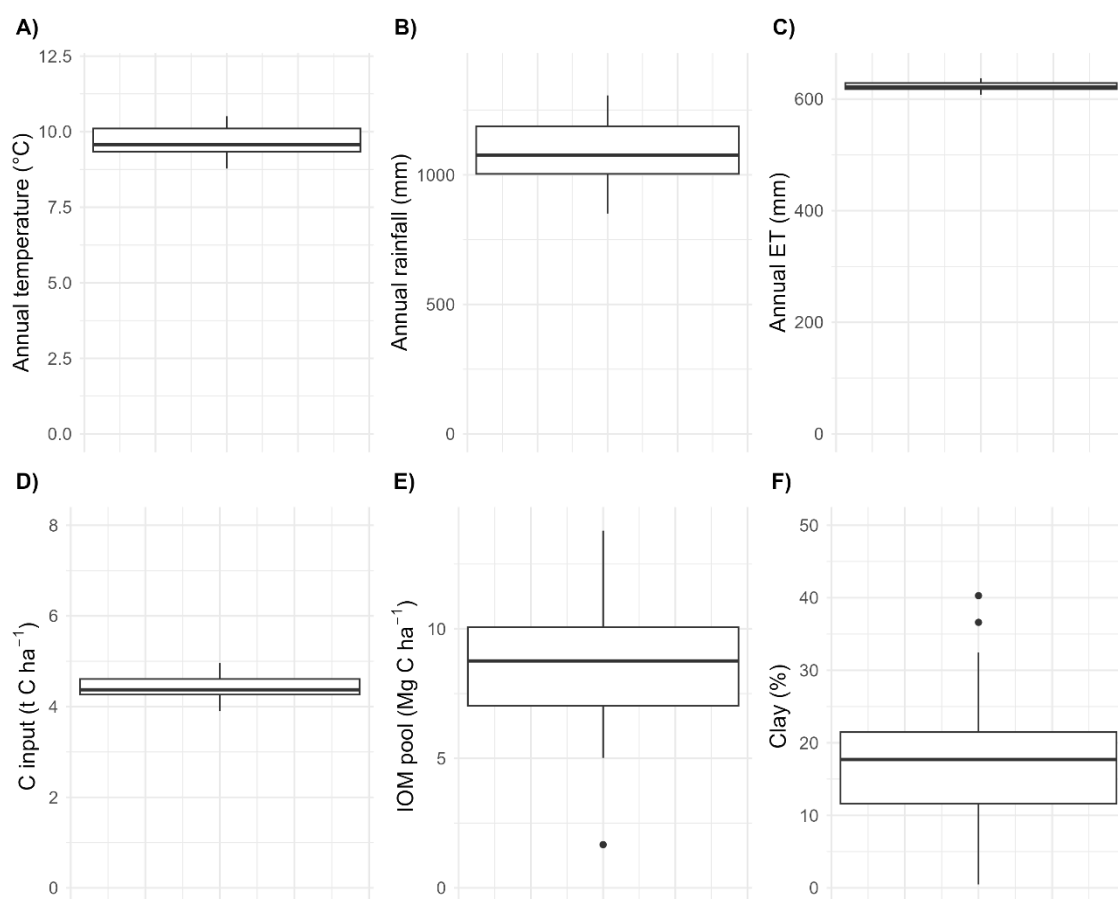


Figure 6.5 Boxplots of the MG model inputs and outputs across the selected SoilC sites. A) Long-term average (LTA, 1961-2007) annual temperature. B) LTA of yearly rainfall. C) LTA of estimated evapotranspiration (ET). D) LTA of estimated C input. E) Estimated inert organic matter (IOM) pool size. F) Clay content. Each boxplot displays the median (central line), interquartile range (IQR; box) and whiskers extending to 1.5 times the IQR. Individual data points beyond this range are shown as outliers (dots).

The MG model produced a narrower range of SOC stock estimates (58.8 to 107 Mg C ha⁻¹) compared to the measured SOC stocks (22 to 141 Mg C ha⁻¹). This indicates a limitation in

the model's ability to capture the variability observed in the measured SoilC dataset. Figure 6.6 compares measured versus modelled SOC stock values across all sites. This suggests that the model underestimates both the lower and upper values of the SOC stock distribution.

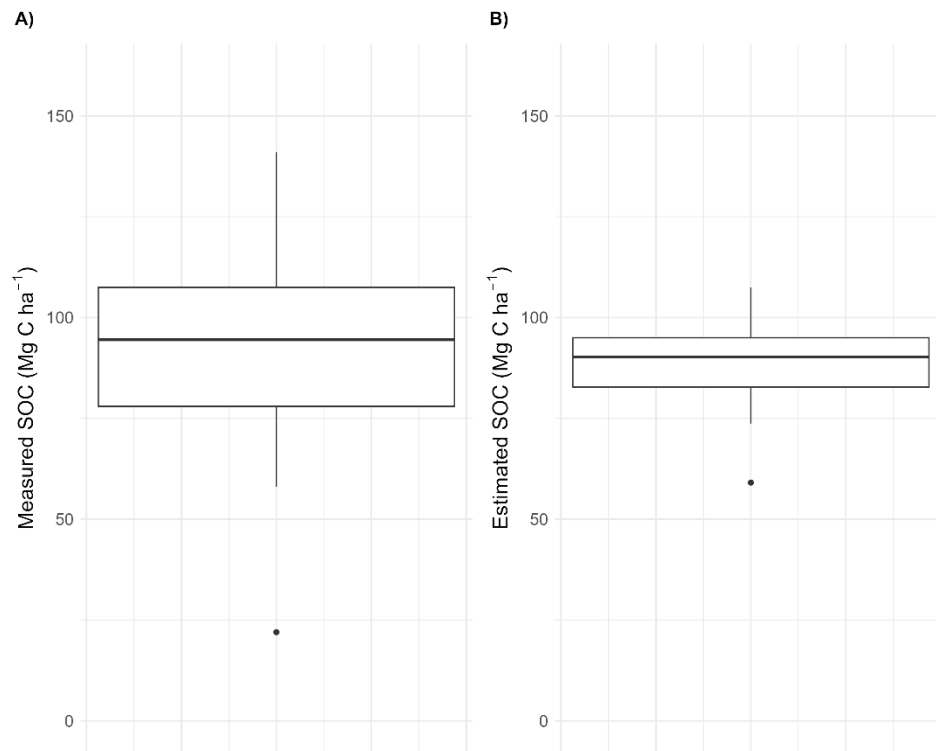


Figure 6.6 Boxplots of the measured soil organic carbon (SOC) stock graph A), and estimated SOC stock graph B) for the mineral grassland sites in the SoilC database. Each boxplot displays the median (central line), interquartile range (IQR; box) and whiskers extending to 1.5 times the IQR. Individual data points beyond this range are shown as outliers (dots).

Figure 6.7 presents individual site-level comparisons between measured and modelled SOC stocks, where each panel shows the long-term SOC trends estimated by the MG model alongside the corresponding measured SOC value. While uniform axis scaling facilitates comparison across sites, it limits the visibility of finer temporal variation in SOC stock dynamics. To overcome this, Figure 6.8 depicts monthly modelled SOC trajectories for four selected sites (126, 358, 773, and 3007), providing a finer resolution of intra-annual variability. These sites were chosen to capture a range of model performance: two sites (773 and 3007) where the model showed strong agreement (classified as excellent and good), and two sites (126 and 358) where the model performed poorly.

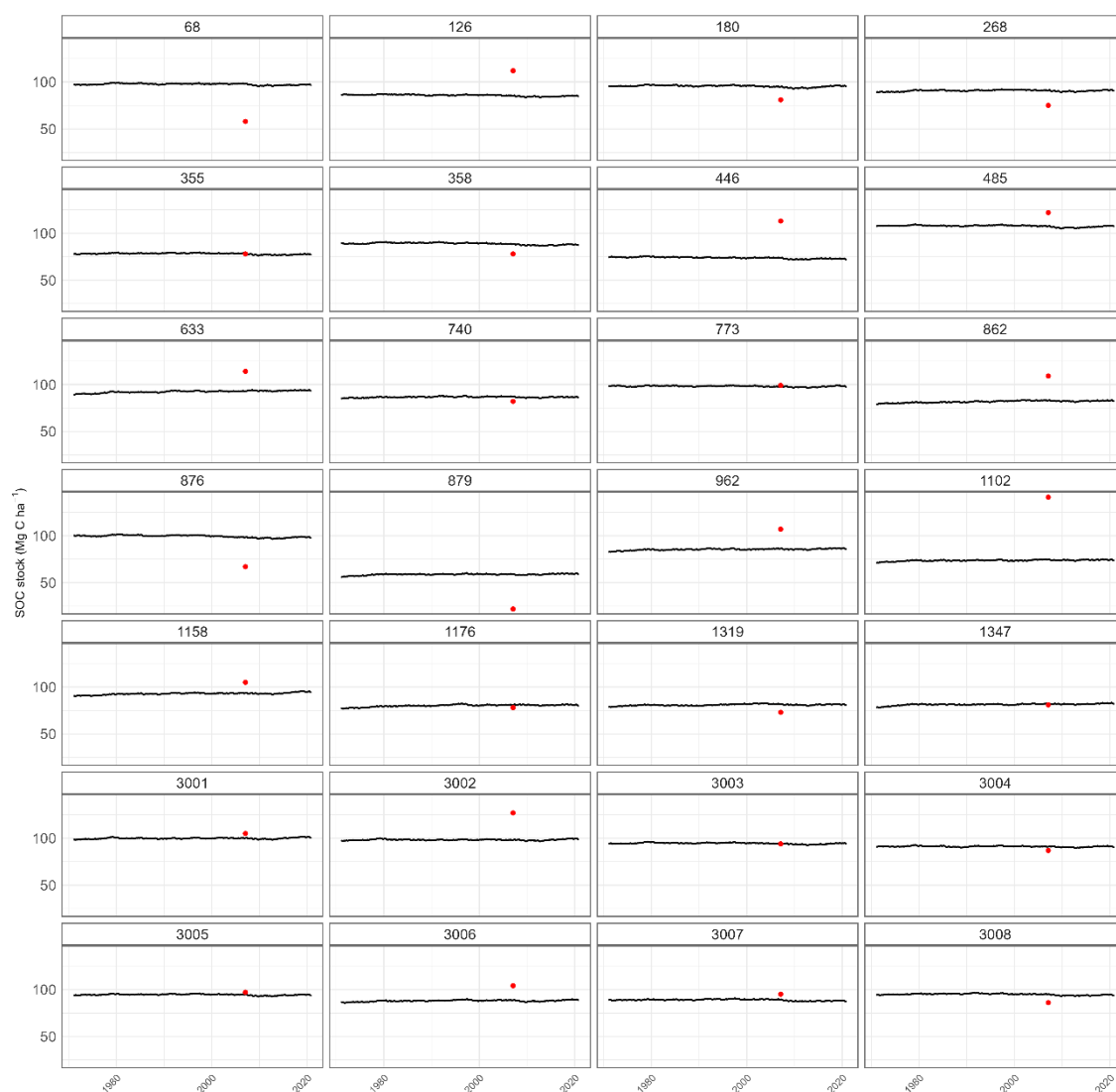


Figure 6.7 Modelled versus measured soil organic carbon (SOC) stock for the 28 mineral grassland sites from the SoilC database. Each graph represents an individual site, where the black line indicates the temporal SOC stocks estimated by the MG model, and the red point marks the measured SOC stock value from the SoilC database.

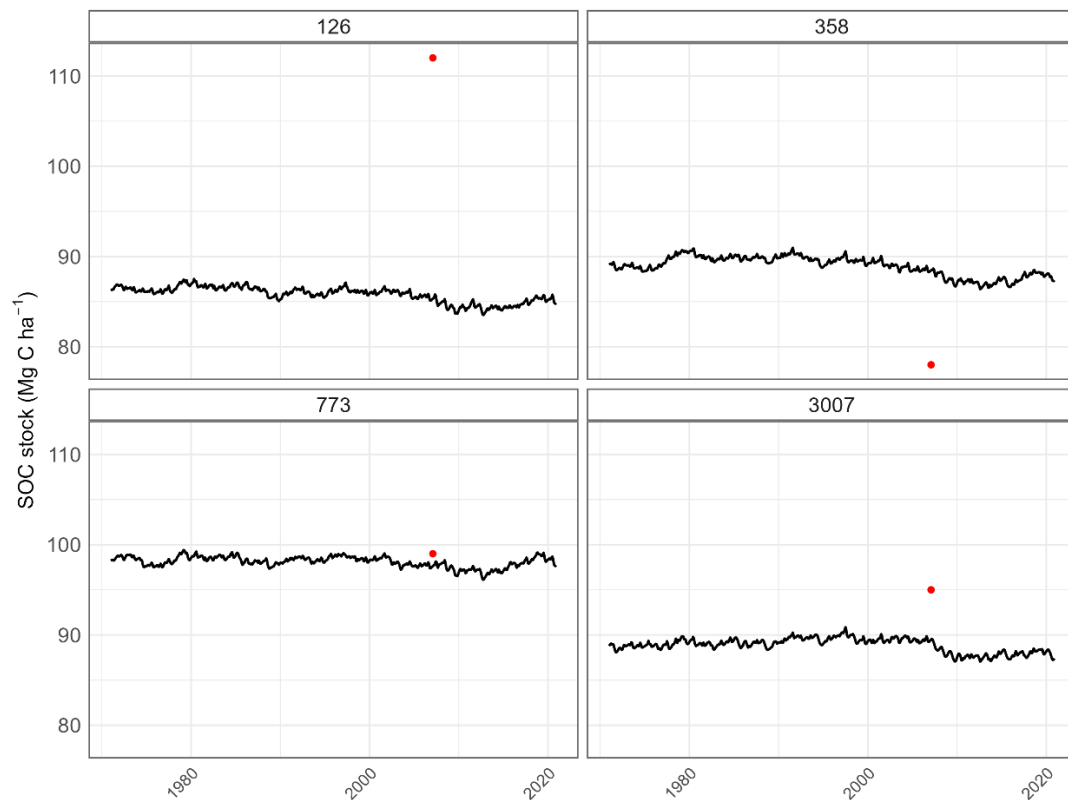


Figure 6.8 Modelled versus measured soil organic carbon (SOC) stock for sites 126, 358, 773 and 3007 from the SoilC database to highlight site-specific SOC stock trajectories. Each graph represents an individual site, where the black line indicates the temporal SOC stocks estimated by the MG model, and the red point marks the measured SOC stock value from the SoilC database.

The MG model exhibited variable agreement between measured and modelled SOC stock across sites. Good to Excellent agreement, defined as $RMSE \leq 10.06 \text{ Mg C ha}^{-1}$, was observed at 13 sites (sites 355, 358, 740, 773, 1176, 1319, 1347, 3001, 3003, 3004, 3005, 3007, 3008). A further 5 sites (sites 180, 268, 485, 1158, 3006) showed moderate agreement with $RMSE \leq 15.72 \text{ Mg C ha}^{-1}$. The remaining 10 sites (sites 68, 126, 446, 633, 862, 876, 879, 962, 1102, 3002) exhibited poor agreement, with RMSE values exceeding 20 Mg C ha^{-1} .

The relationship between RMSE and selected environmental variables, including measured SOC stock, temperature, rainfall, moisture balance (rainfall minus ET), clay content, and C input, is illustrated in Figure 6.9. The MG model appears to perform well when estimating SOC stocks in the range of $\sim 73\text{--}105 \text{ Mg C ha}^{-1}$, while the RMSE increases at and below 60 Mg C ha^{-1} and at and above 110 Mg C ha^{-1} . The narrow spread in simulated C inputs ($3.9\text{--}4.9 \text{ t C ha}^{-1}$; Table 6.4 and Figure 6.5) ultimately propagates into the model SOC estimates, which display a small variation across sites ($\pm 16 \text{ Mg C}$) (Figure 6.6).

This pattern is largely attributable to the current input configuration, in which Miami-derived C inputs (with a uniform allocation coefficient) and Thornthwaite ET estimates do not sufficiently capture variability at the distribution ranges. These findings are consistent

with Moll-Mielewczik *et al.* (2023), who found that RothC was unable to replicate measured SOC at sites with high or low SOC stocks, particularly where input data were uncertain. Consequently, outputs tend to cluster within a restricted range, limiting the model's ability to capture the full spread of observed SOC values. No obvious visible relationships were observed between the RMSE and the remaining variables (temperature, rainfall, moisture, clay content, and C input), with RMSE values evenly distributed across the ranges of values of the driving factors.

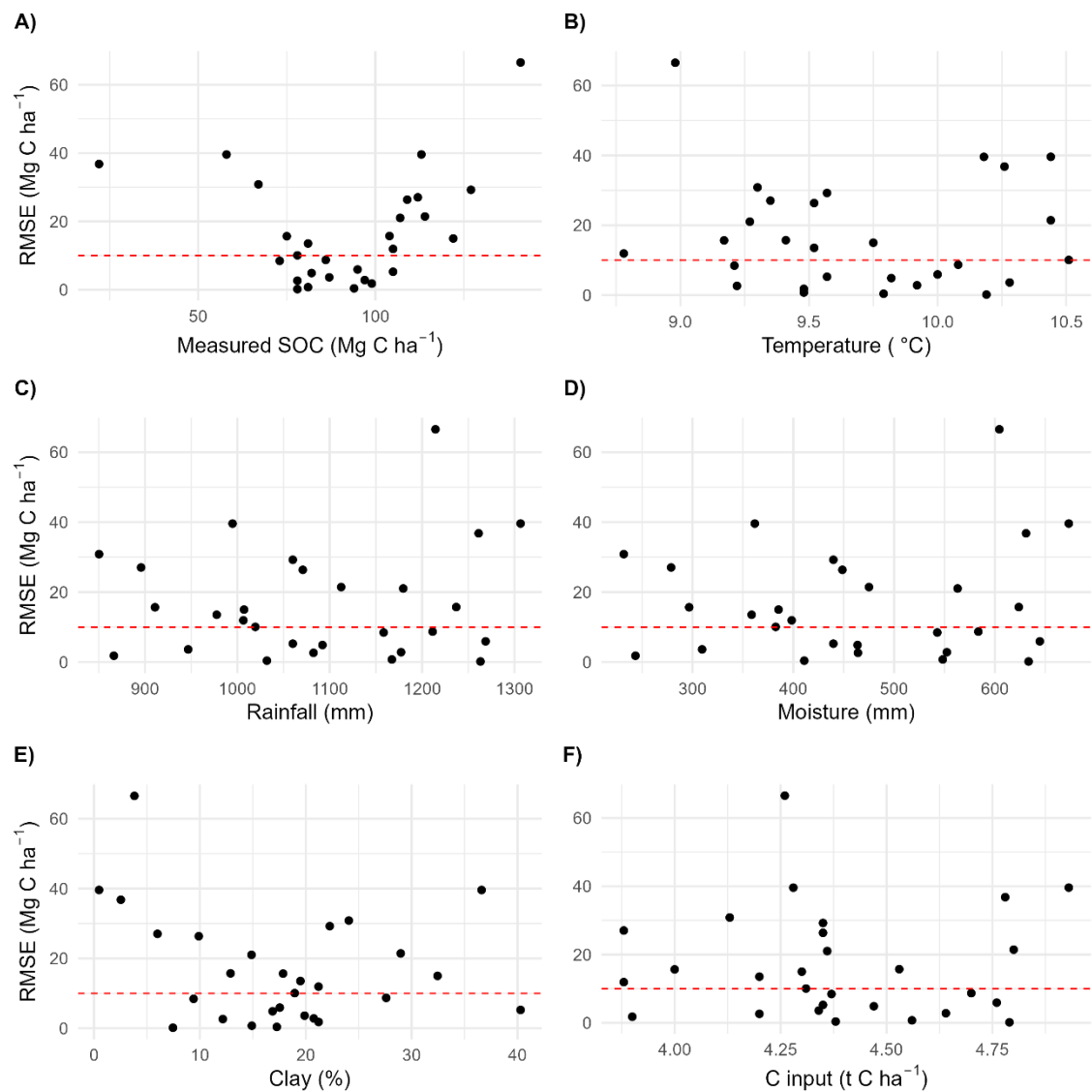


Figure 6.9 Relationship between model performance, expressed as root-mean-square-error (RMSE) and selected site variables across 28 mineral grassland sites from the SoilC database. Graphs show RMSE plotted against A) measured SOC stock; B) Mean annual temperature; C) Mean annual rainfall; D) Mean annual Moisture (rainfall minus evapotranspiration); E) Mean clay as %; and F) Mean annual carbon (C) input. The red dashed line equates to an RMSE of 10 Mg C ha⁻¹, which is considered to indicate a good agreement between measured and modelled SOC stocks for regional studies.

Since %C, OM, BD and C/N ratio were identified as having a significant relationship with SOC stocks, we plotted their relationship against RMSE to investigate any potential association with model performance, as illustrated in Figure 6.10. Carbon as % showed a cluster

between 3-5%, which is expected due to its direct relationship with measured SOC stock. However, no other consistent relationships were evident.

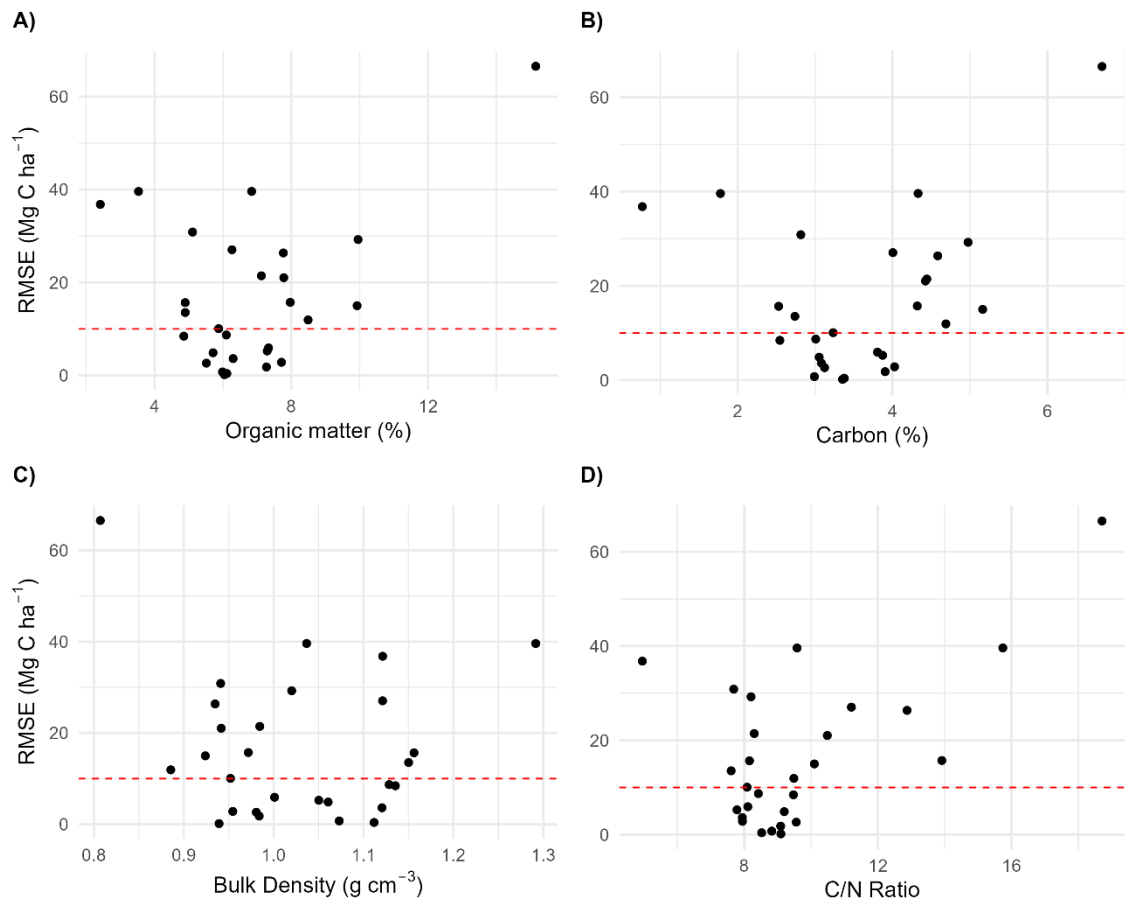


Figure 6.10 Relationship between model performance, expressed as root-mean-square-error (RMSE) and statistically significant variables across 28 mineral grassland sites from the SoilC database. Graphs show RMSE plotted against A) organic matter, B) carbon, C) bulk density, and D) C/N ratio. The red dashed line equates to an RMSE of 10 Mg C ha^{-1} , which is considered a good agreement between measured and modelled SOC stocks for regional studies.

To assess the potential spatial influence on RMSE, the RMSE values were imported into ArcGIS and mapped for visual inspection, as shown in Figure 6.11. However, no spatial signature or patterns were observed that could be directly attributed to climate or environmental conditions.

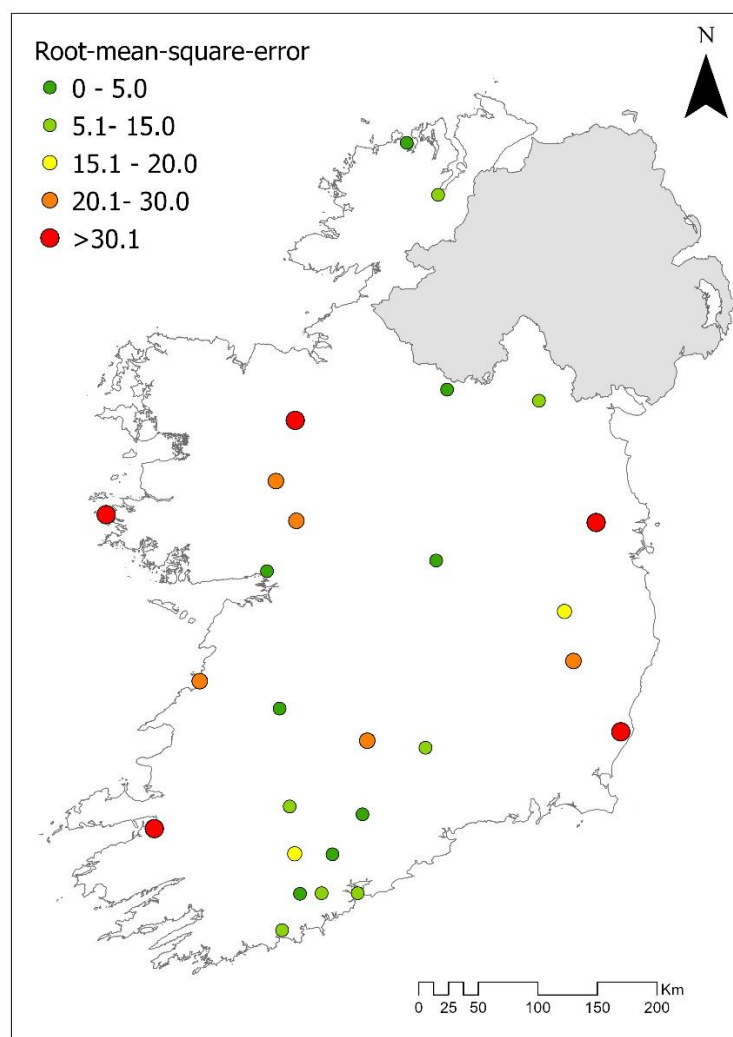


Figure 6.11 Spatial distribution of the root-mean-square-error (RMSE) (Mg C ha^{-1}) for the selected SoilC sites plotted across Ireland.

Across all sites, the MG model yielded an RMSE of $22.7 \text{ Mg C ha}^{-1}$ and an NRMSE (%) of 24.5, indicating a poor agreement between measured and modelled SOC stocks. An overview of the model performance across sites is presented in Figure 6.12. To further explore potential sources of model uncertainty, measured versus modelled SOC stocks were plotted and coloured by mean annual temperature, annual rainfall, annual ET, moisture (rainfall minus ET), C input, and clay content, as illustrated in Figure 6.13. No clear patterns emerged across the environmental gradients assessed, suggesting that these variables do not systematically explain variation in model performance under the current configuration.

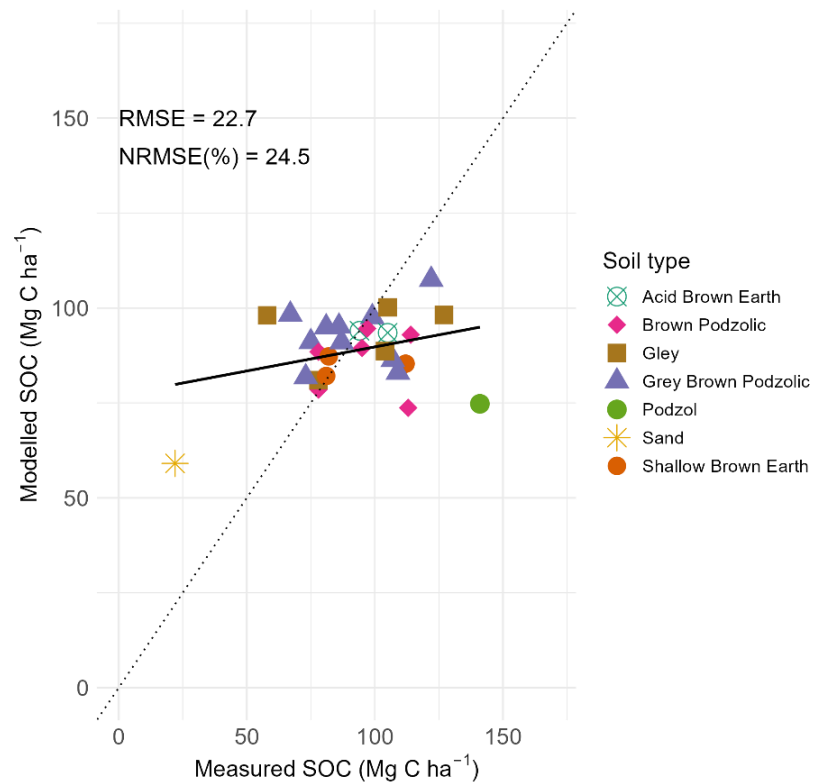


Figure 6.12 Comparison of modelled versus measured SOC stock values across the 28 SoilC grassland sites, categorised by soil type. The black solid line represents the line of best fit, illustrating the overall fit of the MG model performance. The black dotted diagonal line represents the 1:1 line.

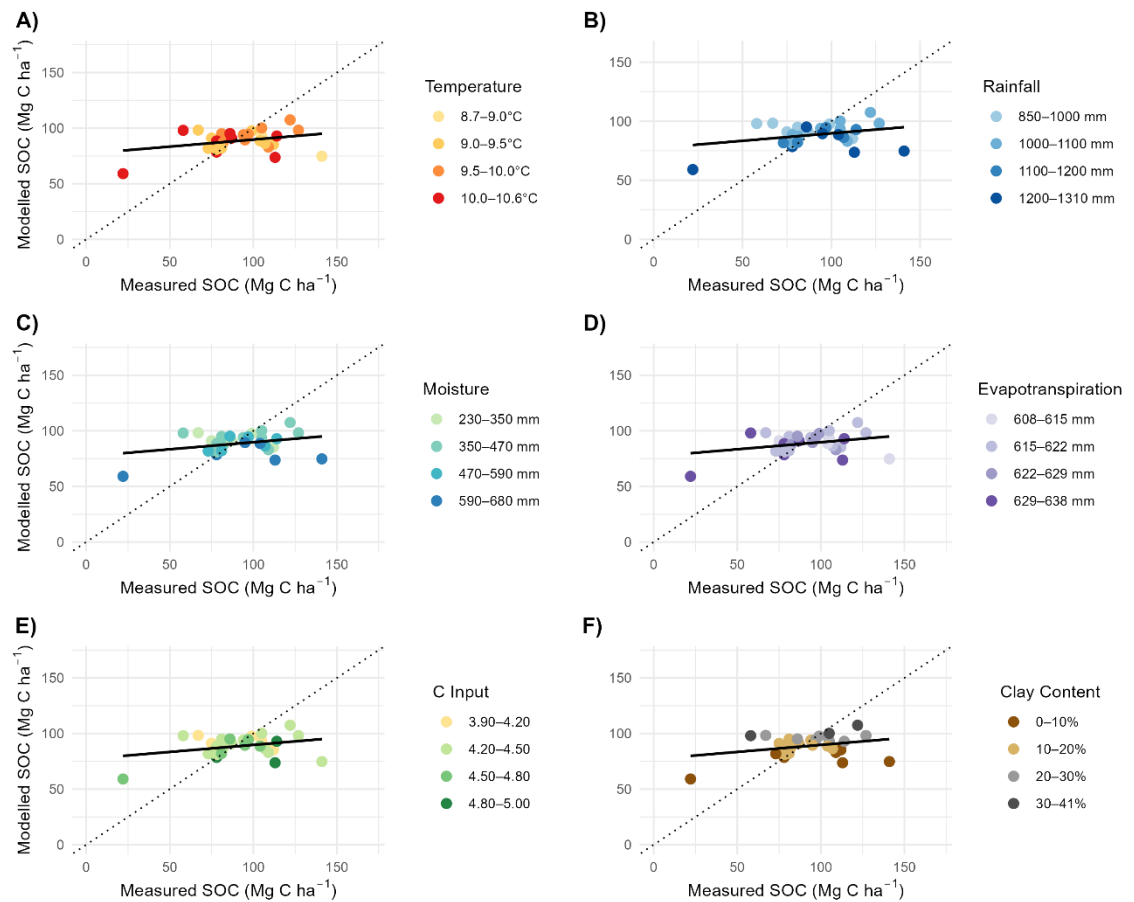
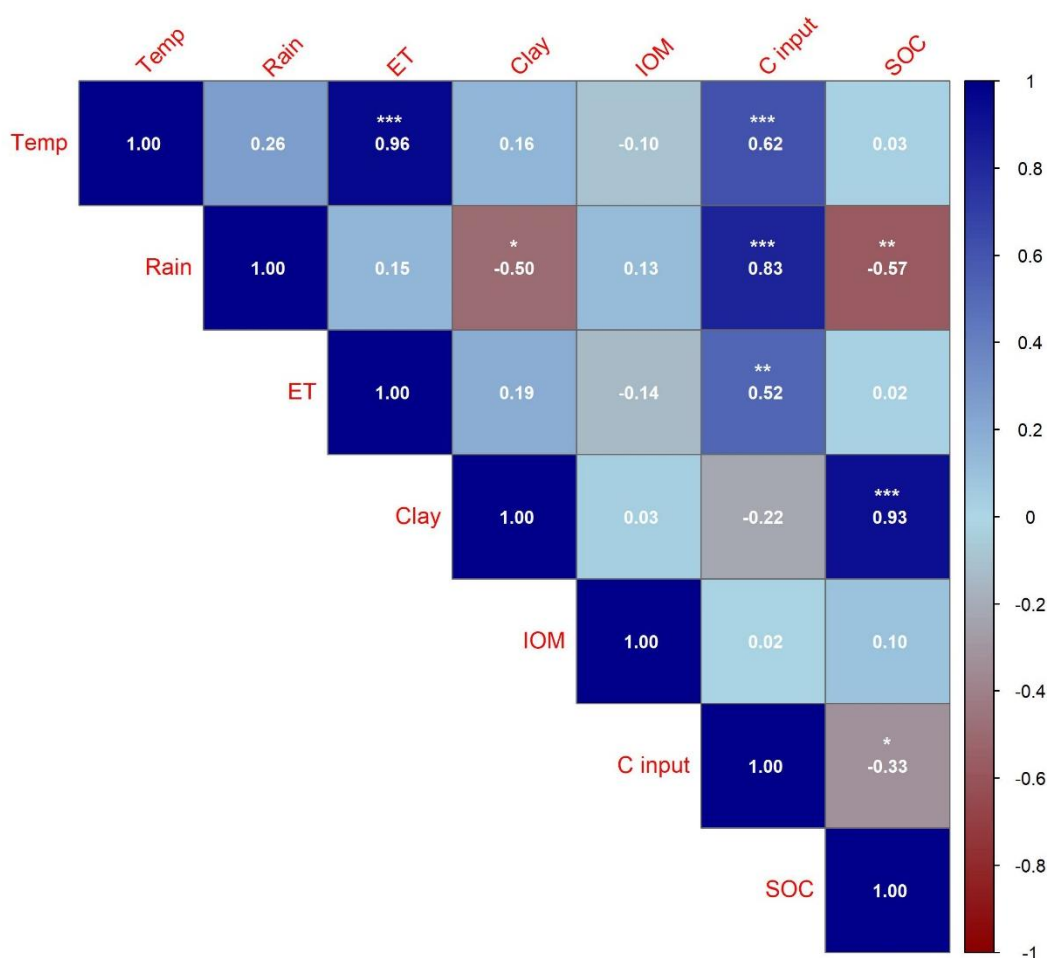


Figure 6.13 Comparison of modelled versus measured SOC stock values across the 28 SoilC grassland sites, categorised by A) average annual temperature ($^{\circ}\text{C}$), B) annual rainfall (mm), C) annual soil moisture (mm) estimated by rainfall minus evapotranspiration (ET), D) annual ET (mm), E) average annual C input (t C ha^{-1}), and F) clay content (as %). The black solid line represents the line of best fit, illustrating the overall fit of the MG model performance. The black dashed diagonal line represents the 1:1 line.

6.3.3 Environmental drivers of SOC: Modelled drivers (RothC)

The correlation analysis of the key variables driving the RothC model is presented in Table 6.5. Several significant relationships were identified, varying in strength. A strong relationship was observed between clay and SOC ($\rho = 0.93$, $p < 0.001$). Moderate to weak relationships were observed between rainfall and SOC ($\rho = -0.57$, $p < 0.01$), and C input and SOC ($\rho = -0.33$, $p < 0.05$).

Table 6.5 Spearman correlation matrix of key variables driving the SOC stock estimates of the RothC model. The colour gradient represents correlation strength, with blue indicating positive and red indicating negative correlations. Asterisks denote significance levels: $p < 0.05$ (*), $p < 0.01$ (**), and $p < 0.001$ (***). The variables are temperature (Temp, °C), rainfall (Rain, mm), evapotranspiration (ET, mm), clay (%), inert organic matter (IOM, Mg C ha⁻¹), carbon input (C input, t C ha⁻¹), and estimated soil organic carbon stock (SOC, Mg C ha⁻¹).



The primary RothC drivers, temperature, moisture, clay and C input, were further examined by plotting each variable against estimated SOC stock to aid visual interpretation, as illustrated in Figure 6.14.

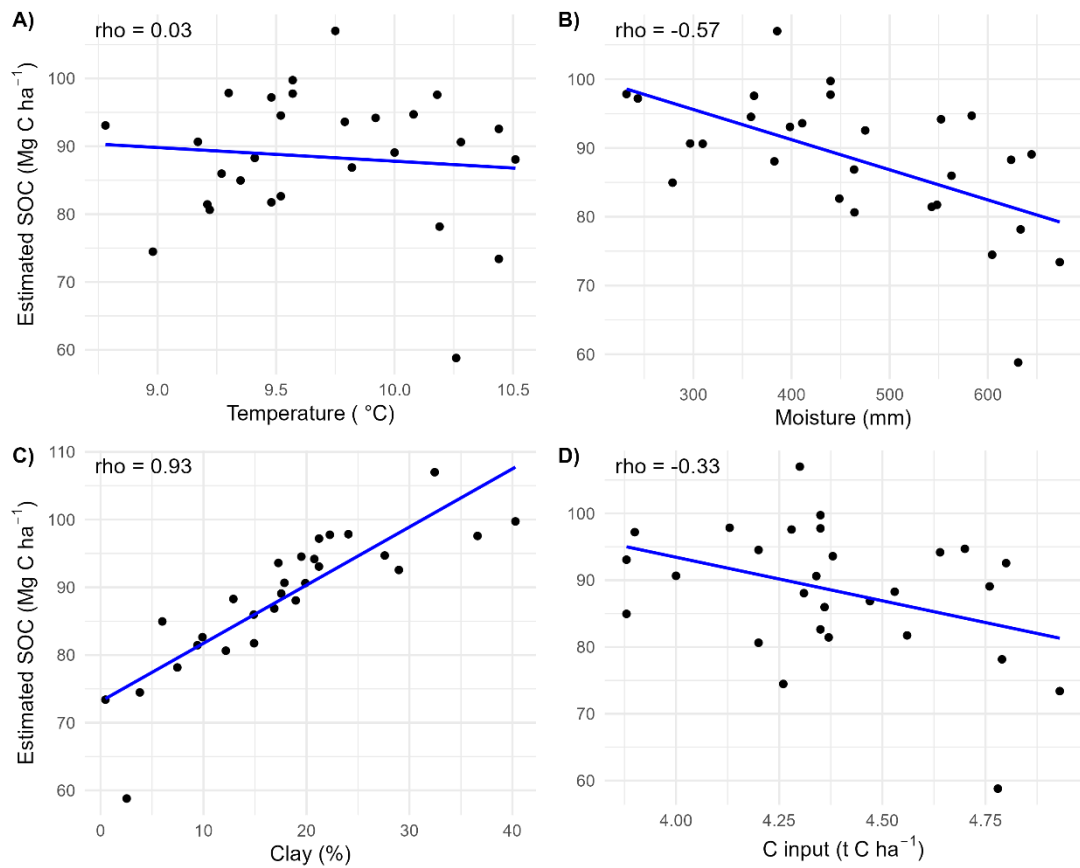


Figure 6.14 Relationship between key RothC model input variables and estimated soil organic carbon (SOC) stocks across 28 Irish mineral grassland sites. Graphs show estimated SOC stock plotted against A) Mean annual temperature; B) Mean annual moisture (rainfall minus evapotranspiration); C) clay content (%), and D) Carbon (C) input. The Spearman's rho value is located in the top left of each graph.

To further investigate the influence of clay content on the relationship between C input and estimated SOC stocks, Figure 6.15 stratifies sites into three clay content groups: low (<16%), medium (16-24%), and high (>24%). Across all clay classes, a consistent negative relationship was observed between C input and estimated SOC stocks. However, this inverse trend is likely an artefact of the MG model structure rather than a true reflection of the underlying RothC and C input relationship.

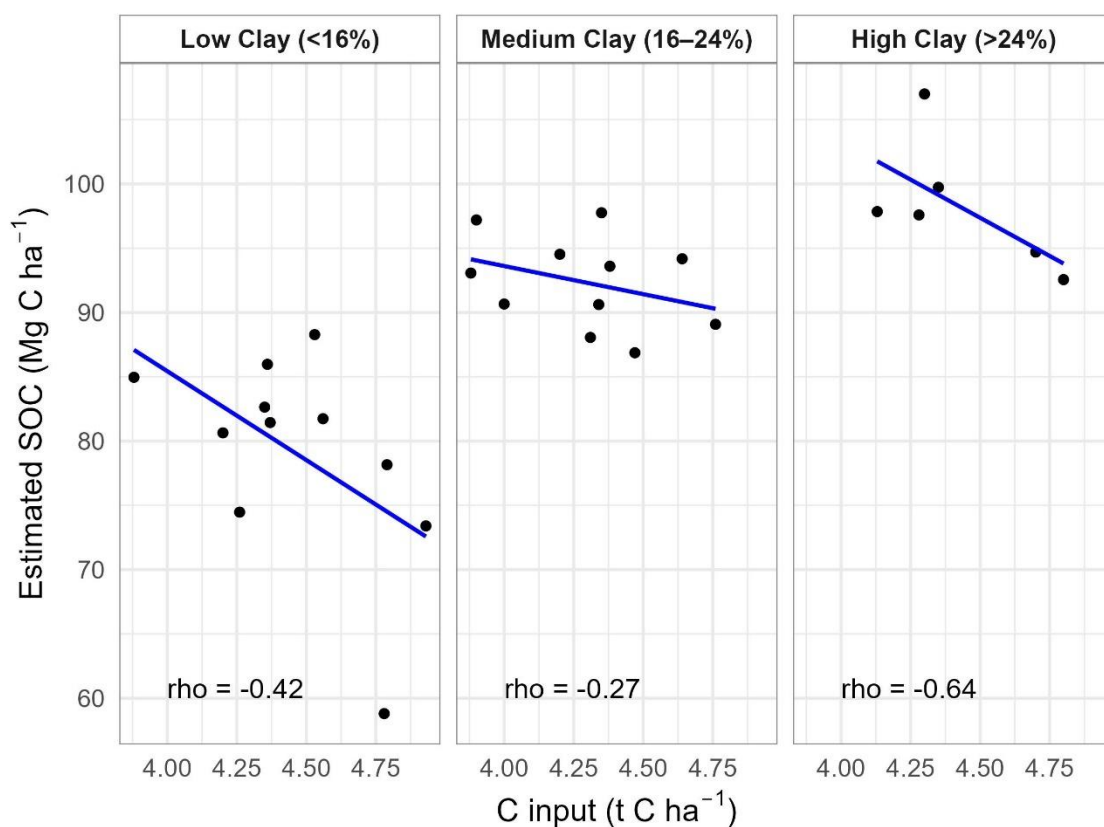


Figure 6.15 Relationship between estimated soil organic carbon (SOC) stock and carbon (C) input stratified by clay content. Sites were grouped into three clay classes: Low Clay (<16%), Medium Clay (16–24%), and High Clay (>24%). Each panel displays a linear regression fit (blue line) and the Spearman correlation coefficient (rho) between C input and estimated SOC.

6.3.4 Johnstown Castle simulation

The MG Model estimated SOC stock across the JC Dairy Enterprise to range from 75.8 to 92.4 Mg C ha⁻¹. Based on the spatial analysis, the total area of the selected paddocks was 66.86 ha, yielding a cumulative SOC stock estimate of 5929.8 Mg C ha⁻¹, with a mean value of 88.7 Mg C ha⁻¹. The variation in SOC estimates was predominantly driven by spatial differences in clay content. The estimated SOC stock for each map unit is provided in Table 6.6. The spatial distributions are outlined in Figure 6.16.

Table 6.6 Estimated soil organic carbon (SOC) stock (Mg C ha⁻¹) and corresponding area (hectares) for each soil map unit.

Map Unit	Estimated SOC stock	Number of hectares
A1	92.44	18.26
A2	92.26	17.89
A3	89.01	4.11
B1	75.82	5.87
B2	75.82	4.37
C1	86.66	9.76
C2	91.36	6.61

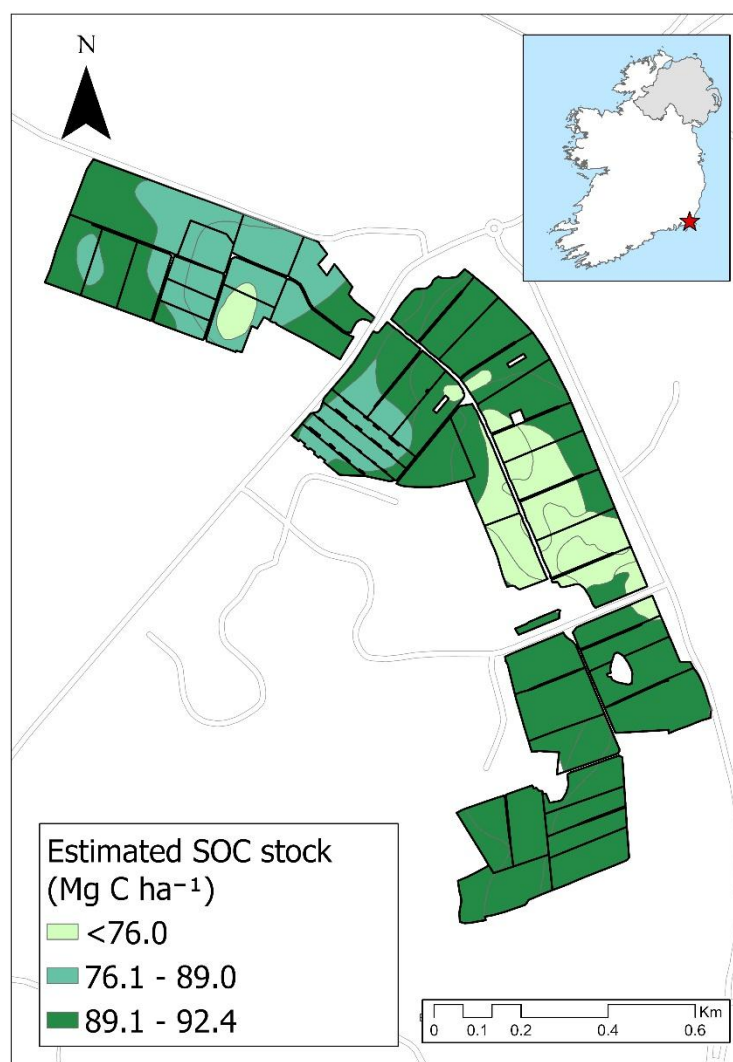


Figure 6.16 Spatial distribution of estimated soil organic carbon (SOC) stocks (Mg C ha⁻¹) across the selected paddocks at Johnstown Castle Dairy Enterprise derived from simulations using the Mineral Grassland (MG) model.

Measured SOC data were available for only two paddocks, with an average SOC stock of 118.2 Mg C ha⁻¹, and the status of the remaining paddocks is unknown. The earlier validation of the MG model indicated that it performed most reliably when simulating SOC stocks within the range of 70 to 100 Mg C ha⁻¹. Considering this, and in the absence of known SOC measurements, the SOC stock estimates of JC Dairy Enterprise from this study should be interpreted with caution. Nonetheless, the results highlight the utility of the MG model approach, providing a valuable approximation of the spatial SOC variability at the farm scale.

6.3.5 Leveraging the generalised framework

Several studies have shown that multi-model analyses can reduce uncertainty in simulated SOC stocks, suggesting that MRV systems should not rely on a single model (Batjes *et al.*, 2024). To illustrate the modularity and future-proofing of the MG framework, we incorporated an additional SOC model, the Introductory Carbon Balance Model (ICBM)

(Andrén and Kätterer, 1997; Kätterer and Andrén, 2001). This is not intended to be exhaustive but seeks to highlight the advantage of using a generalised model framework, such as SoilR. Because SoilR represents SOC models in a common mathematical structure, it can accommodate multiple model variants or even hybrid configurations. For example, SoilR includes a range of temperature and moisture modifiers (see Chapter 3, Tables 3.1 and 3.2), which can be incorporated into the MG model to create customised RothC or ICBM, or hybrid model configurations.

While there was a poor fit between measured and modelled results, indicated by the RMSE of 29.4 Mg C ha⁻¹, as illustrated in Figure 6.17, this is not unexpected. The ICBM we implemented used default values, which may not represent temperate mineral grassland sites, and we did not conduct a cross-model evaluation like the RothC to RothC_R evaluation in Chapter 4; therefore, this result should be treated with caution. However, it strengthens the potential of the overall MG model configuration as it highlights its modular capabilities and application of additional SOC models, which are both crucial to MRV systems (Batjes *et al.*, 2024; Ceschia *et al.*, 2025). The code implementation for the ICBM in the MG model is outlined in Appendix C.3.

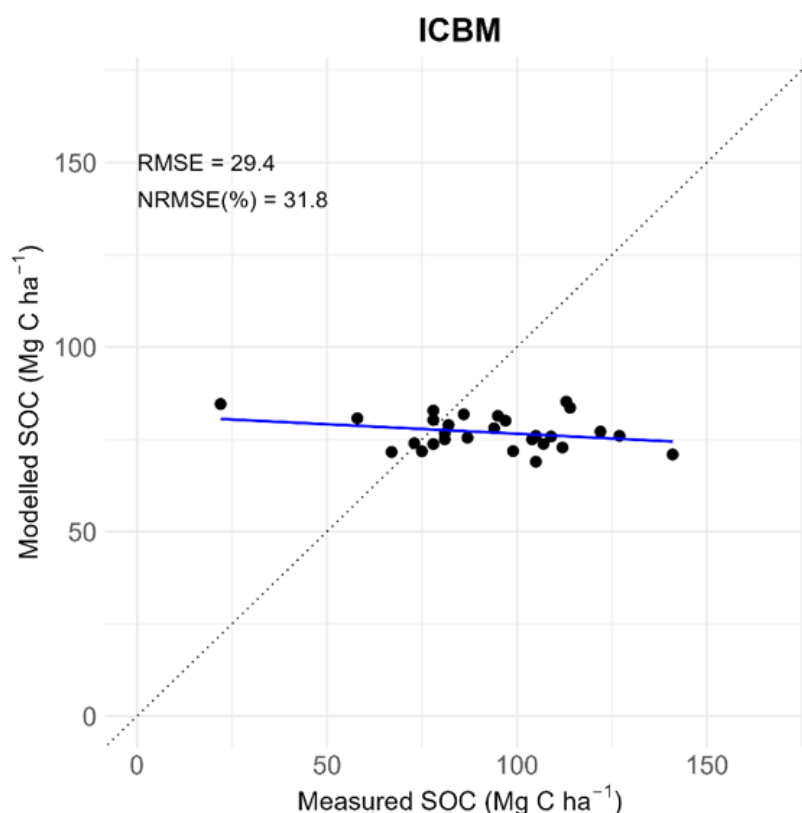


Figure 6.17 Comparison of modelled versus measured SOC stock values across the 28 SoilC grassland sites, using the Introductory Carbon Balance Model (ICBM) implemented in SoilR. The blue solid line represents the line of best fit, illustrating the overall fit of the MG model performance. The black dotted diagonal line represents the 1:1 line.

6.4 Discussion

6.4.1 Model performance

We developed a transparent and standardised model for estimating SOC stocks in Irish mineral grasslands. The MG model was designed to operate at both field and farm scales, requiring minimal data inputs, and offers flexibility for future modifications and refinements. While the model performed well or reasonably at 18 out of 28 sites evaluated, overall agreement between measured and modelled results was poor, as indicated by an RMSE of 22.7 Mg C ha⁻¹ and a NRMSE (%) of 24.5.

The MG model's performance appears dependent on the size of the initial SOC stock. The MG model performed most accurately when measured SOC stocks ranged from 73 to 105 Mg C ha⁻¹, suggesting that the current configuration may exhibit internal biases favouring sites within this range. For SOC stocks outside this range, the model agreement was consistently poor (RMSE > 20 Mg C ha⁻¹). Notably, site 485 recorded the highest modelled SOC stock at 107 Mg C ha⁻¹, which may represent the upper threshold of the MG model under the current configuration. Seven sites in the SoilC dataset had measured SOC stocks greater than 107 Mg C ha⁻¹, indicating that high SOC stock soils are likely to be underestimated under the current model configuration. Similar limitations were observed by Moll-Mielewczik *et al.* (2023), who found that RothC performance declined for several high-SOC alpine sites in Switzerland, suggesting that model calibration outside moderate SOC ranges may contribute to systematic under- or overestimation of stocks.

Similarly, the lowest modelled SOC stock was 58.8 Mg C ha⁻¹. This may indicate the lower predictive threshold, though it appears less significant, as only two sites had measured SOC stocks below this: site 68 (58 Mg C ha⁻¹) and site 879 (22 Mg C ha⁻¹), the latter of which may be considered a statistical outlier. No clear or consistent relationships were identified between model performance and spatial location, temperature, rainfall, clay content, soil moisture, and C input in this investigation.

Additionally, the MG model appears to be less accurate in soils with low clay content. Among the 28 sites analysed, the four with the lowest clay contents (≤6%, sites 126, 879, 446, and 1102) accounted for four of the ten sites exhibiting the poorest agreement between measured and modelled SOC stocks (RMSE > 20 Mg C ha⁻¹). Interestingly, three of these low-clay sites (126, 446 and 1101) also recorded relatively high measured SOC stocks (112, 113, and 141 Mg C ha⁻¹, respectively). This may suggest that RothC struggles to accurately simulate SOC stocks in clay-poor soils with high C contents. However, due to the small sample size and absence of management information, this observation requires further investigation before definite conclusions can be drawn.

Comparisons with previous studies are challenging, as this study is the first application of the RothC model across multiple Irish grassland sites at a depth of 0-25 cm. The only comparable spatial analysis of SOC stock in Irish grasslands was conducted by Saunders *et al.* (2022), who applied the ECOSSE v.6.2b model to 94 sites at a depth of 0-10 cm. They also found poor agreement between modelled and measured values, reporting an RMSE of 17.05 Mg C ha⁻¹ and a NRMSE (%) of 36.84%. Moll-Mielewczik *et al.* (2023) applied the RothC model to 24 Swiss Soil Monitoring Network grassland sites, analysing six sampling campaigns from 1985 to 2014. They found good agreement between measured and modelled SOC for two-thirds of the sites. This is consistent with our findings, where the MG model performed well at approximately 64% of the selected SoilC sites.

Both Saunders *et al.* (2022) and Moll-Mielewczik *et al.* (2023) employed more data-intensive and sophisticated methodologies than our study. For example, Saunders *et al.* (2022) derived C inputs using the land parcel identification system and simple stocking rate categories (e.g., low, medium, and high organic nitrogen rate in kg ha⁻¹ yr⁻¹). Moll-Mielewczik *et al.* (2023) calculated manure-derived C inputs using farm-reported data where available and applied regional estimates from the Swiss GHG inventory for sites lacking management information.

Despite the relative simplicity of our approach, the MG model produced results comparable to those of Saunders *et al.* (2022) and Moll-Mielewczik *et al.* (2023). This suggests that in data-constrained environments, the use of more complex models and input estimation procedures may not substantially improve SOC stock estimates. This interpretation is consistent with findings by Maas and Lal (2023), who emphasised that increasing model complexity does not inherently enhance predictive accuracy in data-limited contexts.

We evaluated the RothC model's performance against independent sites with no empirical relationship to the model's calibration dataset. Although RothC has been successfully applied worldwide, improving the model's accuracy and reliability requires optimised input parameters and regional calibration (Qingsong *et al.*, 2023). Smith *et al.* (2000) emphasised that the RothC model must be tested and, if necessary, recalibrated using data from the specific region where it is applied. For instance, Shirato and Yokozawa (2005) modified the decomposition rate constants at 0.2 and 0.6 times the values in the original RothC model for paddy soils. Similarly, Farina *et al.* (2013) adjusted the rate-modifying factor of moisture to accurately predict the dynamics of SOC in dryland regions.

To expand the model's predictive range and variability, the MG model could incorporate modifiers that better reflect SOC dynamics in Irish mineral grasslands. This includes empirical coefficients based on the C/N ratio and BD to adjust the DPM/RPM ratio and pool-specific decomposition rates, a refined RothC moisture modifier, and improved C input

estimates based on grassland management practices. These additions could enable the model to better estimate higher SOC stocks ($>107 \text{ Mg C ha}^{-1}$).

We incorporated a single generalised calibration factor into the C input model to improve the MG model's performance. Since C input estimates are one of the most influential parameters in SOC stock projections (Wiesmeier *et al.*, 2016), previous studies have incorporated C input adjustment coefficients to systematically adjust C input values into the RothC model (Peralta *et al.*, 2022). The C input derived from the Miami model of NPP initially averaged $7.2 \text{ t C ha}^{-1} \text{ yr}^{-1}$; however, using a C input adjustment coefficient of 0.72 following Peralta *et al.* (2022) methodology reduced the average C input to $4.4 \text{ t C ha}^{-1} \text{ yr}^{-1}$.

To validate our adjusted C input values, we compared them to optimised inverse modelling estimates from European grasslands. Previous studies have determined that a UK grassland requires $3 \text{ t C ha}^{-1} \text{ yr}^{-1}$ (Coleman *et al.*, 1997), Spanish grasslands require $1.32\text{-}3.96 \text{ t C ha}^{-1} \text{ yr}^{-1}$ depending on the sub-region (Doblas-Rodrigo *et al.*, 2022), and French grassland sites require $5.15 \pm 0.12 \text{ t C ha}^{-1} \text{ yr}^{-1}$ (Meermans *et al.*, 2013). Average annual grass DM production on efficient Irish farms ranges from 10 to $15 \text{ DM ha}^{-1} \text{ yr}^{-1}$ (O'Donovan *et al.*, 2022). Assuming a C content of 0.45, consistent with the Miami model conversion, this corresponds to an estimated C input range of 4.5 to $6.75 \text{ t C ha}^{-1} \text{ yr}^{-1}$. This is slightly higher than the C input range derived from the Miami model, which ranges from 3.9 to $4.9 \text{ t C ha}^{-1} \text{ yr}^{-1}$.

Nonetheless, our adjusted C input value falls within the range of previously reported C input estimates for European grasslands and aligns with the lower bound of C input estimates based on national DM production figures. Without this adjustment, the MG model would produce an RMSE of $\sim 46 \text{ Mg C ha}^{-1}$, indicating an even poorer agreement between measured and modelled measurements.

To further explore this, we calculated the required C inputs to match measured SOC stocks at the upper and lower ends of observed SOC stocks. For example, site 1102 had the highest observed SOC stock, measuring at 141 Mg C ha^{-1} . This would require $\sim 9 \text{ t C ha}^{-1} \text{ yr}^{-1}$ to achieve that observed SOC stock. Conversely, site 879 had the lowest SOC stock measurement of 22 Mg C ha^{-1} and would require $\sim 2 \text{ t C input ha}^{-1} \text{ yr}^{-1}$ to achieve that observed SOC stock. These results demonstrate that the Miami model constrains C inputs to a narrow range, which cannot reproduce the lower and higher range of measured SOC stocks.

A C input of $\sim 9 \text{ t C ha}^{-1} \text{ yr}^{-1}$ exceeds realistic values for a grassland system, as it would equate to $\sim 20 \text{ t DM ha}^{-1} \text{ yr}^{-1}$ assuming a C content of 0.45. By contrast, C input of $\sim 2 \text{ t C ha}^{-1} \text{ yr}^{-1}$ falls within the plausible range for low productivity grasslands. This suggests that discrepancies at both ends of the SOC distribution are unlikely to be resolved by C input adjustments alone,

and that refining decomposition parameters under certain conditions (e.g., management practices, soil types, or hydrological status) may provide a more realistic pathway to reproduce observed SOC stocks. These findings highlight the importance of model calibration and refinement for improving SOC stock estimation. In this study, the C input adjustment coefficient was applied as a generalised adjustment rather than a product of nationally representative data, and it substantially improved the model's performance. Ogle *et al.* (2010) highlighted that achieving higher precision in SOC stock estimates requires calibration of model parameters, improved input data quality, and broader site coverage.

Currently, Ireland lacks the comprehensive empirical datasets required to fully support calibration of the MG model and other national SOC modelling attempts. However, recent national initiatives are addressing this data gap. The Signpost Farm Programmes' deep soil sampling campaigns provide a national baseline for SOC stocks using standardised sampling methods across 67 farms, generating over 1,000 samples from 268 soil profiles (Teagasc, 2025). Furthermore, the National Agricultural Soil Carbon Observatory (NASCO) is deploying over 20 eddy covariance towers across grassland systems in Ireland to quantify verifiable rates of SOC sequestration across climatic gradients and management intensities (Haughey *et al.*, 2023). Together, these initiatives will provide critical data to facilitate soil-type and region-specific calibration of national SOC models, improving model performance and policy relevance.

6.4.2 Analysis of measured and modelled environmental drivers of SOC stocks

This study examined the relationship between measured SOC stocks and observed environmental variables, as well as the relationship between modelled SOC stocks and model inputs. The environmental data, obtained from the SoilC database, provided insight into the drivers of SOC dynamics in Irish mineral grasslands. Several observed environmental factors, such as BD, OM, %C, and C/N ratio, showed significant correlations with measured SOC stocks, consistent with findings from previous studies. In our investigation, BD exhibited a negative correlation with measured SOC stock. This is consistent with established understanding, as lower BD improves soil physical properties, such as porosity, water retention, and hydraulic conductivity, which collectively enhance conditions for SOC accumulation (Chenu *et al.*, 2000; Fukumasu *et al.*, 2022; Kätterer *et al.*, 2006; Meurer *et al.*, 2020).

A strong positive correlation was also observed between OM and measured SOC, which is expected given that SOC constitutes the measurable component of soil OM. Soil organic carbon can be estimated from OM using empirically derived conversion factors, demonstrating its intrinsic link (Pribyl, 2010). Similarly, the strong positive correlation

between %C and measured SOC stock reflects the direct role of carbon concentration in SOC stock calculation and is thus expected.

The C/N ratio, which plays a role in determining the rates of SOC decomposition and stabilisation (Blanco *et al.*, 2023; Mattila and Vihanto, 2024), ranged from 5 to 18.4 across our study site, with a median value of 8.95. Mattila and Vihanto (2024) suggest that soil with a C/N ratio near 10 provides an optimal balance for ensuring sufficient nitrogen to support microbial activity and promote C stabilisation, without accelerating decomposition. Assuming similar dynamics apply to Irish agricultural soils, this may help explain the significant positive correlation between C/N ratio and measured SOC stocks in our study. However, the broader influence of the C/N ratio on SOC dynamics remains unclear. Several studies have noted that it may not be a reliable predictor of SOC mineralisation processes (Fornara *et al.*, 2020b; Ostrowska and Porebska, 2015). While our findings suggest that the C/N ratio could influence SOC accumulation in Irish grassland soils, the mechanistic basis of this relationship remains uncertain within the scope of this investigation.

In contrast, climatic variables, spatial coordinates, elevation, soil texture, and pH did not exhibit statistically significant correlations with measured SOC stocks. On a global scale, SOC concentration often increases with higher latitudes, a pattern observed in both hemispheres and attributed to cooler climates and slower decomposition rates (Guo *et al.*, 2024). In Ireland, higher SOC stocks are typically associated with western coastal areas, corresponding to the distribution of peatlands and organic soils (Xu *et al.*, 2011b). Jobbágy and Jackson (2000) emphasised that the distribution of SOC is more strongly associated with vegetation type than with climate. In our study, the dataset was limited to mineral grasslands, which likely limited both the spatial and environmental heterogeneity. This constrained variability may explain the lack of significant dependent relationships observed in our analysis.

The relationship between observed SOC and elevation varies considerably across studies, with reports of positive, negative, or mixed correlations (Bangroo *et al.*, 2017; Leifeld *et al.*, 2005; Li *et al.*, 2024; Wu *et al.*, 2024). In certain cases, SOC concentrations increase with elevation, primarily due to cooler temperatures and higher precipitation rates, which together reduce microbial decomposition rates and favour SOC accumulation (Leifeld *et al.*, 2005; Li *et al.*, 2024; Wu *et al.*, 2024). Conversely, other studies report a decline in SOC with increasing elevation, potentially driven by greater temperature sensitivity of OM decomposition and reduced SOC stabilisation capacity (Bangroo *et al.*, 2017; Gutiérrez-Girón *et al.*, 2015). The elevation range in our study was 8-186m, which is relatively flat compared to studies such as Leifeld *et al.* (2005), where SOC increases were documented

over a 200 to 3000m gradient. This limited elevational range likely constrained our ability to detect any robust SOC-elevation relationship.

Clay content is generally considered an important stabiliser of SOC due to its role in forming organo-mineral complexes and reducing the accessibility of OM to decomposers (Wei *et al.*, 2014). Despite this theoretical expectation, empirical findings remain inconsistent. The relationships between SOC and clay have been shown to vary depending on the mass proportion of clay particles, the type of clay mineral, climate, land use, management practices, and the chemical characteristics of soil OM (Matus, 2021; Schapel *et al.*, 2018). For instance, Wang *et al.* (2013) found no regional differences in the effect of soil texture on SOC content using 900 soil profiles obtained from the Second National Soil Survey of China. Similarly, Zhong *et al.* (2018) found that SOC dynamics in Chinese forest soils were more influenced by vegetation and nutrient status than by clay content. In contrast, Schapel *et al.* (2018) found a positive correlation between SOC and clay content, explaining 46% of the variation for arable sandy soils in South Australia.

In our study, we observed no statistically significant relationship between clay content and measured SOC stocks, suggesting that soil texture alone is not a dominant control on SOC dynamics in Irish mineral grasslands. Similarly, Torres-Sallan *et al.* (2017) found the total quantity of SOC stocks was similar among typical brown earths, luvisols and surface-water gleys across 31 temperate Irish grassland sites. However, other authors have indicated that the relationship between clay content and SOC is not always straightforward. For instance, Torres-Sallan *et al.* (2017) argue that while total SOC stocks may appear similar across soils with varying clay contents, the key distinction lies in the distribution of C across aggregate size fractions, which ultimately reflects differences in SOC stability. Their findings highlight that subsoil layers below 30cm, particularly in clay-illuviated Irish grassland soils, store the most stable forms of C and represent valuable long-term sinks for SOC sequestration.

Similarly, Johannes *et al.* (2017) demonstrated that the SOC:clay ratio declines with decreasing soil structural quality. Their findings suggest that a SOC:clay ratio of approximately 1:8 is indicative of optimal structural conditions, whereas a ratio of 1:13 reflects poor structural integrity. Strong soil structure facilitates both the physical protection of organic matter within aggregates and the regulation of water and air flow, which are essential for microbial activity and plant productivity. As such, robust soil structure is a critical factor in promoting the accumulation and long-term stabilisation of SOC (Bondi, n.d).

The role of soil pH in SOC stabilisation remains complex and context-dependent. Kuśmier *et al.* (2023) found the highest SOC stocks in Polish arable soils under slightly acidic to neutral

conditions and alkaline conditions (pH 6.5-7.2 and >7.2), suggesting that neutral to elevated pH levels may favour SOC preservation. In contrast, Kögel-Knabner (2021) argued that alkaline soils are more prone to SOC losses than acidic ones due to reduced soil organic matter complexation on mineral surfaces via ligand exchange. Liao *et al.* (2016), in a study of nearly 26,000 topsoil samples across Jiangsu Province, China, reported both negative and positive influences on SOC content. SOC increased with pH from 4.2 to 6.5 but declined between 6.5 and 9.2.

In Ireland, Teagasc (2020) recommends an optimum pH of ≥ 6.3 for productive grasslands, as values ranging from 6.0-7.2 improve nitrogen cycling and reduce fertiliser requirements. In our analysis, grassland sites exhibited a pH range of 5.0 to 7.5, with an average of 6.1, indicating predominantly acidic conditions. The observed low pH values could reflect soil acidification, which is common in high rainfall regions and often exacerbated by the intensive application of nitrogenous fertilisers (Teagasc, 2020). However, in the absence of site-specific land-use and management data, it is not possible to determine whether management practices are the primary drivers of soil acidity in these sites.

The relationships between the RothC_R model inputs and modelled SOC stock revealed several notable differences from both the measured SOC correlations and the outcomes of the sensitivity analysis presented in Chapter 5. Most prominently, modelled SOC stock exhibited a strong positive correlation with clay content (Spearman $\rho=0.87$, $p < 0.001$), suggesting clay as the principal driver of SOC variation in this investigation. This is unexpected, as the one-at-a-time (OAT) sensitivity analysis in Section 5.3.1 reported a low sensitivity index for clay (<0.2 , with 0 indicating no effect), indicating limited influence of this parameter on the RothC_R outputs under controlled perturbations.

This apparent contradiction likely reflects the constrained variability of other model inputs within the current MG model configuration. Given the relatively homogeneous climatic conditions and, by extension, C input estimates, clay content emerged as the dominant source of input variation within the current configuration of the MG model. This finding is potentially problematic, as the relationship between clay and SOC is known to be highly context-dependent and inconsistent across ecosystems (Schapel *et al.*, 2018; Wang *et al.*, 2013; Zhong *et al.*, 2018). Furthermore, clay content showed no correlation with the measured SOC stock in Irish mineral grasslands, which may indicate an overall reliance on this parameter.

Another unexpected result was the negative correlation between estimated C input and modelled SOC stock (Spearman $\rho = -0.33$, $p < 0.05$). This finding is not consistent with theoretical expectations. It also contrasts the observation findings from the OAT C input sensitivity analysis in Section 5.3.1, which showed that increasing C input consistently

increased modelled SOC stocks. The inverse correlation is likely an artefact of both the narrow range in estimated C input values (3.9-4.9 t C ha⁻¹) and the dominance of clay content as a driver of SOC variability under the current modelling configuration, rather than a reflection of the true mechanistic relationship between C input and SOC stock.

These findings highlight that correlations between model inputs and outputs can be misleading in contexts where input variability is limited. When key parameters do not exhibit sufficient variation across sites, the current MG model configuration may incorrectly attribute differences in SOC stock to insensitive parameters. This highlights the need for model calibration and evaluation against datasets that span a broad range of environmental conditions. Without such variability, the inferred relationships from model outputs may not reflect the true biophysical drivers of SOC dynamics.

In contrast, one consistent finding between Chapters 5 and 6 is the negative correlation between rainfall and modelled SOC stock. This study found a statistically significant negative correlation (Spearman rho=-0.57, $p < 0.05$) between annual rainfall and modelled SOC stocks. This is consistent with the OAT sensitivity analysis in Chapter 5, where a 15% increase in rainfall resulted in a 5.73% decrease in modelled SOC stocks. However, the modelled relationship was not supported by the measured SOC stock, which exhibited no statistically significant correlation with rainfall. While annual rainfall values in this study are derived from national gridded datasets, which may not fully capture localised site conditions, the absence of empirical rainfall records limits any definitive evaluation of site-level accuracy.

This discrepancy suggests that the RothC model may overestimate the influence of rainfall in driving SOC dynamics compared to empirical observations from mineral grasslands. This overemphasis may partially be explained by the RothC moisture modifier, which regulates decomposition based on soil moisture conditions. The RothC moisture modifier has been known to perform poorly under both very dry and saturated conditions (Farina *et al.*, 2013; Jebari *et al.*, 2021). Therefore, this consistent negative correlation between rainfall and modelled SOC stocks observed across multiple simulations may be an artefact of this limitation, rather than a representation of actual biophysical processes in Irish mineral grasslands.

Of the environmental variables that showed a significant relationship with measured SOC stocks (e.g., bulk density, C/N ratio, %C, and OM), none are explicitly represented in the default RothC model or our configuration of the RothC_R model within the MG model. Organic matter and %C can be excluded from further discussion, as their strong correlation with SOC stock reflects their intrinsic relationship.

Bulk density is required to calculate the known SOC stock used to estimate the IOM pool size; however, the IOM pool is inert and not subjected to decomposition. Consequently, BD is not explicitly represented as a dynamic variable in the RothC model. However, in our study, BD had a negative relationship with measured SOC stocks, likely due to denser soils having suboptimal porosity and soil structure, or a higher susceptibility to physical disturbances such as poaching. These effects could be incorporated into the MG model by adjusting the pool-specific decomposition by a coefficient derived from empirical observations. For example, in sites with lower BD values, decomposition rates could be reduced, allowing for greater SOC accumulation and thus higher SOC stock estimates.

The C/N ratio influences SOC decomposition rates and stabilisation (Blanco *et al.*, 2023; Mattila and Vihanto, 2024). In our study, the C/N ratio exhibited a moderate positive correlation with measured SOC stocks, suggesting its potential importance as a driver of SOC accumulation in Irish mineral grasslands. In the RothC model, and our MG model, the DPM/RPM ratio determines how incoming plant material is partitioned into fast- and slow-decomposing pools, thereby influencing the proportion of organic C that is rapidly decomposed versus stabilised. Our current configuration utilises the default DPM/RPM ratio of 1.44, which is recommended for improved agricultural land (Coleman *et al.*, 2024).

Incorporating C/N ratio-derived coefficients to modify the MG model DPM/RPM ratio could result in higher accuracy. For example, at sites with a high C/N ratio, the DPM/RPM ratio could be reduced, allowing more incoming C to be partitioned into the resistant C pool, which has slower decomposition rates and enables greater SOC accumulation. Conversely, at a site with a lower C/N ratio, a higher DPM/RPM ratio could be applied to reflect rapid decomposition and reduced SOC accumulation.

6.4.3 Farm-scale SOC estimates

Farm-scale estimates for SOC dynamics have been identified as a potential way to provide more accurate emissions and removals estimates for agricultural lands (Bolinder *et al.*, 2007). The MG Model successfully demonstrated its capability to generate farm-scale SOC stock estimates for the JC Dairy Enterprise, despite known limitations in model accuracy. Finer granularity represents a significant advantage over traditional spatial modelling approaches, which typically provide a single SOC estimate per coarse-resolution grid cell (e.g., 1 km² or 5 km²). In the Irish context, applying these traditional methods would result in a single SOC value representing an area equivalent to approximately 3 to 15 average-sized farms, thereby obscuring important within-farm variability.

The availability of SOC measurements and input data for combinations of plant, environment and management is a major limiting factor for farm-scale estimates (Palosuo *et al.*, 2025). The farm-scale SOC stock estimates for the JC Dairy enterprise research centre

were only viable due to previous soil campaigns and soil texture shapefiles, but lack reliable SOC stock measurements to validate or verify our modelling efforts. Furthermore, JC Dairy Enterprise has detailed management data, which we were unable to utilise due to our relatively simple C input model.

It is important to note that our approach represents an initial prototype of a generic model designed for farm-scale SOC estimation across sites. Research farms and commercial operations that use grassland management decision-support tools such as PastureBase Ireland (Hanrahan *et al.*, 2017) and Agrinet (Agrinet Systems Ltd, 2025) typically possess extensive, high-quality datasets that could be leveraged to enhance model parameterisation and performance. However, applying this approach to commercial farms lacking such detailed management information remains challenging. Improved estimation of carbon inputs that better capture management variability, along with additional calibration of coefficients within the MG model, will be essential to ensure accurate SOC predictions and prevent misrepresentation of SOC stocks. Collectively, these refinements will strengthen the model's performance and applicability across different data environments.

6.4.4 Limitations and recommendations

The two primary limitations of our study are the lack of temporal SOC data and the generic parameterisation of the MG model. The lack of temporal SOC data is a persistent issue in many SOC modelling efforts in Ireland. Several studies have cited data availability as a significant obstacle to model input estimates and validation (Dondini *et al.*, 2009; Khalil, 2014; van Groenigen *et al.*, 2011; Saunders *et al.*, 2020). As a result, most modelling studies in Ireland rely on a single SOC measurement, with only a few incorporating two SOC measurements taken at different times.

A single SOC observation significantly increases uncertainty in model validation. For example, site 879 had a measured SOC stock of 22.1 Mg C ha⁻¹, a relatively low SOC stock value compared to the other sites. However, because only a single sample was available, we cannot assess whether this value is representative of long-term site conditions. Regular decadal resampling would enable the detection of long-term trends in SOC stocks (Harbo *et al.*, 2025), and consistent values would enhance the observer's confidence in the measurement. Conversely, significant deviations could indicate that the initial sample was affected by sampling errors or short-term environmental or management variability.

A second major limitation is the generic or default parameterisation of the MG model. In particular, the C input estimation method is very generic and may benefit immensely from further refinements. The current configuration of the Miami model of NPP used to estimate C inputs relies solely on climatic variables, thereby ignoring the impact of management. Grassland sites can have vastly different management systems, including sward

composition, stocking rates, grazing rotations, and fertilisation regimes, but our current modelling methodology does not reflect these factors. However, the impacts of management on SOC stock dynamics remain inconsistent, with different practices often exhibiting mixed results in grasslands (Abdalla *et al.*, 2018; Fornara *et al.*, 2020b; Meng *et al.*, 2022).

In its current configuration, the MG model estimated the upper limit of $\sim 107 \text{ Mg C ha}^{-1}$ for SOC stocks, whereas the highest measured SOC stock was $141.4 \text{ Mg C ha}^{-1}$. This discrepancy highlights the need for further refinement of the model to better capture higher SOC stock potentials. One promising approach is to adjust the C input value based on management. For instance, O'Donovan *et al.* (2022) reported elevated DM production rates on efficient dairy and dry stock farms, which may translate into increased C inputs. Similarly, Byrne and Kiely (2009) applied inverse modelling with the RothC model and estimated C inputs of $8.40 \text{ t C ha}^{-1} \text{ yr}^{-1}$ and $5.37 \text{ t C ha}^{-1} \text{ yr}^{-1}$ to achieve a SOC stock of $136.31 \text{ Mg C ha}^{-1}$ and $78.82 \text{ Mg C ha}^{-1}$ (0-20cm depth) for research farms located in Cork and Wexford, respectively. These results suggest that the current C input range derived from the Miami model may be too constrained and should be broadened to better reflect more grassland conditions, especially for more productive farm systems.

We propose that an empirically derived approach to adjusting C inputs is the most appropriate, considering the limitations on available management data and the inherent site-specific relationship between management practices and the local environmental conditions. For example, the C inputs could be adjusted using the following formulation:

$$C \text{ input} = C_{\text{Miami input}} \times C_{LU} \times C_S \times C_M \quad (6.3)$$

Where, $C_{\text{Miami input}}$ is the baseline C input estimated by the Miami model, adjusted by a land-use coefficient (C_{LU}), soil type coefficient (C_S), and management coefficient (C_M). This adjustment approach is consistent with the IPCC's (2006; 2019) tier 1 and 2 methodologies and allows for greater variability in the MG model predictions by incorporating site-level heterogeneity. Coefficient values could be derived from national or regional data sources, such as those generated by the NASCO and the Signpost Farms deep soil sampling campaigns (Haughey *et al.*, 2023; Teagasc, 2025). These initiatives will provide spatially and temporally resolved baseline SOC stocks and associated drivers, supporting the development of region- and management-specific model calibrations. Such calibration would enhance the capacity of SOC models to simulate SOC dynamics under diverse pedoclimatic and management conditions.

The future of spatial SOC modelling will continue to be constrained unless three critical components, namely SOC database development, improved C input modelling, and refined modelling configuration (e.g., incorporating additional modifiers for BD and C/N ratios to

improve model performance), are integrated into a unified approach, as seen in Figure 6.18. Our research primarily focused on developing a general SOC model. Still, future improvements will require a comprehensive temporal SOC database and more advanced C input estimates that capture the full range of management variability within Irish grasslands. Strengthening these components will enhance the accuracy and reliability of SOC stock estimates at both the farm and national scale.

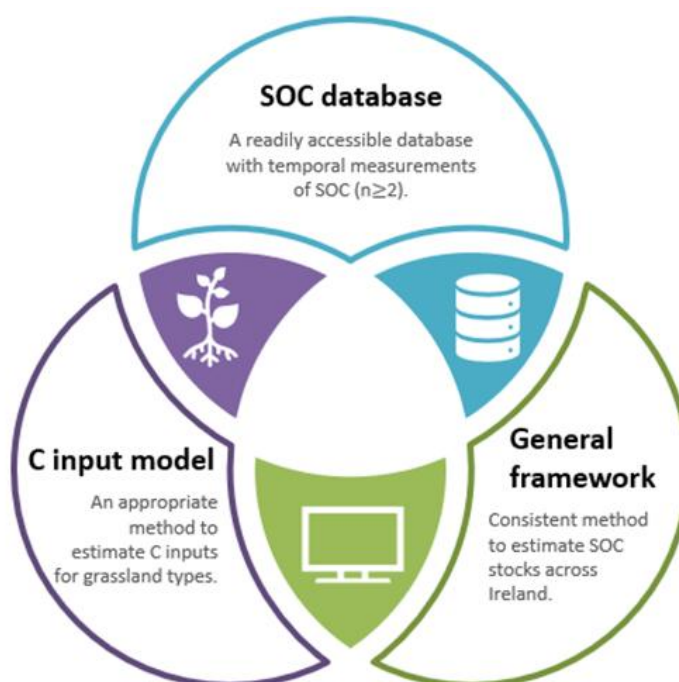


Figure 6.18 Venn diagram illustrating the three key components required for accurate and reliable estimation of soil organic carbon (SOC) stocks: i) a temporal SOC database with repeated SOC measurements, ii) a robust carbon (C) input model suitable for grassland systems, and iii) a consistent general model for spatial SOC stock estimation across Ireland.

6.5 Conclusions

This study presents the first spatial application of the RothC model to estimate SOC stocks in Irish mineral grasslands. We developed a generic and standardised model (MG model) capable of generating SOC stock estimates across diverse sites with minimal input requirements. This design facilitates consistent comparison and applicability in data-limited environments. The MG model performed well at 18 of the 28 evaluated sites; however, overall model agreement was poor, with an RMSE of 22.7 Mg C ha⁻¹ and a NRMSE of 24.5%. Model performance was best at sites with initial SOC stocks between 73–105 Mg C ha⁻¹ but declined noticeably outside this range. Other site variables, including mean annual temperature, annual rainfall, annual soil moisture, clay content and C input estimates, did not exhibit a consistent or predictive relationship with model performance, suggesting that SOC stock magnitude remains the primary determinant of modelling accuracy under the current MG configuration.

C input estimates derived from the Miami-based approach proved problematic: values were too high for low-productivity grasslands, while reproducing the upper observed SOC stocks would require unrealistic dry matter yields. Addressing this limitation will require both the refinement of C input estimates (e.g., through additional coefficients or site-specific adjustments) and the modification of decomposition rates to reflect management practices or soil types. Bulk density and C/N ratio were significantly correlated with measured SOC stocks, but are not explicitly represented in the RothC_R model. Incorporating empirical modifiers based on these variables could enhance predictive accuracy across a wider range of conditions.

Despite these limitations, the MG model shows significant value as a flexible and adaptable framework for estimating SOC stocks at the farm level. One of the key strengths of this study is the use of a generalised modelling framework, implemented in SoilR, which allows for transparent model development and easier code modifications. This flexibility supports the integration of alternative SOC models or input methodologies, enabling intercomparison and multi-model ensemble analyses, where different model structures can be tested and evaluated side by side. These features are vital for MRV systems, where transparency, reproducibility, and performance verification are critical. In summary, this work provides a foundation for ongoing methodological refinement and regional calibration of SOC models. It highlights the importance of generalised modelling approaches in enhancing the accuracy and comparability of SOC assessments.

Chapter 7: Discussion

7.1 Introduction

This chapter synthesises the research outcomes into a broader discussion. The purpose is to assess the overall contribution of the thesis by integrating the key findings, considering their broader implications, and positioning them within the context of SOC modelling. Specifically, this chapter will:

- i. Evaluate the extent to which Tier 3 methodologies, under their current configuration and requirements, can be considered viable to meet the needs of policy,
- ii. Highlight the key findings, the synergies between the research chapters, and their collective advancement of knowledge in this field of research,
- iii. Identify potential fundamental limitations that arise from reliance on a single SOC model as the basis for national modelling frameworks,
- iv. Identify limitations within the current research,
- v. Outline future advancements required for the refinement of a Tier 3 modelling approach for Irish mineral grasslands; and,
- vi. Provide recommendations to policymakers.

7.2 Performance of process-based (Tier 3) SOC models'

There is increasing pressure from policy makers to transition towards Tier 3 methodologies for national emission reporting, particularly under regulatory frameworks such as the Carbon Removal and Carbon Farming Certification (CRCF) Regulation (EU 2024/3012) and the LULUCF Regulation (EU 2023/839). For example, the CRCF Regulation mandates that carbon farming quantification must follow either a measure-remeasure or a measure-model approach, with Tier 3 models encouraged as best practice. This evolving regulatory landscape makes the question of the feasibility of advanced SOC modelling approaches directly relevant to all EU member states.

However, the viability of Tier 3 approaches remains uncertain, particularly when compared with the practicality and performance of existing Tier 1 and Tier 2 methods. Several recent studies have attempted to evaluate the comparative performance of models across the IPCC tiers, with mixed outcomes regarding whether higher-tiered models consistently outperform simpler approaches (e.g., Del Grosso *et al.*, 2016; Obi-Njoku *et al.*, 2024; Peter *et al.*, 2016; Vázquez-Amábile *et al.*, 2025).

Del Grosso *et al.* (2016) compared process-based models (CQESTER and DayCent) with the IPCC Tier 1 model to estimate SOC changes under varying tillage and nitrogen fertiliser

treatments in Oregon and Colorado. In Oregon, all three models correctly identified the direction of change in SOC as losses, but the Tier 1 method substantially underpredicted their magnitude. In Colorado, all models underestimated the SOC losses, though the Tier 3 models outperformed the Tier 1 approach, producing more realistic SOC changes as indicated by stronger agreement with the observations.

Similarly, Peter *et al.* (2016) evaluated GHG emissions associated with two wheat cropping systems in Germany and two peach orchards in Italy. While the Tier 2 methods were applied for N₂O emissions, both Tier 1 and Tier 3 methods were used to estimate SOC stock changes. The study revealed that Tier 1 estimates overestimated SOC stock changes in annual crops (up to +90%) and underestimated emissions in perennial systems (by as much as -75%) compared to Tier 3 model outputs (RothC) and field measurements. The authors concluded that the higher-tiered methods should be strongly recommended for land-based emission accounting due to their improved ability to capture system-specific dynamics.

Vázquez-Amábile *et al.* (2025) compared a Tier 2 model, the Steady-State Method (SSM), against two Tier 3 models, the Agricultural Model for Greenhouse gases (AMG) and RothC, using experimental data from two sites in the Pampean Region of Argentina. All models were consistent in their predictions, with agreement on the direction of change in SOC stocks (e.g., SOC decreased under full tillage and increased under pasture or no-till systems), even if the magnitude of change varied. However, the Tier 2 model outperformed both Tier 3 models in quantitative accuracy, likely due to better alignment with regional conditions and more appropriate calibration.

In a similar study focused on N₂O emissions rather than SOC dynamics, Obi-Njoku *et al.* (2024) compared Tier 1, 2, and 3 methodologies for estimating emissions from soils amended with biosolids. The study analysed data from eight experimental plots across three ecozones in Quebec, Nova Scotia, and Alberta in Canada. The authors reported that the Tier 3 model, the Denitrification Decomposition Model (DNDC), provided the most accurate estimates, showing the closest agreement with measured N₂O fluxes. This was followed by a modified Tier 2 approach that included regionally calibrated correction factors, the standard Tier 2 methodology, and the Tier 1 method, which performed the poorest. These findings reinforce the broader conclusions that higher-tier models outperform the simple empirical approach of Tier 1 methods, likely attributable to the inclusion of site-specific information in Tier 3 models.

These studies collectively highlight the well-known limitation of Tier 1 methodologies, their limited responsiveness to local variations in soil, climate, and management practices (IPCC, 2006; 2019). As noted by Peter *et al.* (2016), this can lead to misleading results due to oversimplified interpretations of C input factors and the omission of local pedo-climate

influence. However, direct comparison between Tier 1 and Tier 3 models may not be entirely fair; Tier 1 methods were never designed for field-scale applications, and their underperformance in such contexts is expected (Del Grosso *et al.*, 2016). Recognising these constraints, recent comparative studies have tended to only focus on comparing Tier 2 and Tier 3 methodologies (e.g., Vázquez-Amábile *et al.*, 2025).

Notwithstanding concerns about fairness, it is crucial to compare the outcomes of Tier 1 and Tier 2 methods at finer scales, even if this only reveals their limitations. Without testing, it is impossible to determine whether Tier 1 approaches consistently perform poorly or if, in some circumstances, they can produce acceptable estimates or results. Additionally, investigating Tier 1 approaches helps justify the use of higher-tier methods, thereby reinforcing the case for further research and investment in advanced modelling. In principle, the simplest method that yields satisfactory results should be prioritised, especially in data-limited environments, regardless of tier level.

Tier 3 methods rely on computationally complex models to simulate SOC dynamics, often based on sparse datasets, to improve SOC stock estimates (Davoudabadi *et al.*, 2024). While these models offer higher resolution of SOC stock estimates at finer scales, many datasets cannot support this level of fine resolution. For instance, Vázquez-Amábile *et al.* (2025) argue that Tier 2 approaches may be more appropriate for regional- and national-scale SOC stock inventories, especially when well-calibrated with regional datasets. This raises an important methodological question: is the current requirement for Tier 3 implementation fully justified, or should greater emphasis be placed on improving Tier 2 frameworks to ensure comparability, accuracy, consistency and practical viability? If the overarching goal is to improve the accuracy of SOC stock reporting, there may be a flawed assumption underpinning current policy direction, primarily based on the assumption that complexity automatically leads to more accurate estimates.

In many scenarios, higher-tiered or more complex methods can improve estimates (e.g., Del Grosso *et al.*, 2016; Obi-Njoku *et al.*, 2024; Peter *et al.*, 2016). In contrast, numerous authors have found counterintuitive results (e.g., Davoudabadi *et al.*, 2024; Jebari *et al.*, 2021; Maas and Lal, 2023; Vázquez-Amábile *et al.*, 2025). For example, Davoudabadi *et al.* (2024) demonstrated that a simplified three-pool RothC model, embedded within a Bayesian state-space framework, outperformed the standard five-pool RothC model for two Australian datasets, which consist of a wheat rotation experiment at Tarlee and a semi-arid Brigalow site in Queensland, including continuous cropping, pasture, and native forest systems. Their work illustrates that reduced model complexity, when appropriately structured, can yield greater predictive accuracy. Similarly, Vázquez-Amábile *et al.* (2025) found that a Tier 2 SSM model provided more accurate SOC estimates than two Tier 3 models (AMG and RothC).

across multiple Argentinian cropping systems. In this context, model structure and calibration outweighed model complexity.

Further evidence comes from intra-comparison of SOC model configurations, showing that increasing complexity can sometimes decrease accuracy. For example, Maas and Lal (2023) reported that simpler ET model inputs for the RothC model can improve model performance compared to more complex alternatives, aligning with findings from Chapter 5 (see Section 5.4.3). Similarly, Jebari *et al.* (2021) found that a RothC configuration with three extra sub-model modifications outperformed one with four sub-models, even though the latter was more complex. These results highlight that model performance often depends more on the quality and availability of input data and the model structure rather than complexity alone. However, a common reason for poor performance in more complex models is their higher data requirements. A complex model with all inputs and parameters correctly adjusted using sufficient, site-specific data will almost always perform better. Nonetheless, in many situations, these model inputs and parameters are unavailable.

These studies emphasise that the principal challenge in SOC modelling is not the complexity itself, but in the data-scarce environments in which such models are frequently applied. This adds further uncertainty to the broader question of Tier 3 feasibility. Addressing this issue requires a twofold approach. First, instead of focusing on modelling tiers, a more practical approach involves aiming for the desired accuracy, regardless of whether the method is formally Tier 2 or Tier 3. Second, there is a crucial need for enhanced data collection, including repeated soil surveys and carbon measurements, to build reliable databases that can inform SOC models and increase confidence in their predictions.

It is also important to acknowledge that the feasibility of Tier 3 implementation depends not just on scientific accuracy but also on the administrative and operational costs of MRV frameworks. The resources needed for high-resolution data collection, model parameterisation, and managing national databases can be considerable. Although these factors are outside the scope of this study, they are crucial in determining the scalability and sustainability of Tier 3 SOC modelling frameworks.

In the Irish context, current national reporting for mineral grasslands relies on Tier 1 methods, which apply fixed SOC stock change factors with no regional differentiation. While comparison between our MG model (Tier 3 prototype) and Tier 1 estimates might appear as an attractive case study, it is premature, as such an exercise would be methodologically insufficient for three key reasons:

1. The MG model remains a working prototype, with current limitations on its configuration (e.g., limited output range, varying from 73 to 105 Mg C ha⁻¹). There

are known weaknesses of the model that should be addressed before evaluation against the current approach.

2. Comparing Tier 1 outputs with site-specific Tier 3 SOC model simulations introduces a scale mismatch. A fairer comparison would require aggregating the Tier 3 outputs to a spatial resolution consistent with Tier 1 reporting.
3. Inconsistent sampling depth, the SoilC dataset was harmonised to the 0-25cm depth interval using a mass-weighted averaging approach, where Tier 1 methodology is defined for 0-30cm. This mismatch in depth would need to be resolved to ensure a fair comparison of SOC stock estimates.

7.3 Key findings, synergies and contribution to knowledge

As SOC cannot be measured everywhere, models are essential to provide estimates where observations are absent (Smith *et al.*, 2020). While the development of finer-scale Tier 3 modelling approaches at the European level remains a priority, SOC modelling faces a broader global challenge related to consistency and data availability. Most SOC models share a broadly similar structure (e.g., pool-based decomposition models with environmental modifiers) (McGill, 1996; Senapati *et al.*, 2014; Sierra *et al.*, 2012), but they often produce divergent SOC stock estimates (e.g., Palosuo *et al.*, 2012; Riggers *et al.*, 2019; Smith *et al.*, 1997). These differences stem from a combination of factors, including variations in pool definitions, underlying assumptions, parameterisation, environmental modifiers, and the long-term experimental sites used to derive model structures and decomposition rates (Falloon and Smith, 2002; LeNoë *et al.*, 2023; Maas and Lal, 2023). Furthermore, many SOC models are hard-coded in specific programming languages, which prevents intercomparison studies and hinders their flexibility (Sierra *et al.*, 2012). This thesis contributed to this broader issue through four supporting objectives:

- **Transition towards a general modelling framework.** Chapter 3 offered a methodological investigation of the diversity of SOC models and highlighted the challenges involved in comparing models that vary in structure, complexity, and conceptual assumptions (LeNoë *et al.*, 2023; Parton, 1996b; Smith *et al.*, 1997). However, many of these models share similar elements but are represented differently (Campbell and Paustian, 2015; Senapati *et al.*, 2014). Through its standardised, matrix-based formalism, SoilR allows explicit comparison of model structures within a generalised modelling framework (Sierra *et al.*, 2012). This approach enables users to reproduce existing models, create hybrids, and test simplified variants by adjusting decomposition functions, pool structures, or environmental modifiers (e.g., Riggers *et al.*, 2019). A key outcome of this chapter is demonstrating that SoilR offers a flexible and transparent platform to harmonise

SOC model design and facilitate direct structural comparisons. Importantly, it shifts the focus from comparing outputs alone to examining the underlying behaviour and assumptions of models. While SoilR does not eliminate all challenges, particularly those related to model parameterisation, it provides a reproducible framework for model development, intercomparison, and integration. The chapter concludes that frameworks like SoilR are vital for advancing model transparency and reproducibility, but must be carefully benchmarked against legacy models (e.g., RothC, CENTURY) to ensure behavioural fidelity before deployment.

- **Implementation of a generalised modelling framework that can accommodate future model modifications and enhance reproducibility and transparency.**

Chapter 4 evaluated the SoilR implementation of RothC (RothC_R) as an alternative to the original RothC model. RothC_R is not a direct emulation but a generalised framework that can replicate RothC's core structure (Sierra *et al.*, 2012). Unlike earlier studies that focused only on SOC stock output (e.g., Lefebvre *et al.*, 2020; Riggers *et al.*, 2019), our validation also compared rate modifier values, which directly influence decomposition rates. Two key insights emerged: (i) RothC_R can replicate the outputs from RothC when modified appropriately, and (ii) comparisons across software implementations (R, Python, Excel) are as important as comparisons between models, since differences in coding environments can alter outcomes. These findings are particularly relevant for soil carbon modellers who may assume RothC and RothC_R are equivalent or interchangeable without verifying their implementation. Translating a faithful RothC model to a flexible open-source scripting language, such as the R environment, unlocks more potential as it allows model functions and structure to be modified and improved as research advances. Importantly, it also provides a generalised model structure to enable fair comparison for intermodal studies or model ensembles. We acknowledge that the developers of RothC have recognised this shortcoming and have transitioned the model to Python, which was released after this study commenced.

- **Identification of an optimal model configuration that balances model performance with minimal data requirements, adaptable to typical farm-scale conditions.** Chapter 5 systematically categorises C input and ET estimation methods by simple, intermediate, and complex to explore the influence of model input complexity on the RothC model performance. As RothC requires both externally estimated C and ET values to operate, understanding the effect of the methodology used to derive these values is essential. The results showed that RothC

was sensitive to the choice of C inputs, while alternative methods for calculating ET were less impactful on the model outcomes. A key, counterintuitive finding was that simpler methods for estimating C inputs and ET resulted in the RothC_R model performing as well as, or in some cases better than, more complex estimation methods for these variables. This challenges the common assumption that more data intensive methods will result in greater accuracy. However, in data-limited environments, simpler methods may yield more reliable results. Key insights from Chapter 5 were: (i) RothC is more sensitive to C inputs than ET methods, and (ii) in data-limited situations, simple C and ET methods may outperform their more complex counterparts.

- **Development and evaluation of an appropriate methodology for estimating SOC at the farm scale, while supporting Tier 3 requirements.** Chapter 6 integrated the findings from Chapters 3 to 5 to develop the MG model, using readily available and open-source software libraries. This modular Tier 3 prototype is a multi-point model capable of estimating topsoil SOC stock at the farm scale with limited data inputs for mineral grasslands. While none of its components are unique, as RothC_R (e.g., Lefebvre *et al.* 2020; Riggers *et al.*, 2019), gridded meteorological data (e.g., Oyesiku-Blakemore, 2022; Peralta *et al.*, 2022), or the Miami model coupled with RothC (e.g., Gottschalk *et al.*, 2012; Gutiérrez *et al.*, 2023), have been applied before. Their integration into a coherent and transparent modelling system capable of operating at the field or farm scale is novel. The MG model represents a significant advancement, as it allows the same modelling framework, data sources, and parameterisation to be applied consistently across different sites and landscapes. This consistency enhances comparability between locations and enables coherent intercomparison of multiple models. Consequently, the MG model functions not only as a farm-scale operational tool and a proof-of-concept for Tier 3 implementation, but also as a foundation for harmonised and replicable SOC modelling to support climate change mitigation efforts, multi-model ensembles, and intercomparison studies.

Collectively, these research chapters provide advances in SOC modelling across three areas: (i) evaluation of generalised model frameworks, (ii) systematic testing of input configurations, and (iii) development of a prototype Tier 3 SOC modelling approach. Nearly three decades after the release of RothC-26.3 (Coleman and Jenkinson, 1996), this work demonstrates that new configurations, such as the MG model, can extend the model's utility. Although conceptually similar to global approaches like the Global Soil Sequestration Potential (GSOCseq; Peralta *et al.*, 2022), the MG model operates at a finer resolution and is

designed for farm-scale SOC stock simulations, and with further refinement, can aid or be scalable to national applications.

The most immediate application is to generate baseline SOC stocks at the farm scale to improve national inventory reporting. However, the research findings here have wide application across schemes that require SOC modelling at finer scales in data-limited environments, including measuring, reporting and verification (MRV) systems for policy compliance, carbon markets and certification programmes, and agri-environmental sustainability schemes. For example, the Australian Carbon Credit Union (ACCU) scheme specifies that soil carbon projects can quantify sequestration using a measure-model approach (Australian Government, 2021), which the MG model could facilitate.

Similarly, the Agri-Climate Rural Environment Scheme (ARCES), introduced under Ireland's Common Agricultural Policy Strategic Plan 2023-2027 by the Department of Agriculture, Food and the Marine (DAFM), has multiple objectives such as climate change mitigation and adaptation, efficient management of natural resources such as soil, and enhancing ecosystem services (DAFM, 2023). The MG model can directly support these objectives by estimating C sequestration rates and using SOC stock estimates as an indicator of soil health and ecosystem robustness.

Beyond SOC modelling, the MG model also has relevance for farm system analysis and agricultural life cycle assessment (LCA). Agricultural research has adopted whole farm system models and LCA to determine the environmental impact of different products, production systems, and to assess the effects of management practices (Herron *et al.*, 2022; Hutchings *et al.*, 2018; Goglio *et al.*, 2015; O'Brien *et al.*, 2014). Agricultural LCA studies take a holistic approach of an agricultural system up to the point at which the product leaves the farm (e.g., cradle to farm-gate), where all of the major processes that occur on the farm and those associated with the production of farm inputs are included (Herron *et al.*, 2022; Petersen *et al.*, 2013; O'Brien *et al.*, 2014).

Soil C sequestration can strongly influence the GHG intensity of agricultural products. Herron *et al.* (2022) found that when grassland C sequestration was included, the global warming potential per kilogram of fat and protein-corrected milk was reduced between ~15.1% and 16.4%. Similarly, Sevenster *et al.* (2020) found that SOC changes can significantly impact crop carbon footprints, as wheat carbon footprint varied from 0.13 to 0.71 kg CO₂-eq/kg depending on region and crop type. Furthermore, the variability highlights why farm system models and agricultural LCAs rarely include soil C sequestration. This process is excluded due to methodology inconsistencies as multiple accounting approaches exist (e.g., IPCC emission factors, empirical models, process-based models), and each method gives different results (Goglio *et al.*, 2015; Petersen *et al.*, 2013).

The MG model and LCA both operate at the farm scale, allowing for finer resolution estimates that reflect local soil, climate, and management conditions. Furthermore, the MG model enables multiple SOC models to be run under a consistent input configuration. Variation between models will still occur, but differences would reflect inherent model structures (e.g., decomposition rates, environmental modifiers) rather than inconsistencies in input data or programming language. By generating a consistent range of SOC stock estimates across popular SOC models, the MG model supports fair and transparent estimation of soil C sequestration potential and offers a pathway to reduce methodological inconsistencies in farm-scale assessments.

7.4 From single models to ensemble approaches

All models have inherent biases. This is often regarded as a disadvantage, given that it potentially limits the reliability of SOC projections outside the conditions under which the model was parameterised initially and calibrated. However, within a well-structured MRV framework, such biases can also be strategically utilised. By incorporating a suite of validated SOC model, their specific biases can be strategically harnessed to improve predictive robustness and overall performance across a diverse range of ecosystems (Ceschia *et al.*, 2025). In Section 2.6, we discuss approaches to estimate SOC stock for national inventories, which include popular SOC models such as RothC (Richards, 2001; Shiratio and Taniyama, 2003; Smith *et al.*, 2020), DayCent (Del Grosso *et al.*, 2005), CENTURY (Parton, 1987), and C-Tool (Taghizadeh-Toosi *et al.*, 2014). Most national inventories rely on a single model approach that is calibrated to their local conditions. However, no single model can satisfactorily quantify SOC changes across all combinations of soils, climates, crops and management practices at various scales (Basso *et al.*, 2025; Ceschia *et al.*, 2025), so why do national inventories and other MRV systems rely on a single SOC model?

Traditionally, multi-model ensembles in SOC research were limited and have been used for comparative analysis, where the same input configurations are run across several models to evaluate performance and variability (e.g., Riggers *et al.*, 2019). Recently, multi-model ensemble studies have become more common, ranging from practical applications (e.g., Basso *et al.*, 2025; Couëdel *et al.*, 2024; Farina *et al.*, 2021) to discussion points for improvements in SOC modelling systems (Batjes, 2024; Ceschia *et al.*, 2025). This transition towards a multi-model ensemble may be inspired by climate science (Basso *et al.*, 2025). In climate science studies, coupled model intercomparison projects (CMIP) are routinely done. This involves operating multiple coupled earth system models within a flexible framework, with model configurations and methodology standardised to ensure simulations are comparable across different high-performance computing systems, and their performance

assessed (Döscher *et al.*, 2022). CMIPs are effectively a large coordinated multi-model ensemble for Earth system models and climate models.

SOC modelling has yet to adopt a similar framework; however, this point has been recently emphasised (Batjes, 2024; Flattery *et al.*, 2018; Ceschia *et al.*, 2025). Batjes (2024) emphasised the importance of developing a modular, integrative MRV framework that can be evaluated against a list of key characteristics. Similarly, Ceschia *et al.* (2025) acknowledged that no single SOC model can adequately represent the diversity of global soils, advocating for multi-model assessment approaches to improve accuracy, reduce uncertainty, and increase reliability (Ceschia *et al.*, 2025). Both Batjes (2024) and Ceschia *et al.*, (2025) further recommend the establishment of standardised protocols for the assessment of SOC models. This research, through the development of the MG model, represents an initial step towards a standardised assessment framework. The MG model's modular architecture allows for the implementation of multiple SOC models using harmonised input datasets, standardised parameter configurations, and consistent methodologies across a range of sites. This design, therefore, provides a practical foundation for facilitating multi-model ensemble analyses and intercomparison studies.

Although SOC studies have no equivalent to CMIPs, multi-model ensemble studies have recently demonstrated the ability to improve model estimates. Riggers *et al.* (2019) found that a multi-model ensemble improved the prediction trends in SOC stock in German croplands. Farina *et al.* (2021) demonstrated that a multi-model ensemble provides more robust predictions of SOC change trends compared to single-model runs in long-term bare-fallow soils. Couëdel *et al.* (2024) assessed the accuracy of each individual model and the multi-model ensemble in reproducing crop yield and SOC stocks. They found that the latter had greater accuracy, especially with full calibration, and model improvement was larger for maize yields (NRSME 47 vs 18%) and topsoil SOC (NRMSE 22 vs 14%) in sub-Saharan Africa. Basso *et al.* (2025) validated a multi-model ensemble approach against long-term trials in US Midwest croplands and found that the multi-model ensemble showed greater accuracy and lower uncertainty. All these SOC multi-model ensemble studies indicate that the performance of model combinations exceeds individual capabilities. The development of a standardised SOC modelling comparison study like CMIPs may result in similar improvements and advancements as found in climate sciences (Basso *et al.*, 2025; Döscher *et al.*, 2022).

Furthermore, a multi-model ensemble component can also be embedded directly into a SOC MRV system, which can reduce the risk of over-calibration associated with a single model, improve accuracy and reduce uncertainty in SOC change assessments (Batjes, 2024; Ceschia *et al.*, 2025). For example, the MG model performed reliably when initial SOC stocks were

within the range of 73-105 Mg C ha⁻¹, but consistently underestimated sites with high SOC stocks, particularly in low-clay soils. Instead of recalibrating RothC to perform more accurately in these specific conditions, which could compromise its performance elsewhere or overfit the model to specific conditions, it may be more effective to introduce alternative SOC models that have been demonstrated to improve the estimation of SOC at these lower or higher values.

Aiteew *et al.* (2024) evaluated the Model of Nitrogen and Carbon dynamics in Agroecosystems (MONICA) against long-term SOC observations from 46 German agricultural sites and benchmarked its performance relative to five established SOC models (CANDY Carbon Balance; CENTURY, C-Tool, ICBM, and RothC). The uncalibrated MONICA systemically overestimated decomposition rates and produced, on average, a ~17% greater mean absolute error than the other models. This highlights that specific SOC model initial parameters have inherent differences and mathematical affinities to specific SOC stock ranges, which could be incorporated into a multi-model ensemble to improve SOC monitoring, reporting and verification.

Ideally, more SOC models need to be faithfully translated into the R environment and incorporated into the MG model to ensure a genuine multi-model ensemble approach. However, integrating additional SOC model(s) would likely require additional modifications to the MG model configuration. For example, the C input value is currently calibrated for RothC simulations, so that model-specific coefficients may be needed for different models. Integrating an additional SOC model into the MG model would involve a similar process to that undertaken in this research:

1. Implement the selected model in the R environment and validate it against the original version.
2. Conduct a model input sensitivity analysis to determine the most appropriate configuration.
3. Perform measured versus modelled comparisons to assess the model's strengths, weaknesses, and suitability for different soil types, climate conditions, grasslands and management practices (if data is available).

Even in its current configuration, the MG model enables a standardised approach that can support multi-model ensembles and intercomparison studies, providing a foundation for more transparent and robust SOC modelling studies and robust MRV systems.

7.5 Limitations

This research was constrained by several overarching limitations that are not unique to this project but reflect broader SOC modelling, particularly in data-limited environments. The

most significant of these relate to data availability, representativeness, and parameterisation. These issues influenced both the methodological choices in this study and our overall results. The recurring limitations were:

- *Limited temporal and spatial SOC stock measurements*

Despite the growing interest in SOC stocks, information on long-term SOC dynamics across large scales remains scarce (Chen *et al.*, 2025; Yang *et al.*, 2025). This limitation arises not only from the paucity of repeated SOC measurements but also from the general lack of consistent soil data, including management information, soil texture variables and bulk density. Collectively, these data gaps constrain the robustness of model validation and hinder efforts to represent SOC dynamics across diverse agroecosystems accurately.

- *Restricted geographical representativeness:*

Many authors have recognised that most long-term SOC measurement sites and global SOC stock observations for agricultural areas are concentrated in temperate zones of Europe and North America (Smith *et al.*, 2020; Stockmann *et al.*, 2013). As a result, many SOC models and their parameterisations are based on geographically limited datasets, often centred on these regions, which restricts their applicability to other soil types and climatic zones. However, this bias is less significant for the current study, as it focuses on England and Ireland, both located within the temperate zone where much of the empirical evidence originates. Relying on temperate data means that applying such approaches to other grassland systems, particularly those with contrasting climatic or edaphic conditions, would need further validation and possible recalibration.

- *Generic parameterisation:*

In the absence of adequate site-specific data, default parameterisation values were used. Reliance on default values in a complex model is known to lead to inaccuracies and decrease the model's performance (Davoudabadi *et al.*, 2024; Heikkinen *et al.*, 2014). In our simulations, this limitation most likely had a greater impact on the input data rather than the model calibration, since the Rothamsted site shares broader, similar environmental conditions to sites in Ireland. For example, both the Miami model of net primary production (Lieth, 1973) and the Poeplau (2016) C input methodology were applied using general or literature-derived values, which ignore local soil and management effects. While this enables modelling in data-limited contexts, it reduces the capacity to capture site-specific contexts.

These limitations likely introduced systematic bias into the results. For example, reliance on generic parameterisation may have underestimated SOC stocks in high-productivity systems. At the same time, restricted geographic coverage reduces confidence in applying our methodologies across a diverse range of mineral grassland soils without further investigation.

7.6 Future refinements and requirements

This research is an early prototype of a Tier 3 SOC methodology for mineral grasslands for Ireland. Despite our research focusing on sites in England and Ireland, the MG model configuration can be applied to many temperate zones, and with further investigation, it can be adapted to other land uses and climatic zones. The MG model performed reasonably well, despite operating with limited data inputs, demonstrating both its feasibility and its considerable potential for refinement. With targeted improvements, the MG model could deliver more accurate and spatially representative SOC stock estimates, thereby increasing its suitability for farm-scale assessments and potentially aiding national inventory reporting.

Batjes *et al.* (2024) outlined a set of best-practice design features for an operational MRV SOC stock tool. Table 7.1 summarises their five key general considerations and compares them with the current capabilities of the MG model.

Table 7.1 Batjes *et al.* (2024) recommendations for best practice design features for monitoring, reporting, and verification of a soil organic carbon stock model, compared to the Mineral Grassland (MG) model prototype.

Batjes <i>et al.</i> recommendations		MG model approach
a	Define the project's name, boundaries, duration, scope and ecosystem under consideration.	The Mineral grassland (MG) model, which operates on grasslands at the farm scale.
b	Permit uploading of activity data and other relevant spatial data layers, with preference for local data when available.	Uses gridded weather data and local soil data; can incorporate local management data if adapted.
c	Define the relevant method for designing the baseline and test different scenarios to increase SOC stock and reduce GHG emissions.	In our approach, baseline pool sizes are typically initialised using a spin-up run to establish equilibrium in the absence of data. However, in policy frameworks such as the CRCF Regulation (EU) 2024/3012, the baseline is a measured reference period (commonly three years of SOC observations). These policy requirements can be met when sufficient data is available.
d	Produce biophysical products derived from earth observation data that will eventually be assimilated in Tier 3 modelling approaches or used in machine learning and artificial intelligence approaches.	Not currently implemented or discussed within our research, though earth observation data, machine learning and artificial intelligence are capable within R.
e	Utilise a decision tree to select and run the appropriate methodology for monitoring (e.g., Tier 1 to Tier 3).	The model can be expanded to include multiple SOC methodologies, such as the ICBM utilised in Chapter 6. The decision tree is not currently implemented, but possible to implement.

The current MG model configuration addresses 4 out of the 5 recommendations of Batjes *et al.* (2024). However, these areas can still be improved, and further research is required on additional model integration and database integration. Future development of the MG model can be structured into three complementary pathways:

1. Strengthening data collection and centralisation

While outside the scope of this study, the development and centralisation of a national SOC database remain essential for advancing SOC modelling. Many existing datasets (e.g., the Irish Soil Information System, National Soil Database) are based on single sampling campaigns and thus provide limited temporal resolution. Emerging initiatives such as the National Agricultural Soil Carbon Observatory (NASCO), the Signpost deep soil sampling and the Teagasc heavy soil programme represent significant steps forward, offering repeated measurements and improved spatial coverage across diverse land-use systems.

Leveraging these new developments through coordinated data integration would markedly enhance Ireland's capacity for Tier 3 SOC modelling. A centralised and harmonised database combining historical, emerging, and management datasets would enhance model calibration, validation, and uncertainty assessment while improving consistency across projects and research institutions. Moreover, aligning national monitoring initiatives like NASCO with emerging national modelling frameworks could facilitate more dynamic, data-driven assessments of SOC change and strengthen Ireland's evidence base for climate action and carbon accounting. This topic is discussed in greater detail in Section 7.7.

2. Model performance improvements

Improving the MG model can be achieved through further calibration and the incorporation of additional models, but these adjustments must be derived from empirical data from field-based measurements. Calibration may involve refinement of existing parameters (e.g., DPM/RPM ratio, decomposition rate coefficients, initial pool sizes) to better reflect site conditions. Additional adjustments include supplementary coefficients for overgeneralised parameters. For example, Miami-derived C inputs neglect management practices but could be incorporated with the addition of management coefficients, as outlined in Equation 6.3, to allow for a more diverse range of C inputs tailored to local management conditions. At the same time, consideration must be taken to avoid over-calibration, which can improve fit locally but reduce performance elsewhere. To mitigate this, incorporating complementary empirical or process-based SOC models (e.g., IPCC Tier 2 approach, CENTURY) would allow model selection to be based on site characteristics that are better suited to certain SOC models. This would prevent over-calibration of a single SOC model, while improving accuracy.

3. Improved user experience

The MG model currently operates in R, which ensures transparency and reproducibility, but it is not user-friendly. In its current configuration, data must be manually entered or imported from CSV files. An ideal SOC stock tool should automate data retrieval seamlessly from various national databases. In practice, this could allow users to input a location (e.g., latitude/longitude) and receive SOC stock estimates from linked soil, climate and management, supplemented with minimal user-supplied information. The most practical format for such a tool would likely be a web-based platform, accessible to the public, policymakers, landowners, and agricultural businesses. Transitioning towards an open code environment and generalised model frameworks represents the first step towards this goal. Such a transition would enhance transparency, expand model utility, enable multi-model ensembles, and facilitate future model modifications, while reducing the barrier to entry. This would improve accessibility and ensure alignment with best-practice design features for SOC MRV tools outlined by Batjes *et al.* (2024).

7.7 Implications for policy

The lack of appropriate and sufficient data to operate SOC models remains one of the most significant issues (e.g., Jebari *et al.*, 2021; Moll-Mielewicz *et al.*, 2023; Saunders *et al.*, 2022). Many SOC policies and guidelines focus on the transition to Tier 3 models (e.g., IPCC, 2006, 2019; Regulation (EU) 2024/3012, 2023/839); however, our research highlights the limitations of and the lack of appropriate datasets to operate and assess Tier 3 modelling attempts sufficiently. Acknowledging this critical flaw, we suggest four key policy recommendations based on the findings of this research. We recommend the following measures for policymakers:

7.7.1 Establish repeated national SOC surveys

Monitoring SOC content is crucial for understanding the role of agricultural soils in C sequestration and climate change mitigation (Cornu *et al.*, 2023; Harbo *et al.*, 2025; Paustian *et al.*, 2019a; Smith *et al.*, 2020). Repeated SOC surveys (e.g., routinely sampling the same site every 5-10 years) programmes have been conducted in several countries, such as England and Wales, Denmark, Belgium, and New Zealand, which have supported detecting long-term SOC trends, verifying model predictions, and supporting national GHG inventories and carbon accounting efforts (Cornu *et al.*, 2023; Harbo *et al.*, 2025; Smith *et al.*, 2020).

Many countries, including Ireland, do not conduct repeated national SOC surveys. Generally, national SOC surveys are conducted every 5-12 years (Harbo *et al.*, 2025; Smith *et al.*, 2020). Annual sampling can detect short-term fluctuations, but the associated increase in labour

and cost may not justify the improvement in trend detection (Harbo *et al.*, 2025). Harbo *et al.* (2025) suggest that an interval of 3-5 years, potentially in combination with a rolling campaign (e.g., where 20-30% of sites are sampled at that interval) to help maintain the continuity of field expertise and laboratory capacity, ensuring consistent data quality over time. Furthermore, in addition to temporal SOC observations, complementary data on bulk density, vertical SOC profile, clay content, moisture content, plant-derived C inputs, and microbial biomass may be required to validate other model outputs (LeNoë *et al.*, 2023).

Repeated national surveys are crucial for advancing SOC modelling efforts, as temporal SOC observations can strengthen SOC model performance and improve the reliability of SOC assessments (LeNoë *et al.*, 2023; Paustian *et al.*, 2019a; Petropoulos *et al.*, 2025). Countries without repeated national soil surveys may be at a disadvantage. Therefore, we recommend a policy that highlights this need and advocates for the routine resampling of pre-existing sites every 3-10 years, as well as the continuous improvement of our existing SOC databases.

7.7.2 Development of an integrated soil database

There is a large disparity in the number of databases, datasets and soil information systems among European countries (n=24), ranging from 1 to 19, with a median of 6 (Cornu *et al.*, 2023). However, the number of soil databases is not an indicator of soil data quantity or quality because soil databases are organised differently in each country (Cornu *et al.*, 2023). Nevertheless, this variation does highlight the lack of harmonisation of national and international soil datasets.

Ireland has two established national soil databases (e.g., the Irish Soil Information System and the National Soil Database), as well as additional projects such as the SoilC database, which extended and deepened SOC-focused measurements on a subset of National Soil Database sites. More recent initiatives, including the NASCO, the Signpost Programme deep-soil sampling, and the Teagasc Heavy Soils Programme, together with several local or smaller-scale SOC observation efforts, contribute valuable new data on soil properties and management practices.

To enable coherent national and international assessments, these diverse datasets need to be consolidated into a unified and central database. While substantial soil information is already available on various parameters at the national level, differences in sampling strategies, and soil properties differ across surveys and monitoring programmes, require harmonisation (Cornu *et al.*, 2023). Establishing an overarching coordination or oversight mechanism, such as a centralised data governance body or national soil data platform would help ensure consistency in data collection, improve comparability across programmes, and secure the long-term management of Ireland's soil datasets. Such coordination would not

only enhance data quality and accessibility but also strengthen Ireland's capacity to deliver robust SOC monitoring, model evaluation, and national greenhouse gas emission reporting.

The European Joint Programme on Agricultural Soil Management (EJP-Soil) similarly advocates the consolidation of standardised national and international inventory practices (EJP-Soil, 2025). However, adherence to these recommendations remains voluntary (Cornu *et al.*, 2023). To advance progress, we suggest the introduction of additional national regulations requiring that future SOC databases conform to standardised formats compatible with the EJP-Soil framework. This would facilitate cross-country collaboration, enable identification of large-scale SOC stock trends, and support integration into European SOC modelling efforts. Paustian *et al.* (2019a) emphasised that achieving these objectives can be enhanced by engaging land users directly in the provision of management data through participatory or crowdsourcing approaches, thereby improving the spatial and contextual detail of soil management information.

7.7.3 Development of testing sites

Long-term experiments serve as a record of long-term SOC change and a testing bed for SOC models (Smith *et al.*, 2020). Still, many countries lack the appropriate long-term experiments, making it challenging to adapt SOC models to local conditions. Ireland has the capacity for a series of short-term testing sites; however, this potential has not been fully acted upon. For example, the Teagasc research centre in Johnstown Castle has SOC measurements from 2006 and 2021, along with detailed management records and soil information. Similar Teagasc research centres, such as Solohead and Oakpark, also conduct SOC observations and modelling studies (e.g., Dondini *et al.*, 2009; Necpálová *et al.*, 2014; van Groenigen *et al.*, 2011).

If these sites were resampled to provide updated SOC observations and paired with detailed management and soil data, they could form a network of Irish SOC model testing sites with over 15 years of data, offering a strong foundation for model development and standardised datasets for model intercomparison. Such an initiative would also align closely with the objectives of the NASCO, which aims to establish a national framework for long-term soil carbon monitoring. Integrating these Teagasc research sites with the NASCO network would create a more comprehensive, spatially distributed system for model validation and calibration, enhancing Ireland's capacity for Tier 3 SOC modelling and long-term carbon accounting.

7.7.4 Assessment protocols

Currently, there is no standardised method to assess the performance of SOC models. Many policies demand a sufficient level of accuracy but rarely provide explicit evaluation criteria.

The draft CRCF methodology is one of the few to introduce such criteria. It requires 90% statistical power at a 5% significance level on initial SOC baselines to ensure robust detection of SOC change, and it mandates verification of model-based estimates through resampling 20% of the area. If resampling shows that model outputs overestimated removal by more than 20%, the corresponding certified C credits are invalidated (EC, 2024). These criteria are important for maintaining reliability, but they are verification rules rather than systemic model evaluation protocols.

This highlights the need for broader and standardised protocols to evaluate the model performance and behaviours. We recommend developing a national and international protocol for assessing Tier 3 models. At a national level, protocols should require SOC models to be tested against a series of testing bed sites (as outlined in Section 7.7.3). To ensure comparability, data inputs should be harmonised, and methodology standardised (similar to the MG model approach). This would enable users to validate, verify, and compare models under consistent datasets while allowing methodological differences to be systematically evaluated.

At an international level, we suggest adopting a similar approach to the CMIPs in climate science (e.g., Döscher *et al.*, 2022). In such an approach, multiple coupled SOC models would operate within a standardised framework with consistent model configurations and methodologies, with their performance assessed against a set number of high-quality international testing bed sites. This would provide a universal procedure for assessing SOC models, highlight their respective strengths and weaknesses, and help identify suites of complementary models capable of improving national and international GHG inventory reporting across diverse soils, climates, and land uses.

Both national and international protocols should include defined performance metrics. These protocols may have to be lenient at first, given the difficulty of achieving high accuracy across a diverse range of soil, climate and management. Regardless, minimum standards are essential. For example, a threshold of RMSE $<15 \text{ Mg C ha}^{-1}$ and other equivalent metrics (e.g., absolute mean error, model efficiency) could be adopted. Ultimately, having a universal assessment protocol supported by testing bed sites that are routinely sampled with clear performance-based criteria would strengthen the reliability of Tier 3 SOC models and deliver more accurate estimates for national GHG inventory reporting and farm-scale climate change mitigation efforts.

7.8 Conclusions

This thesis addresses key challenges and uncertainties in SOC modelling by systematically evaluating model frameworks and input configurations and applying them to mineral grasslands at both the field and farm scales. While each chapter has contributed to the

current scientific knowledge, together this research supports the broader transition towards Tier 3 approaches for modelling, reporting, and policy requirements.

This research advances SOC modelling by:

- Establishing that generalised frameworks can extend model utility and reproducibility of established models.
- Demonstrating that model input methodology is a critical determinant of model performance, and more complex methodology do not consistently outperform simpler choices.
- Developing the MG model as a proof-of-concept Tier 3 tool for estimating SOC stocks on mineral grasslands at farm-scale.

These contributions establish a foundation for future research and policy that aims to integrate Tier 3 models into operational MRV systems for farms. More broadly, our research highlights the importance and flexibility of generalised frameworks that support model modifications, multi-model ensembles, and systematic intercomparison, thereby advancing SOC modelling from research prototypes towards policy-relevant tools.

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Appendix A: Chapter 4 supporting material

Appendix A.1

The original RothC model operates with monthly carbon (C) inputs. The comparison of the RothC model with different C distributions is outlined in Table 4A.1

Table 4A.1 Outlines the monthly C input (t C/ha) for each method used in the simulation.

Month	RothC single	RothC default	RothC equal
January	3	0.05	0.25
February	0	0.05	0.25
March	0	0.05	0.25
April	0	0.2	0.25
May	0	0.2	0.25
June	0	0.2	0.25
July	0	0.05	0.25
August	0	0.05	0.25
September	0	0.7	0.25
October	0	0.7	0.25
November	0	0.7	0.25
December	0	0.05	0.25
Total	3	3	3

Appendix A.2

The RothC_R model was amended to incorporate a soil cover factor, consistent with the original RothC implementation. The process is fully documented in the accompanying R Markdown file, with code and outputs included here to facilitate transparency and enable independent replication of the results presented in Chapter 4. The following presents the output from this R Markdown file.

RothC_R: Adding a soil cover factor

2025-08-30

Introduction

The RothC model is a popular soil organic carbon (SOC) stock. The RothC model is described in detail in its user guide (see Coleman *et al.* 2024). The RothC model was originally published in Microsoft Windows format, however, this format has some limitations (e.g., obtaining values from outside the system), is cumbersome to operate for multiple sites, and is not suitable for future modifications. As a result, the RothC model has been implemented in various coding languages. One popular implementation is operating the RothC model through the R environment called SoilR developed by Sierra *et al.* (2012). However, SoilR is a general modelling framework, not a RothC model emulator. This workbook will discuss differences between the RothC operated through the R environment using the SoilR package (RothC_R) and the original RothC model.

Packages

```
library(tibble)
library(SoilR)
library(tidyverse)
library(dplyr)
library(lubridate)
library(tidyr)
library(ggplot2)
library(RColorBrewer)
library(cowplot)
library(readxl)
```

Model Inputs

We used the Park Grass dataset and values as practice data. Park Grass For the model inputs, we use values from Coleman *et al.* (1997) Park Grass plot 3d simulation. Park Grass

```
soil.thick = 23      # Soil thickness (organic layer topsoil) in cm
clay = 23.4          # Percent clay
IOM = 6.9            # IOM assumed to be 6.9
Cinput = 3           # t C ha
```

We assume long-term weather averages for temperature, rainfall and evaporation over water. These values were calculated off the Rothamsted meteorological weather station for the period 1960-1990.

```
LTA_values <- data.frame(
  month = 1:12,
  Temp = c(3.06, 3.23, 5.27, 7.57, 10.9, 13.9, 15.9, 15.8, 13.6, 10.4, 5.98, 3.99),
  Rain = c(65.4, 48.0, 57.1, 53.2, 53.0, 57.3, 47.0, 53.4, 54.8, 65.9, 64.4, 69.3),
  Evap = c(5.46, 12.6, 35.3, 61.4, 95.5, 111.0, 111.0, 89.2, 55.2, 23.4, 6.72, 3.91))
```

Models' selection

We operated three RothC models using the same data inputs. The three models used to demonstrate variability.

1. Microsoft Windows RothC model
2. RothC_R with no code amendments, referred to as RothC_R_{def}
3. RothC_R with code amendments, referred to as RothC_R_{mod}

RothC_R does not have a soil cover factor (SCF). The original RothC model contains a modifier to reduce decomposition by 0.60. RothC_R_{mod} has been amended to account for the SCF.

RothC Modifiers

We discussed how to implement the SCF into the RothC modifiers. The Microsoft Windows RothC model has a default spin-up simulation of 10,000 years. To ensure equal comparison, all RothC variants will have a spin-up of 10,000 years.

```
years10000 = seq(1/12, 10000, by=1/12) # Spin-Up Run Time Vector
```

The default modifiers can be described as:

```
SPIN_ft = fT.RothC(LTA_values$Temp)
SPIN_fw = fW.RothC(P=(LTA_values$Rain),
  E=(LTA_values$Evap),
  S.Thick = soil.thick, pClay = clay,
  pE = 0.75, bare = FALSE)$b

SPIN_xi.def = data.frame(years10000,rep(SPIN_ft*SPIN_fw,length.out=length(years10000)))
```

The modifier rates accounting for the SCF can be implemented as:

```
SCF <- 0.6 # Define the annual soil cover factor (SCF)

SPIN_xi.mod = data.frame(years10000,rep(SPIN_ft*SPIN_fw*SCF,length.out=length(years10000))) # SCF is added here.
```

It's important to note that the SCF for the RothC_R model is described annually.

Running the Model

The RothC_R_{def} model and RothC_R_{mod} can be operated now that site settings and modifying rates are defined. The RothC_R_{def} The model can be operated as:

```
SpinUP_SoilR.def = RothCModel(
  t=years10000,
```

```

C0 = c(DPM=0, RPM=0, BIO=0, HUM=0, IOM=IOM),
In = Cinput,
clay = clay,
xi = SPIN_xi.def)

SpinUP_SoilR.def_Ct = getC(SpinUP_SoilR.def)

SpinUP_SoilR.def_Pool = as.numeric(tail(SpinUP_SoilR.def_Ct,1))
names(SpinUP_SoilR.def_Pool)<-c("DPM", "RPM", "BIO", "HUM", "IOM")
SpinUP_SoilR.def_Pool

##          DPM          RPM          BIO          HUM          IOM
## 0.2691597 6.3868205 0.9276948 36.2226714 6.9000000

sum(SpinUP_SoilR.def_Pool)

## [1] 50.70635

```

The same process can be done with the RothC_R_{mod} model:

```

SpinUP_SoilR.mod = RothCModel(
  t=years10000,
  C0 = c(DPM=0, RPM=0, BIO=0, HUM=0, IOM=IOM),
  In = Cinput,
  clay = clay,
  xi = SPIN_xi.mod)

SpinUP_SoilR.mod_Ct = getC(SpinUP_SoilR.mod)

SpinUP_SoilR.mod_Pool = as.numeric(tail(SpinUP_SoilR.mod_Ct,1))
names(SpinUP_SoilR.mod_Pool)<-c("DPM", "RPM", "BIO", "HUM", "IOM")
SpinUP_SoilR.mod_Pool

##          DPM          RPM          BIO          HUM          IOM
## 0.4301126 10.6810056 1.5537401 60.3797813 6.9000000

sum(SpinUP_SoilR.mod_Pool)

## [1] 79.94464

```

We operated the Microsoft Windows RothC model on the officially released model, which can be downloaded and accessed from here: <https://www.rothamsted.ac.uk/rothamsted-carbon-model-rothc>. The Microsoft Windows version of the RothC model spin-up values cannot be accessed continuously; instead, the model displays time stamps of the 10,000-year simulation. To circumvent this issue, we ran the model for 30 years after equilibrium with the same data to produce values for comparison. We need to create new modifiers for the 30-year period.

```

years = seq(1/12, 30, by=1/12)

xi.frame_30.def = data.frame(years,rep(SPIN_ft*SPIN_fw,length.out=length(years)))

xi.frame_30.mod = data.frame(years,rep(SPIN_ft*SPIN_fw*SCF,length.out=length(years)))

```

Now lets rerun the RothC_R_{def} model and RothC_R_{mod} for 30 years.

```

# SoilR default model operated for 30 years
SoilR30.def = RothCModel(
  t=years,
  C0 = c(DPM = tail(SpinUP_SoilR.def_Pool["DPM"],1),
        RPM = tail(SpinUP_SoilR.def_Pool["RPM"],1),
        BIO = tail(SpinUP_SoilR.def_Pool["BIO"],1),
        HUM = tail(SpinUP_SoilR.def_Pool["HUM"],1),
        IOM = IOM),
  In = Cinput,

```

```

    clay = clay,
    xi = xi.frame_30.def)

SoilR30.def_Ct = getC(SoilR30.def)

SoilR30.def_Pool = as.numeric(tail(SoilR30.def_Ct,1))
names(SoilR30.def_Pool)<-c("DPM", "RPM", "BIO", "HUM", "IOM")
SoilR30.def_Pool

##          DPM          RPM          BIO          HUM          IOM
## 0.2691612  6.3867042  0.9276519 36.2140061  6.9000000

sum(SoilR30.def_Pool)

## [1] 50.69752

# SoilR modified model operated for 30 years
SoilR30.mod = RothCModel(
  t=years,
  C0 = c(DPM = tail(SpinUP_SoilR.mod_Pool["DPM"],1),
        RPM = tail(SpinUP_SoilR.mod_Pool['RPM'],1),
        BIO = tail(SpinUP_SoilR.mod_Pool["BIO"],1),
        HUM = tail(SpinUP_SoilR.mod_Pool["HUM"],1),
        IOM = IOM),
  In = Cinput,
  clay = clay,
  xi = xi.frame_30.mod)

SoilR30.mod_Ct = getC(SoilR30.mod)

SoilR30.mod_Pool = as.numeric(tail(SoilR30.mod_Ct,1))
names(SoilR30.mod_Pool)<-c("DPM", "RPM", "BIO", "HUM", "IOM")
SoilR30.mod_Pool

##          DPM          RPM          BIO          HUM          IOM
## 0.4301126 10.6798272  1.5535811 60.3700602  6.9000000

sum(SoilR30.mod_Pool)

## [1] 79.93358

```

The values from Microsoft Windows RothC for 30 years were saved in an excel workbook and read in.

```
RothC_LTA <- read_excel("~/Chapter_4/Modelling_Results/Model_Comparison_13.07.2024/Model_Comparison_13.07.24/RothC_Output_1961-1990.xlsx")
```

Data Visualization

We need to create and organise our values to plot. We can calculate the total for each model simulation:

```

SpinUP_SoilR.def_Ct <- as.data.frame(SpinUP_SoilR.def_Ct)
SpinUP_SoilR.def_Ct$Total <- rowSums(SpinUP_SoilR.def_Ct[,1:5])

SpinUP_SoilR.mod_Ct <- as.data.frame(SpinUP_SoilR.mod_Ct)
SpinUP_SoilR.mod_Ct$Total <- rowSums(SpinUP_SoilR.mod_Ct[,1:5])

SoilR30.def_Ct <- as.data.frame(SoilR30.def_Ct)
SoilR30.def_Ct$Total <- rowSums(SoilR30.def_Ct [,1:5])

SoilR30.mod_Ct <- as.data.frame(SoilR30.mod_Ct)
SoilR30.mod_Ct$Total <- rowSums(SoilR30.mod_Ct [,1:5])

```

Now we create the data frames to graph:

```
SpinUp_df <- data.frame(Month = 1:length(SpinUP_SoilR.def_Ct$Total),
                        SoilRdef = SpinUP_SoilR.def_Ct$Total,
                        SoilRmod = SpinUP_SoilR.mod_Ct$Total)

df <- data.frame(Month = 1:360,
                 RothC = RothC_LTA$TOTAL,
                 SoilRdef = SoilR30.def_Ct$Total,
                 SoilRmod = SoilR30.mod_Ct$Total)
```

We can create a graph for the 10,000-year spin-up runs.

```
# Pivot the data frame to a longer format
SpinUp_df_long <- SpinUp_df %>%
  pivot_longer(cols = c(SoilRdef, SoilRmod),
               names_to = "Model",
               values_to = "Total")

# Graph the Long dataframe
SpinUp_Graph <- ggplot(data = SpinUp_df_long, aes(x = Month, y = Total, color = Model)) +
  geom_line(linewidth=1) +
  labs(title = "",
       x = "Month",
       y = expression("SOC stock (Mg C ha-1*)"),
       color = "Model") +
  theme_minimal() +
  ylim(0,85) +
  scale_color_manual(values = c("#666666", "#1F78B4"),
                    labels = c(expression("RothC_R"["def"]), expression("RothC_R"["mod"]))) +
  scale_linetype_manual(values = c("dashed", "dashed"),
                       labels = c(expression("RothC_R"["def"]), expression("RothC_R"["mod"]))) + theme(
    plot.title = element_text(size = 12),
    axis.title.x = element_text(size = 12),
    axis.title.y = element_text(size = 12),
    axis.text.x = element_text(size = 12),
    axis.text.y = element_text(size = 12),
    legend.text = element_text(size = 14),
    legend.title = element_text(size = 14),
    legend.text.align = 0)
```

Then we create the 30-year simulation comparison graphs.

```
cb_palette <- c("#D95F02", "#666666", "#1F78B4")

# Transform the dataframe to Long format
df_long <- pivot_longer(df, cols = c(RothC, SoilRdef, SoilRmod),
                       names_to = "Model", values_to = "Value")

# Create the plot
LTA_Comparison_graph <- ggplot(df_long, aes(x = Month, y = Value, color = Model)) +
  geom_line(linewidth = 1) +
  labs(title = "",
       x = "Month",
       y = "",
       color = "Model") +
  ylim(0,85) +
  theme_minimal() +
  scale_color_manual(values = cb_palette,
                    labels = c("RothC", expression("RothC_R"["def"]), expression("RothC_R"["mod"]))) +
  scale_linetype_manual(values = c("solid", "dashed", "dashed"),
                       labels = c("RothC", expression("RothC_R"["def"]), expression("RothC_R"["mod"]))) + theme(
    plot.title = element_text(size = 12),
    axis.title.x = element_text(size = 12),
    axis.title.y = element_text(size = 12),
```

```
axis.text.x = element_text(size = 12),
axis.text.y = element_text(size = 12),
legend.text = element_text(size = 14),
legend.title = element_text(size = 14),
legend.text.align = 0)
```

Now we can plot them together:

```
# Combine plots and add Labels A) and B)
Total_SpinUp <- plot_grid(
  SpinUp_Graph + theme(legend.position = "none"), # Subplot 1
  LTA_Comparison_graph + theme(legend.position = "none"), # Subplot 2
  ncol = 2, # Arrange in 2 columns
  labels = c("A)", "B)"), # Add Labels A) and B)
  label_size = 12 # Adjust label size if needed
)

# Extract Legend
legend <- cowplot::get_legend(LTA_Comparison_graph)

# Combine the Labeled subplots with the Legend
Total_SpinUp_plot <- plot_grid(
  Total_SpinUp, # Labeled subplots
  legend, # Extracted Legend
  ncol = 2, # Arrange in 2 columns
  rel_widths = c(0.8, 0.2) # Adjust relative widths
)

# Print the final combined graph
print(Total_SpinUp_plot)
```

Discussion

The SCF for RothC_R will have to be tailored for different management and land-use systems. In our scenario, it was a grassland site that is permanently vegetated, so a uniform rate of 0.60 is applied. For other systems with soils that are bare for x amount of months during the year, a SCF value that reduces the decomposition on an annual basis. As RothC_R SCF operates on a yearly basis, the SCF reduction coefficient should also reflect this.

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Appendix B: Chapter 5 supporting material

Appendix B contains supporting information for Chapter 5.

Appendix B.1

Multiple RothC studies were reviewed to investigate the common C and ET inputs model version, objectives and results from the study. These findings are tabulated in Table 5B.1.

Table 5B.1 Summary of studies that have applied the RothC model to grassland sites. Studies that do not mention a specific RothC model or modifications are assumed to be default¹. Many studies reference the national or local meteorological stations to obtain ET values, but do not specifically state which methodology was used.

Study	Land-use	Scale	Location	Model version	Objectives	C inputs	Evaporation inputs	Results
Afzali <i>et al.</i> (2019)	Rangelands	Field and regional	Ghir-O-Karzins BandBast, Iran	Default ¹	Model validation and climate change scenarios	RothC inverse C inputs estimates	Evaporation over water using Penman's (1948)	RMSE values were 0.014 Mg C ha ⁻¹ for model validation. Under climate change scenarios, SOC stock was reduced by 2.36% and 3.53%.
Barančíková <i>et al.</i> (2023)	Semi-natural, over-sown and temporary grasslands	Field and regional	Suchy Vrch, Slovakia	Default ¹	Model validation, climate change, and management scenarios	C inputs calculated from plant residues and livestock manure following Bielek and Jurcova (2010)	ET method not specified	RMSE values ranged from 8 to 15 Mg C ha ⁻¹ for model validation. SOC stocks decreased under increasing temperatures.
Coleman <i>et al.</i> (1997)	Managed grasslands, unmanaged grassland, arable and forestry	Field	Europe	Default ¹	Model validation across a range of sites in different regions experiencing different climate, management and soil conditions	RothC inverse C input estimates	Actual OPE measurements	RothC simulated an acceptable approximation to the measurements for 14 of the experiments.
Doblas-Rodrigo <i>et al.</i> (2022)	Grassland	Field and regional	Basque Country, Spain	Default ¹ and Excel version	Model validation at field scale and climate scenario at regional	Inverse C input estimates and forage yield data are used to estimate C inputs based on an R:S of 1.5.	Hargreaves and Samani ET	Field results were R ² was 0.71, and RMSE was 9.31 Mg C ha ⁻¹ . Regional SOC stock projections varied depending on initial SOC and climate subregions.

Doblas-Rodrigo <i>et al.</i> (2023)	Grassland	Regional	Basque Country, Spain	Excel version	Model validated in Doblas-Rodrigo <i>et al.</i> (2022), and additional modifications and climate change scenarios	Inverse C input estimate and forage yield data to estimate C inputs based on R:S of 1.5.	Hargreaves and Samani ET	The model was run on grassland soils under different climate scenarios and with exogenous organic matter modifications.
Dondini <i>et al.</i> (2023)	Grasslands	Global		RothC spatial version	Evaluate the current state of SOC stocks in global livestock systems and their potential for C sequestration.	C inputs were estimated using RothC inversely, the Global Livestock Environmental Assessment Model (GLEAM 2.0) and IPCC Tier 2 methodology.	ET method not specified	On average, in 2010, SOC in global grasslands was about 51 Mg C ha ⁻¹ to a soil depth of 30cm.
Fallon and Smith (2002)	Grassland, natural and arable	Field and regional	Europe	Default ¹ and CENTURY plant C input sub-model	Model validation using the RothC model and RothC model + CENTURY C input sub-model	Inverse C input estimate and CENTURY model derived C inputs	ET method not specified for multiple sites	RMSE ranged from 1.68 to 12.69, depending on treatment and C input estimate
Francaviglia <i>et al.</i> (2012)	Pastures, semi-natural grasslands, and hay crop	Regional	Sardinia, Italy	Default ¹	Climate change scenarios	Inverse C input estimates	ET method, not specified	Land use at lower intensity was more efficient than intensive agricultural systems for SOC storage in the order hay crop > pasture > cork oak forest > semi-natural systems
Geremew <i>et al.</i> (2024)	Cultivation land, forest, grassland,	Regional	Ethiopia	SoilR	Model validation and SOC dynamics under	Normalised Difference Vegetation Index (NDVI) was	Thornthwaite (1948) ET	R-square ³ = 0.86 and 0.77,

	and fallow land				management scenarios	extracted from MODIS (Moderate Resolution Imaging Spectroradiometer) and converted to NPP using the Miami Model. C inputs were derived from the Miami model estimate.		RMSE ³ = 0.013 and 0.074, (For 2021 and 1997, SOC measured values). Model projection increase in SOC stocks under different future climate scenarios and land-use cover.
Gonzalez-Molina <i>et al.</i> (2011)	Forests, grasslands and rangelands	Field	Mexico	Default ¹	Model validation against multiple grassland or rangeland sites	RothC inverse C input estimates	ET method, not specified	The model performed well with a grassland RMSE of 0.18 and rangeland RMSE = 0.40
Gottschalk <i>et al.</i> (2012)	Arable, grassland ² and forest	Global	Global	Modified RothC model, combined with additional models.	SOC dynamics under climate change scenarios	C inputs based on inverse C input estimates, IMAGE model and Miami model of NPP.	ET was calculated from monthly temperature and cloudiness described according to Prentice <i>et al.</i> (1993) and Sitch <i>et al.</i> (2003).	SOC stock gains and losses are dependent on context-specific conditions
Gutierrez <i>et al.</i> (2023)	Agriculture with temporary crops, permanent crops, and grasslands	Regional	Denmark	Spatial RothC version	Sequestration potential, climate change and land-use change scenarios	RothC inversely C inputs scaled with the Miami model of NPP	Hargreaves and Samani ET	The projection showed a SOC loss of 8.1 Mg C ha ⁻¹ , strongly influenced by warmer temperatures and clay content.
Heikkinen <i>et al.</i> (2014)	Cropland to managed	Field	Pushchino, Russia	Modified RothC for	Model validation and comparison	Annual C input estimates using	Hargreaves (1994) ET	RothC performed reasonably well

	and unmanaged grasslands			Russian conditions operated in MATLAB		above- and belowground biomass, similar to the Bolinder et al. (2007) method		with a modelling efficiency of 0.72.
Jebari et al. (2021)	Managed grasslands	Field	Ireland, France, Switzerland, Scotland	Excel	Model validation and additional RothC model modifications	C input method following Poeplau (2016) and additional C input modifications for above- and belowground inputs and animal excreta.	ET method not specified	The default RothC average RMSE was 11.36 Mg C ha ⁻¹ , and the model efficiency was 0.78. The best-performing modified RothC model average RMSE was 2.77 Mg C ha ⁻¹ , and model efficiency was 0.99.
Koco et al. (2016)	Grasslands, grassland conversion to arable, and arable conversion to grasslands	Regional	Ondavska vrchovina highland, Slovakia	Default ¹	SOC dynamics under future land-use change scenarios	C inputs derived from national statistics following the Bielek and Jurcova (2010) method	ET method not specified	Cropland conversion to grassland increased SOC stock by 15-28% between 1970 and 2020.
Kooch et al. (2022)	Forest, arable and rangeland	Regional	Salahedin Kala region, Iran	Default ¹	SOC dynamics under future climate change and land-use scenarios	RothC inverse C inputs	Open-pan evaporation, and if not available, Thornthwaite and Mather (1955) ET	Changes in SOC stock simulated for land cover. SOC stock increased by 15 to 28% during the simulated period of 1970 – 2020.
Liu et al. (2011)	Annual pastures (AP) and	Field	Wagga Wagga, Australia	Default ¹	Simulation of SOC dynamics under	C inputs based on recorded biomass yields and inverse	ET method not specified	Modelling efficiency was 0.96, 0.97, 0.91 and 0.89

	perennial pastures (PP) with lime (+) or without lime (-)				different pasture management	modelling techniques to calculate the optimised root-to-shoot ratio.		for AP-, AP+, PP-, and PP+
Moll-Mielewczik <i>et al.</i> (2023)	Intensive, semi-intensive and extensive grasslands	Field	Swiss Soil Monitoring Network, Switzerland	SoilR	Model validation against multiple grassland sites in Switzerland	C inputs are assumed constant, with manure-derived C inputs estimated from farm management records or national values.	ET rates are calculated according to Priestley and Taylor (1972).	Good model fit in two-thirds of sites.
Morais <i>et al.</i> (2019)	Grasslands ²	Global	Global	MATLAB implementation of RothC	Global SOC modelling in cropland, grassland and forest soils	FAOSTAT dataset was used to obtain crop yield data, and IPCC guidelines were used to estimate above- and below-ground residues. Constant C content is assumed.	Thornthwaite ET	Regional and detailed understanding of C sequestration.
Oyesiku-Blakemore and Dondini (2022)	Managed mineral soils	National	Scotland	SoilR	Regional estimate of SOC sequestration rates	Miami model of NPP and national grazing intensity to derive C input estimates.	ET method not specified	1-2.5 additional tonnes of C stored per ha ⁻¹ , where C inputs to soils can be increased by 10% for 30 years.
Paramesh <i>et al.</i> (2022)	Cashew, pasture, coconut, forest and arecanut	Regional	Goa, India	Default ¹	SOC dynamics under climate change scenarios	RothC inverse estimated C inputs	Actual OPE measurements	Pasture soils showed a decrease, a negligible positive or a decrease depending on the climate change scenario

Peralta <i>et al.</i> (2022)	Forestry, cropland and grassland	Global		Spatial RothC model	Development of a spatial RothC modelling framework to estimate SOC sequestration potential.	Miami model and land-use coefficients	Penman-Monteith ET	Successful development of the spatial model with practical examples and a detailed guide.
van Wesemael <i>et al.</i> (2010)	Cropland and grassland	National	Belgium	Default ¹	Model validation and SOC dynamics under management and land-use scenarios	Grassland C inputs are assumed constant due to a lack of national data.	Thornthwaite ET	Model validation produced an R^2 that ranges from 0.40 to 0.88, depending on the management.

Appendix B.2

To simulate extreme wet and dry climatic conditions, monthly adjustment factors were applied to baseline climate inputs. We created adjustment factors to adjust the monthly values for temperature, rainfall and evapotranspiration (ET) to mimic extreme wet and dry climatic conditions. The adjustment factors (AF) were determined by calculating the long-term average from 1961-1990 and comparing the monthly values to those recorded for the extreme wet year (2012) and dry year (2022). The adjustment factors for the wet year and dry year are outlined in Table 5A.1 and Table 5A.2.

Table 5B.2 Adjustment factors for monthly values under an extreme wet year to replicate these climatic conditions.

Month	Temperature	Rainfall	Evapotranspiration
Jan	73.02	-12.93	46.82
Feb	0.57	-89.07	14.86
March	46.02	-58.0	19.63
April	-3.13	67.93	3.46
May	9.12	0.19	6.08
June	-1.16	64.1	-6.42
July	-0.98	61.45	-0.27
August	9.21	-1.28	8.47
September	-1.84	-48.76	22.19
October	-5.15	40.21	16.55
November	8.21	33.56	15.70
December	12.34	39.68	-4.32

Table 5B.3 Adjustment factors for monthly values under an extreme dry year to replicate these climatic conditions.

Month	Temperature	Rainfall	Evapotranspiration
Jan	33.32	-179.91	-31.67
Feb	99.74	40.81	38.54
March	39.63	-60.88	22.30
April	19.00	-161.35	26.11
May	19.79	-56.08	17.41
June	10.071	-36.30	23.13
July	19.68	-323.08	31.68
August	23.76	-34.38	34.19
September	7.01	22.65	8.99
October	27.10	31.52	32.36
November	52.30	49.27	8.76
December	-18.15	-1.92	-54.40

For each month (i), the adjusted value (AV_i), for a given variable (e.g., temperature, rainfall, or ET) was calculated as:

$$AV_i = V_i \times \left(1 + \frac{AF_i}{100}\right)$$

Where V_i is the monthly value for month i, and AF_i is the adjustment factor for month i.

In cases where AV_i became negative, these values were substituted with recorded monthly values from the corresponding month for the wet or dry year.

Appendix B.3

The model ensemble of the RothC_R with various C and ET inputs is fully documented in the accompanying R Markdown file. This code and outputs included here facilitate transparency and enable independent replication of the results presented in Chapter 5. The following presents the output from this R Markdown file.

RothC Model Input Sensitivity

2025-09-01

Introduction

Model performance in soil carbon simulations is strongly influenced by the quality and accuracy of the data input. The RothC model is a widely used model for estimating soil organic carbon (SOC) turnover. Key inputs such as plant-derived carbon inputs (C inputs) and evapotranspiration (ET) are not generated internally but must be derived from external sources. The selection of methods to estimate these inputs can significantly impact model outputs, potentially leading to different interpretations of soil carbon dynamics. This document provides a calculation for estimating popular RothC C input and ET estimation methods.

For this analysis, the following packages are:

```
library(readxl)
library(tidyverse)
library(lubridate)
library(dplyr)
library(FA056)
library(SoilR)
library(ggplot2)
library(reshape2)
library(SPEI)
library(cowplot)
library(tidyr)
```

Site description

This analysis uses data from the Park Grass Long-Term Experiment, a historic field trial at Rothamsted Research. The site was selected for the following reasons:

4. It is one of the longest-running agricultural grassland experiments in the world and has been widely used in SOC modelling studies (e.g., Coleman *et al.*, 1997).
5. The data set is rich and detailed, enabling complex model input calculations.
6. The data are freely available and easily accessible from the Electronic Rothamsted Archive (e-RA; <https://www.era.rothamsted.ac.uk/>).

The baseline simulation for this analysis follows the approach described in Coleman *et al.* (1997), as previous work has replicated this simulation with high accuracy (see Chapter 4). All required model inputs can be obtained from Coleman *et al.* (1997) or the e-RA database. The model inputs obtained from Coleman *et al.* (1997) are:

```
# Taken from Coleman et al. (1997)
soil.thick = 23 # Soil thickness (organic layer topsoil), in cm
```

```
clay = 23.4          # Percent clay
IOM = 6.9            # IOM assumed to be 6.9
```

The management and weather data can be obtained from the e-RA database. Once downloaded, they can be imported and formatted as follows:

```
setwd("~/Ch5_Model_input_sensitivity/Model_input_sensitivity")

#-----
# Management data
#-----
PG_DM_yields <- read_excel("ParkGrass_DM_yields_3d_14d.xlsx")

# Calculate the total DM_t/ha for each year for each plot
DM_yields_Total <- PG_DM_yields %>%
  group_by(plot, year) %>%
  summarize(total_DM_t_ha = sum(DM_t_ha))

## `summarise()` has grouped output by 'plot'. You can override using the
## `.groups` argument.

# Determine the first and final years
first_year_3d <- PG_DM_yields %>%
  filter(plot == "3d") %>%
  summarize(first_year = min(year))
first_year_14d <- PG_DM_yields %>%
  filter(plot == "14d") %>%
  summarize(first_year = min(year))

final_year_3d <- PG_DM_yields %>%
  filter(plot == "3d") %>%
  summarize(final_year = max(year))
final_year_14d <- PG_DM_yields %>%
  filter(plot == "14d") %>%
  summarize(final_year = max(year))

# Create a filter to plot 3d years to match the same length as plot 14d
plot_3d_filtered <- DM_yields_Total %>%
  filter(plot == "3d", year >= 1965, year <= 1989)

# Now filter plot 14d
plot_14d_filtered <- DM_yields_Total %>%
  filter(plot == "14d", year >= 1965, year <= 1989)

#-----
# Read in weather file
#-----
# Obtained from ROTHMET weather station via e-RA.
ROTHMET <- read_excel("Rothamsted_WeatherFile.xlsx",
  sheet = "ROTHMET")

## New names:
## • `relh` -> `relh...10`
## • `relh` -> `relh...14`

ROTHMET <- ROTHMET[-1, ] # Remove first row (units)

# Generate the daily sequence
ROTHMET_dates <- seq.Date(from = as.Date("1854-01-01"),
  to = as.Date("1995-12-31"),
  by = "day")
ROTHMET$day <- ROTHMET_dates
```

Evapotranspiration methods

Three ET estimation methods of varying complexity were selected for comparison:

- **Penman-Monteith** (PEN; Monteith, 1965): An energy balance-based approach that integrates radiation, temperature, humidity and wind speed data, representing the most complex approach.
- **Hargreaves** (HAR; Hargreaves, 1994): An empirical method requiring only temperature and extraterrestrial radiation, representing an intermediate level of complexity.
- **Thornthwaite** (THO; Thornthwaite, 1948): A simple temperature-based method that estimates ET using only mean monthly air temperature and day length.

These can be calculated as follows:

```
#-----
# Penman-Monteith ET
#-----
PG_elevation <- 133 # Elevation of Park Grass site in meters
PG_lat <- 51.81 # Latitude of Rothamsted Park Grass experiment
# https://www.era.rothamsted.ac.uk/Park#site/

# Filter data from 1960 to 1993
PG_Weather_filtered <- ROTHMET %>%
  filter(year(day) >= 1965 & year(day) <= 1989)

# Read in windsp
ROTHMET_windsp <- read_excel("Rothamsted_WeatherFile.xlsx",
                             sheet = "ROTHMET_windsp")

ROTHMET_windsp_filtered <- ROTHMET_windsp %>%
  filter(year(day) >= 1965 & year(day) <= 1989)

PG_Weather_filtered$windsp <- ROTHMET_windsp_filtered$windsp

# Convert to numeric
numeric_columns <- c("tmax", "tmin", "rad", "rain", "rad (calc)", "svap", "vap",
                     "hrday", "windrun", "dryb", "wetb", "relh...10",
                     "relh...14", "dda", "accdda", "ddb", "accddb",
                     "evapg", "evapw", "smd", "psmd", "dewp", "avtemp")

PG_Weather_filtered <- PG_Weather_filtered %>%
  mutate(across(all_of(numeric_columns), ~ as.numeric(gsub("NaN|NA|test| ", NA, .))))
apply(PG_Weather_filtered, class)

##           day           tmax           tmin           rain           sun
##           "Date"         "numeric"        "numeric"        "numeric"        "character"
##           windrun        dryb           wetb           rad           relh...10
##           "numeric"      "numeric"        "numeric"        "numeric"        "numeric"
##           rad (calc)     svap           vap           relh...14         dda
##           "numeric"      "numeric"        "numeric"        "numeric"        "numeric"
##           accdda         ddb           accddb         avtemp         hrday
##           "numeric"      "numeric"        "numeric"        "numeric"        "numeric"
## test - ea_grass test - ea_water           evapg           evapw           day nB
##           "character"    "character"        "numeric"        "numeric"        "character"
##           smd            psmd            dewp           windsp
##           "numeric"      "numeric"        "numeric"        "numeric"

# d_r
PG.d_r <- EarSunDis(PG_Weather_filtered$day)
# delta
PG.delta <- SolDec(PG_Weather_filtered$day)
# phi
PG.phi <- DD2Rad(PG_lat)
# omega_s
PG.omega_s <- SunHA(phi = PG.phi, delta = PG.delta)
```

```

# Extraterrestrial Radiation
PG.R_a <- ExRad(d_r = PG.d_r,
               omega_s = PG.omega_s,
               phi = PG.phi,
               delta = PG.delta,
               G_sc = 0.082)

# Calculate radiation
R_s <- PG_Weather_filtered$`rad (calc)`*0.01
R_ns <- NSRad(R_s)
R_so <- CSSRad(elev = PG_elevation, R_a = PG.R_a)
R_nl <- NLRad(PG_Weather_filtered$tmax, PG_Weather_filtered$tmin, PG_Weather_filtered
              $vap/10, R_s, R_so)
R_n <- NRad(R_ns, R_nl)

# Penman-Monteith daily estimate
PG_PEN_daily <- ETo_FPM(R_n = R_n,
                       u_2 = PG_Weather_filtered$windsp*0.78,
                       e_a = PG_Weather_filtered$vap/10,
                       T_min = PG_Weather_filtered$tmin,
                       T_max = PG_Weather_filtered$tmax,
                       phi_deg = PG_lat,
                       elev = PG_elevation,
                       date = PG_Weather_filtered$day,
                       n = PG_Weather_filtered$hrday)

# Convert daily to monthly values
PG_PEN_df = data.frame(Date = PG_Weather_filtered$day,
                       PG_PEN_daily)

# Add month and year columns
PG_PEN_df <- PG_PEN_df %>%
  mutate(
    year = year(Date),
    month = month(Date))

# Calculate monthly averages
PG_PEN <- PG_PEN_df %>%
  group_by(year, month) %>%
  summarise(PG_PEN = sum(PG_PEN_daily, na.rm = TRUE)) %>%
  ungroup()

#-----
# Hargreaves ET
#-----
# Extraterrestrial Radiation
PG.R_a <- ExRad(d_r = PG.d_r,
               omega_s = PG.omega_s,
               phi = PG.phi,
               delta = PG.delta,
               G_sc = 0.082)
C.R_a <- PG.R_a*0.408

# Hargreaves daily estimates
PG_HAR_daily <- ETo_Hrg(T_min = PG_Weather_filtered$tmin,
                       T_max = PG_Weather_filtered$tmax,
                       R_a = C.R_a)

# Convert daily to monthly values
PG_HAR_df = data.frame(Date = PG_Weather_filtered$day,
                       PG_HAR_daily)

# Add month and year columns
PG_HAR_df <- PG_HAR_df %>%
  mutate(
    year = year(Date),
    month = month(Date)
  )

```

```

# Calculate monthly averages
PG_HAR <- PG_HAR_df %>%
  group_by(year, month) %>%
  summarise(PG_HAR = sum(PG_HAR_daily, na.rm = TRUE)) %>%
  ungroup()

#-----
# Thornthwaite ET
#-----
# Calculate the monthly average temperature
monthly_avg_temp <- PG_Weather_filtered %>%
  group_by(year = year(day), month = month(day)) %>%
  summarise(monthly_avg_temp = mean(avtemp, na.rm = TRUE)) %>%
  ungroup()

PG_TH0 <- thornthwaite(Tave = monthly_avg_temp$monthly_avg_temp, lat = PG_lat)

## [1] "Checking for missing values (`NA`): all the data must be complete. Input type
is vector. Assuming the data are monthly time series starting in January, all regular
(non-leap) years."

```

For comparison of ET methodologies, we can combine them into a singular data frame and plot:

```

#-----
# ET comparison
#-----
ET_df <- data.frame(Month = month.abb,
                    Thornthwaite = PG_TH0,
                    Hargreaves = PG_HAR$PG_HAR,
                    Penman_Monteith = PG_PEN$PG_PEN)

# Create the ET_long_df with Method in the desired order
ET_long_df <- ET_df %>%
  pivot_longer(
    cols = c(Thornthwaite, Hargreaves, Penman_Monteith),
    names_to = "Method",
    values_to = "Value"
  ) %>%
  mutate(Method = recode(Method,
                        Thornthwaite = "Thornthwaite",
                        Hargreaves = "Hargreaves",
                        Penman_Monteith = "Penman-Monteith")) %>%
  mutate(Method = factor(Method, levels = c("Penman-Monteith", "Hargreaves", "Thornthwaite"))) # <- Reorder Legend & graph

# Plot with reordered legend and group
ET_boxplot <- ggplot(ET_long_df, aes(x = Month, y = Value, colour = Method, fill = Method)) +
  geom_boxplot(alpha = 0.8, color = "black", outlier.shape = NA, width = 0.6) +
  labs(
    x = "",
    y = expression("Evapotranspiration (mm)")
  ) +
  theme_minimal(base_size = 16) +
  theme(
    panel.grid.major = element_line(color = "grey80"),
    panel.grid.minor = element_blank(),
    axis.text.y = element_text(size = 16),
    axis.text.x = element_text(size = 16, angle = 45, hjust = 1),
    legend.position = "right"
  ) +
  scale_x_discrete(limits = month.abb) +
  scale_colour_manual(values = c(
    "Penman-Monteith" = "#7570b3",
    "Hargreaves" = "#1b9e77",
    "Thornthwaite" = "#d95f02"
  )) +

```

```
scale_fill_manual(values = c(
  "Penman-Monteith" = "#7570b3",
  "Hargreaves" = "#1b9e77",
  "Thornthwaite" = "#d95f02"
))
```

ET_boxplot

Carbon inputs

Three different methods of C input methods were utilised. The RothC inverse methodology, Poeplau (2016) methodology, Miami model of net primary production (NPP), to represent complex, intermediate, and simple, respectively.

Each method is described in detail in its respective literature and documentation. For further information, refer to:

- **RothC inverse:** Coleman *et al.* (1997, 2024)
- **Poeplau methodology:** Poeplau (2016)
- **Miami model of NPP:** Lieth (1973)

An additional Poeplau (2016) methodology was utilised, which alters the root-to-shoot ratio (R:S) by nitrogen application, as done by Jebari *et al.* (2021)

The C input methods can be calculated as:

```
#-----
# Miami model
#-----
# Calculate the monthly sum rainfall
monthly_sum_rain <- PG_Weather_filtered %>%
  group_by(year = year(day), month = month(day)) %>%
  summarise(monthly_sum_rain = sum(rain, na.rm = TRUE)) %>%
  ungroup()

## `summarise()` has grouped output by 'year'. You can override using the
## `.groups` argument.

# Create monthly time sequence for data frame
start_date <- as.Date("1965-01-01")
end_date <- as.Date("1989-12-31")
monthly_sequence <- seq.Date(from = start_date,
                             to = end_date,
                             by = "month")

# Convert to Year-Month format
monthly_sequence_ym <- format(monthly_sequence, "%Y-%m")

PG_Temp_and_Rain_df <- data.frame(Date = monthly_sequence_ym,
                                  Temperature = monthly_avg_temp$monthly_avg_temp,
                                  Rainfall = monthly_sum_rain$monthly_sum_rain,
                                  Month = monthly_avg_temp$month)

# Calculate the Long-Term Average (LTA) for each month
PG_Temp_and_Rain_LTA <- PG_Temp_and_Rain_df %>%
  group_by(Month) %>%
  summarize(
    LTA_temp = mean(Temperature, na.rm = TRUE),
    LTA_rain = mean(Rainfall, na.rm = TRUE))

AnnualAvg_Temp <- mean(PG_Temp_and_Rain_LTA$LTA_temp)
AnnualSum_Rain <- sum(PG_Temp_and_Rain_LTA$LTA_rain)
```

```

# Miami model
library(soilassessment)

## Warning: package 'soilassessment' was built under R version 4.3.3

MiamiModel_Output <- NPPmodel(rain = AnnualSum_Rain, temperature = AnnualAvg_Temp, model = "miami")

# Outputs as g DM m2
MiamiModel_Cinput <- round(MiamiModel_Output * 0.01 * 0.45, 2)
MiamiModel_Cinput <- MiamiModel_Cinput*0.72

#-----
# Poeplau (2016) Method
#-----
Plot3d_HB <- plot_3d_filtered$total_DM_t_ha
Plot14d_HB <- plot_14d_filtered$total_DM_t_ha

# Aboveground net primary production (ANPP)
ANPP_3d <- (Plot3d_HB / 0.7) * 0.45
ANPP_14d <- (Plot14d_HB / 0.7) * 0.45

# ACin
FC_in = 0 # There is no organic manure added to these plots, this value is left zero as a place holder.
AC_in_3d <- (ANPP_3d * 0.3) / 2 + FC_in
AC_in_14d <- (ANPP_14d * 0.3) / 2 + FC_in

# Below-ground net primary production (BNPP)
# BNPP is where the C inputs estimates vary more.
# It requires a root to shoot ratio (R:S), which depends on vegetation and management type.
# Two R:S differents were used:
# Fertilised or Unfertilised: R:S = 5.9 +/- 1.9 or 2.4 +/- 1.5 (Poeplau_F).
# R:S based on nitrogen application was obtained from Jebari et al. (2021) (Poeplau_N).

# Poeplau_F
Plot3d_RS_poeplau_F = 5.9
Plot14d_RS_poeplau_F = 2.4

# Poeplau_N
Plot3d_N_application = 0      # Control plot with no additives
Plot14d_N_application = 96    # 96 kg N (MacDonald et al. 2018)

Plot3d_RS_poeplau_N <- exp(-0.004290241511 * Plot3d_N_application) * 4.737504746
Plot14d_RS_poeplau_N <- exp(-0.004290241511 * Plot14d_N_application) * 4.737504746
# Equation obtained from Jebari et al. (2021)

# BNPP Parameters
soil.thickness = 23 # To match Coleman et al. (1997)
dr = 150
d50 = 15
d = soil.thickness
BNPPd = (d*(d50+dr))/(dr*(d50+d))

# Poeplau_F Plot 3d
BNPP_3d_poeplau_F = ANPP_3d*Plot3d_RS_poeplau_F
BCin_3d_poeplau_F = BNPP_3d_poeplau_F/2
BCin_d3d_poeplau_F = BCin_3d_poeplau_F*BNPPd
TCind_3d_poeplau_F = BCin_d3d_poeplau_F + AC_in_3d # Poeplau_F total C input

# Poeplau_N Plot 3d
BNPP_3d_poeplau_N = ANPP_3d*Plot3d_RS_poeplau_N
BCin_3d_poeplau_N = BNPP_3d_poeplau_N/2
BCin_d3d_poeplau_N = BCin_3d_poeplau_N*BNPPd
TCind_3d_poeplau_N = BCin_d3d_poeplau_N + AC_in_3d # poeplau_N total C input

```

```

# Poeplau_F Plot 14d
BNPP_14d_poeplau_F = ANPP_14d*Plot14d_RS_poeplau_F
BCin_14d_poeplau_F = BNPP_14d_poeplau_F/2
BCin_d14d_poeplau_F = BCin_14d_poeplau_F*BNPPd
TCind_14d_poeplau_F = BCin_d14d_poeplau_F + AC_in_14d # Poeplau_F total C input

# Poeplau_N Plot 14d
BNPP_14d_poeplau_N = ANPP_14d*Plot14d_RS_poeplau_N
BCin_14d_poeplau_N = BNPP_14d_poeplau_N/2
BCin_d14d_poeplau_N = BCin_14d_poeplau_N*BNPPd
TCind_14d_poeplau_N = BCin_d14d_poeplau_N + AC_in_14d # poeplau_N total C input

#-----
# RothC Inverse C inputs
#-----
rothc_plot3d = 2.5688 # C inputs calculated on original windows RothC model & used
in Chapter 4.
rothc_plot14d = 2.2688

```

A comparison of Poeplau's methods can be graphed:

```

DM_yields_df <- data.frame(Year = plot_3d_filtered$year,
                           Plot3d = plot_3d_filtered$total_DM_t_ha,
                           Plot14d = plot_14d_filtered$total_DM_t_ha)
DM_yields_long <- melt(DM_yields_df, id.vars = "Year",
                      variable.name = "Plot", value.name = "DM_yields")

# Modify the Plot Labels
DM_yields_long$Plot <- factor(DM_yields_long$Plot,
                             levels = c("Plot3d", "Plot14d"),
                             labels = c("3d", "14d"))

# DM Comparison Plot
DM_Comparison_plot <- ggplot(DM_yields_long, aes(x = Plot, y = DM_yields, fill = Plot)) +
  geom_boxplot(color = "black") +
  scale_fill_manual(values = c("3d" = "#7570b3", "14d" = "#d95f02")) +
  labs(title = "",
       x = "",
       y = expression("DM yields (t ha-1yr-1")) +
  theme_minimal() +
  ylim(0,13) +
  theme(text = element_text(size = 12),
        plot.title = element_text(size = 12))

```

The Poeplau outputs need to be organised for easier retrieval during the RothC simulations:

```

# Poeplau Results
Poeplau_methods_3d <- data.frame(Plot = rep("3d", length(plot_3d_filtered$year)),
                                Poeplau_F = TCind_3d_poeplau_F,
                                Poeplau_N = TCind_3d_poeplau_N)

Poeplau_methods_14d <- data.frame(Plot = rep("14d", length(plot_14d_filtered$year)),
                                Poeplau_F = TCind_14d_poeplau_F,
                                Poeplau_N = TCind_14d_poeplau_N)

# Combine the two dataframes
Poeplau_methods_combined <- rbind(Poeplau_methods_3d, Poeplau_methods_14d)

# Reshape the data from wide to Long format
Poeplau_methods_long <- melt(Poeplau_methods_combined,
                             id.vars = "Plot",
                             measure.vars = c("Poeplau_F", "Poeplau_N"),
                             variable.name = "Metric",
                             value.name = "Value")

Poeplau_methods_long$Plot <- factor(Poeplau_methods_long$Plot,
                                   levels = c("3d", "14d"))

```


RothC Modifiers

To calculate the rate of decomposition from the different ET methods, we need to calculate the environmental modifiers (xi) for each ET method. The temperature modifier will be the same for each approach:

```
fT = fT.RothC(monthly_avg_temp$monthly_avg_temp)
```

The ET method is an input for the moisture modifier. Therefore the PEN, HAR and THO moisture modifier can be calculated as:

```
fw_THO = fw.RothC(P=(monthly_sum_rain$monthly_sum_rain),
                  E=(PG_THO),
                  S.Thick = soil.thick, pClay = clay,
                  pE = 1.0, bare = FALSE)$b

fw_HAR = fw.RothC(P=(monthly_sum_rain$monthly_sum_rain),
                  E=(PG_HAR$PG_HAR),
                  S.Thick = soil.thick, pClay = clay,
                  pE = 1.0, bare = FALSE)$b

fw_PEN = fw.RothC(P=(monthly_sum_rain$monthly_sum_rain),
                  E=(PG_PEN$PG_PEN),
                  S.Thick = soil.thick, pClay = clay,
                  pE = 1.0, bare = FALSE)$b
```

Now we can create the xi dataframe for each method:

```
SCF <- 0.6 # Soil Cover factor
years <- seq(1/12, 25, by=1/12) # Length of the simulation

THO_xi.frame = data.frame(years,rep(fT*fw_THO*SCF,length.out=length(years)))
HAR_xi.frame = data.frame(years,rep(fT*fw_HAR*SCF,length.out=length(years)))
PEN_xi.frame = data.frame(years,rep(fT*fw_PEN*SCF,length.out=length(years)))
```

The differences in decomposition rate for each modifier can be graphed as:

```
Rate_modifiers <- data.frame(
  Time = years,
  Thornthwaite = THO_xi.frame[,2],
  Hargreaves = HAR_xi.frame[,2],
  Penman_Monteith = PEN_xi.frame[,2])

# Prepare data with desired order
Rate_modifiers_long <- Rate_modifiers %>%
  pivot_longer(
    cols = c(Thornthwaite, Hargreaves, Penman_Monteith),
    names_to = "Method",
    values_to = "Values"
  ) %>%
  mutate(Method = recode(Method,
    Thornthwaite = "Thornthwaite",
    Hargreaves = "Hargreaves",
    Penman_Monteith = "Penman-Monteith")) %>%
  mutate(Method = factor(Method, levels = c("Penman-Monteith", "Hargreaves", "Thornthwaite")))

# Plot with correct order
Modifiers_box <- ggplot(Rate_modifiers_long, aes(x = Values, y = Method, colour = Method, fill = Method)) +
  geom_boxplot(alpha = 0.4, color = "black", outlier.shape = NA, width = 0.6) +
  geom_jitter(width = 0, height = 0.1, alpha = 0.25, size = 1.2) +
  labs(
    x = expression("Rate modifier (xi)"),
    y = NULL
  ) +
```

```

theme_minimal(base_size = 14) +
theme(
  axis.text.y = element_text(size = 12),
  axis.text.x = element_text(size = 12),
  legend.position = "none"
) +
scale_colour_manual(values = c(
  "Penman-Monteith" = "#7570b3",
  "Hargreaves" = "#1b9e77",
  "Thorntwaite" = "#d95f02"
)) +
scale_fill_manual(values = c(
  "Penman-Monteith" = "#7570b3",
  "Hargreaves" = "#1b9e77",
  "Thorntwaite" = "#d95f02"
)) +
xlim(0, 1.4)

# Display plot
Modifiers_box

```

Appendix B.4

Appendix B.4 provides supplementary results from the sensitivity analysis, including RMSE values for each model input combination, graphical summaries by ET, and an assessment of the importance of initial starting values in the OAT analysis. Table 5B.4 presents detailed results for the different model input configurations.

Table 5B.4 Results from the model input sensitivity analysis showing the influence of evapotranspiration (ET) estimation method (THO = Thornthwaite; HAR = Hargreaves; PEN = Penman-Monteith) and carbon (C) input model (Miami, Poeplau_P, Poeplau_J, RothC inverse) on simulated SOC stocks for Park Grass plots 3d and 14d. Reported values include final SOC stock (Mg C ha⁻¹), absolute SOC stock difference (Mg C ha⁻¹), relative difference (%), and root mean square error (RMSE, Mg C ha⁻¹) compared to benchmark simulations.

Plot	ET model	C input model	End SOC stock	SOC stock diff	Difference (%)	RMSE
3d	THO	miami	83.2	8.5	11.3	7.1
3d	THO	poeplau_P	83.7	9	12	7.2
3d	THO	poeplau_J	79.1	4.3	5.8	4.1
3d	THO	rothc	76	1.2	1.6	2
3d	HAR	miami	85.2	10.4	13.9	4.8
3d	HAR	poeplau_P	85.7	10.9	14.6	4.9
3d	HAR	poeplau_J	80.9	6.1	8.2	2
3d	HAR	rothc	77.7	2.9	3.9	5.6
3d	PEN	miami	81.7	7	9.3	5.7
3d	PEN	poeplau_P	82.3	7.5	10	2.8
3d	PEN	poeplau_J	77.8	3	4	0.8
14d	THO	miami	80.3	10.4	14.9	8.3
14d	THO	poeplau_P	87	17.1	24.5	14.5
14d	THO	poeplau_J	95.2	25.3	36.2	20.6
14d	THO	rothc	71	1.1	1.6	1.8
14d	HAR	miami	82.2	12.3	17.6	6.2
14d	HAR	poeplau_P	89.2	19.4	27.7	12
14d	HAR	poeplau_J	97.7	27.9	39.9	17.8
14d	HAR	rothc	72.5	2.6	3.8	6.9
14d	PEN	miami	78.9	9	12.8	12.8
14d	PEN	poeplau_P	85.4	15.5	22.1	18.7
14d	PEN	poeplau_J	93.2	23.4	33.4	0.7

In Chapter 5, we plotted the model input simulations by C inputs. We have attached the same simulated results, but plotted the ET method. Figure 5B.1 displays the difference C inputs have on the simulations.

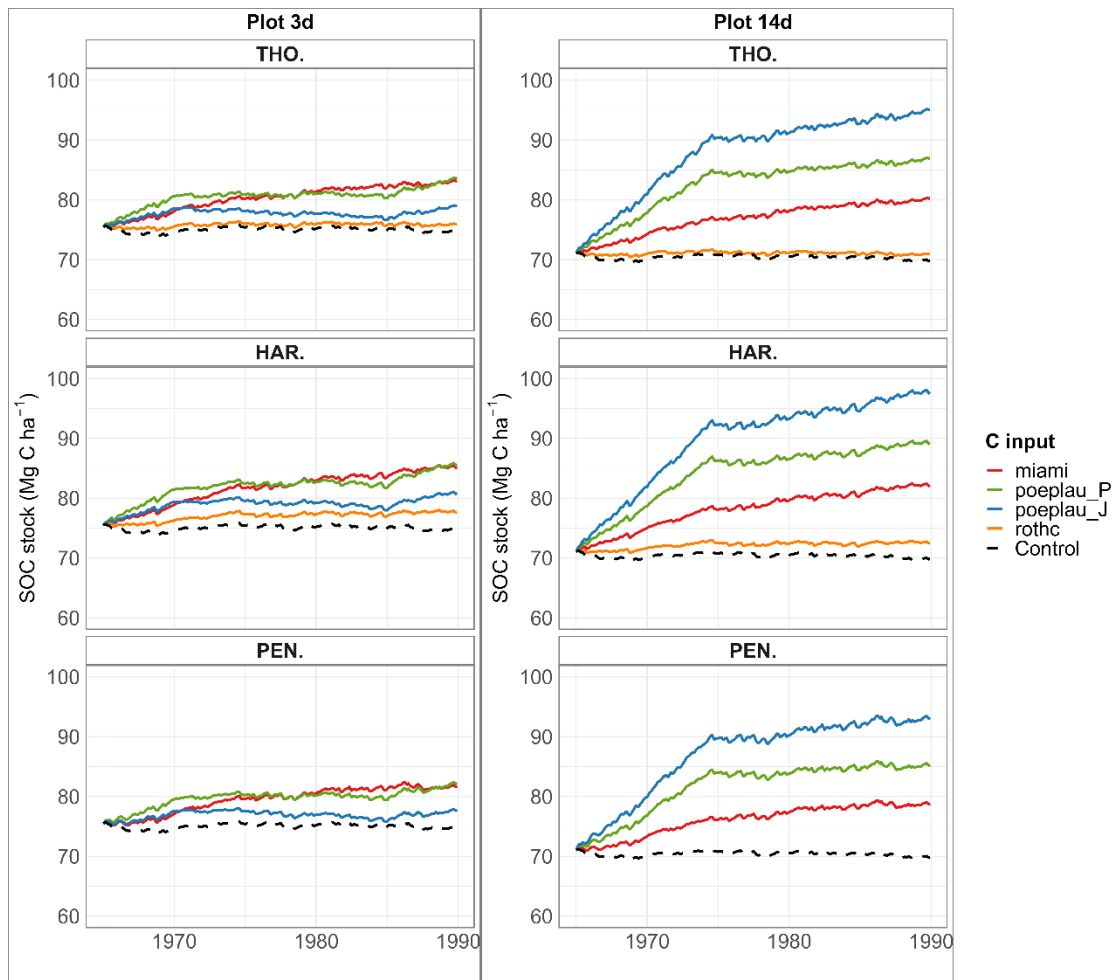


Figure 5B.1 Simulated SOC stocks (Mg C ha⁻¹) for Park Grass plots 3d (left) and 14d (right) under different evapotranspiration (ET) estimation methods: Thornthwaite (THO), Hargreaves (HAR), and Penman-Monteith (PEN). Each panel compares SOC trajectories using alternative C input methods: Miami (red), Poeplau_P (green), Poeplau_J (blue), and RothC default (orange). The black dashed line represents measured SOC values. Results highlight the influence of ET and C input methods on simulated SOC dynamics, with larger divergences observed in the managed plot (14d).

Figure 5B.2 demonstrates the difference in the clay OAT SA if the control value is changed to 5%. The S_i is significantly reduced, showing how the initial control value can influence the S_i values.

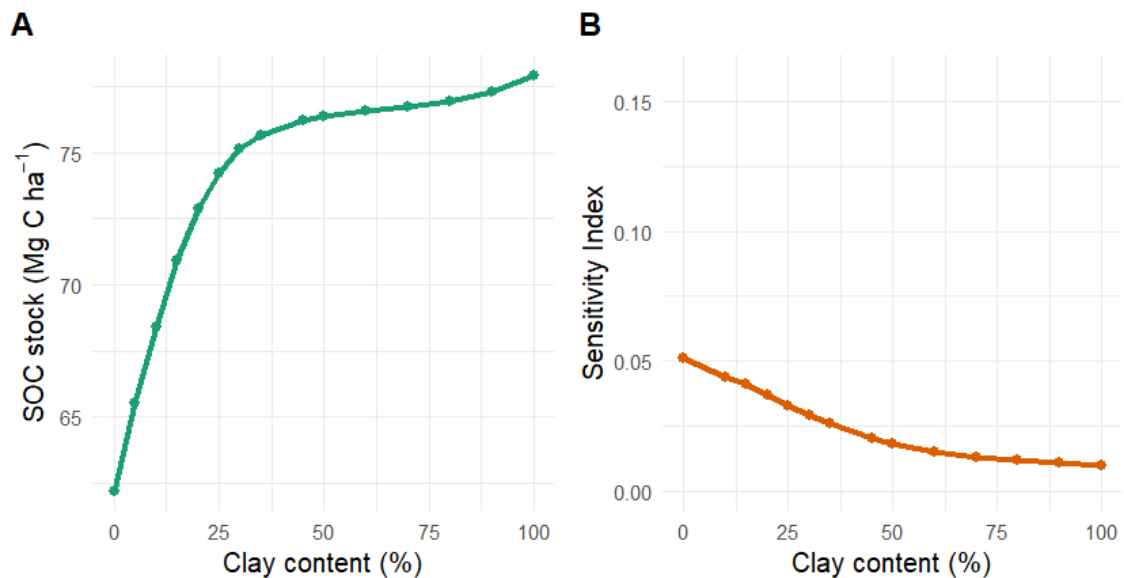


Figure 5B.2 One-at-a-time sensitivity analysis of modelled soil organic carbon (SOC) stock in response to changes in clay inputs (Graph A). The corresponding sensitivity index is calculated as the relative change in SOC stocks divided by the relative change in the clay parameter (Graph B).

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Appendix C: Chapter 6 supporting material

Appendix C contains information and code on how to convert the SoilC database into appropriate model inputs, the Mineral Grassland (MG) model user guide, and MG model amendments to incorporate the Introductory Carbon Balance Model (ICBM).

Appendix C.1

The SoilC dataset used in this experiment is publicly available online and can be accessed at: <https://eparesearch.epa.ie/safer/iso19115/displayISO19115.jsp?isoID=107>. The relevant file is "Att 5 SoilC_FinalData_04-Sept-08". Prior to use, a minor correction is required within the Excel file: in the "Soil_Texture" tab, the site ID 663 should be changed to 633. Additional information on the SoilC project is available through the link above. The following presents the output from an R Markdown file that generates RothC data inputs from the SoilC database.

Organising SoilC database

2025-08-28

```
setwd("~/Chapter_6_Modelling_Irish_SOC/SoilC_data")

#-----
# Read in database
#-----
library(readxl)
SoilC_df <- read_excel("SoilC_FinalData_04-Sept-08.xls",
                      sheet = "Site_Attributes")
head(SoilC_df)

## # A tibble: 6 × 15
##   Site Easting_ING Northing_ING LandUse   LandUse_Secondary SoilType
##   <dbl>      <dbl>      <dbl> <chr>      <chr>              <chr>
## 1    43      300999      131000 Arable     <NA>              Gley
## 2    61      245992      146014 Arable     <NA>              Grey Brown Podzolic
## 3    68      315853      145600 Grassland <NA>              Gley
## 4   107      281001      170999 Arable     <NA>              Grey Brown Podzolic
## 5   126      291003      181000 Grassland <NA>              Shallow Brown Earth
## 6   143      221027       81004 Forest    Broad-leaf        Brown Podzolic
## # 9 more variables: ParentMaterial <chr>, Rainfall_mm <dbl>,
## #   Elevation_GPS_m <dbl>, Elevation_GIS_m <dbl>, Slope_GIS_Degree <dbl>,
## #   Aspect_GIS <dbl>, Aspect_Category <chr>, County <chr>, Name <chr>

#
SoilC_BD <- read_excel("SoilC_FinalData_04-Sept-08.xls",
                      sheet = "Bulk_Density")

SoilC_CP <- read_excel("SoilC_FinalData_04-Sept-08.xls",
                      sheet = "Chemical_Properties")

SoilC_ST <- read_excel("SoilC_FinalData_04-Sept-08.xls",
                      sheet = "Soil_Texture") # One small change i
s required. Change the site id on "Soil_Texture" from 663 to 633.

SoilC_NS <- read_excel("SoilC_FinalData_04-Sept-08.xls",
```



```

sheet = "Nutrient_Stocks")

#-----
# Create filter for grasslands
#-----
library(dplyr)

##
## Attaching package: 'dplyr'

## The following objects are masked from 'package:stats':
##
##   filter, lag

## The following objects are masked from 'package:base':
##
##   intersect, setdiff, setequal, union

# We are only interest in grassland sites
SoilC_grassland <- SoilC_df %>% filter(LandUse == "Grassland")
SoilC_grassland <- SoilC_grassland %>% filter(Site != 872) # Site 872 soil type is
peat and has no soil texture.

#-----
# Removing rows where sites from other SoilC sheets are not grassland
#-----
# Create list of sites to keep
SoilC_grassland_site <- SoilC_grassland$Site
print(SoilC_grassland_site)

## [1] 68 126 180 268 355 358 446 485 633 740 773 862 876 879 962
## [16] 1102 1158 1176 1319 1347 3001 3002 3003 3004 3005 3006 3007 3008

# Remove other sites
SoilC_BD_grasslands <- SoilC_BD[SoilC_BD$Site %in% SoilC_grassland_site, ]
SoilC_CP_grasslands <- SoilC_CP[SoilC_CP$Site %in% SoilC_grassland_site, ]
SoilC_ST_grasslands <- SoilC_ST[SoilC_ST$Site %in% SoilC_grassland_site, ]
SoilC_NS_grasslands <- SoilC_NS[SoilC_NS$Site %in% SoilC_grassland_site, ]

#-----
# Bulk Density
#-----
head(SoilC_BD_grasslands)

## # A tibble: 6 × 6
##   Site Depth   Number_SampleRings `Apparent_BD_g/cm^3` `Actual_BD_g/cm^3`
##   <dbl> <chr>           <dbl>           <dbl>           <dbl>
## 1    68 0-5 cm                5             0.901           0.886
## 2    68 5-10 cm               5             1.52           1.50
## 3    68 15-20 cm              5             1.47           1.45
## 4    68 20-25 cm              5             1.35           1.33
## 5    68 40-45 cm              5             1.40           1.37
## 6    68 45-50 cm              5             1.29           1.27
## # i 1 more variable: `FineSoilDensity_g/cm^3` <dbl>

# Carbon_% is divided by 0-10 and 10-25, we need BD to match this.

#-----
# Filter for depths "0-5 cm" and "5-10 cm"
#-----
Depths_0_to_10cm <- SoilC_BD_grasslands %>%
  filter(Depth %in% c("0-5 cm", "5-10 cm"))

# Group by Site and calculate the mean for each group
Mean_BD_0_to_10cm <- Depths_0_to_10cm %>%
  group_by(Site) %>%
  summarise(
    Apparent_BD_0_to_10 = mean(`Apparent_BD_g/cm^3`),
    Actual_BD_0_to_10 = mean(`Actual_BD_g/cm^3`),

```

```

        FineSoilDensity_0_to_10 = mean(`FineSoilDensity_g/cm^3`)
      )

#-----
# Filter for depths "15-20 cm" and "20-25 cm"
#-----
Depths_15_to_25cm <- SoilC_BD_grasslands %>%
  filter(Depth %in% c("15-20 cm", "20-25 cm"))

# Group by Site and calculate the mean for each group
Mean_BD_15_to_25cm <- Depths_15_to_25cm %>%
  group_by(Site) %>%
  summarise(
    Apparent_BD_15_25cm = mean(`Apparent_BD_g/cm^3`),
    Actual_BD_15_25cm = mean(`Actual_BD_g/cm^3`),
    FineSoilDensity_15_25cm = mean(`FineSoilDensity_g/cm^3`)
  )

#-----
# Bulk Density (0-25cm)
#-----
Depths_0_to_25cm <- SoilC_BD_grasslands %>%
  filter(Depth %in% c("0-5 cm", "5-10 cm", "15-20 cm", "20-25 cm"))

# Define weights for existing depth intervals
weights <- c("0-5 cm" = 0.2, "5-10 cm" = 0.2, "15-20 cm" = 0.2, "20-25 cm" = 0.2)

# Calculate depth-weighted averages
Weighted_Mean_BD_0_to_25cm <- Depths_0_to_25cm %>%
  group_by(Site) %>%
  summarise(
    Depth = "0-25 cm", # Set a new depth label
    Apparent_BD_g_cm3 = sum(`Apparent_BD_g/cm^3` * c(weights["0-5 cm"], weights["5-10
cm"], weights["15-20 cm"], weights["20-25 cm"]))) / sum(weights),
    Actual_BD_g_cm3 = sum(`Actual_BD_g/cm^3` * c(weights["0-5 cm"], weights["5-10
cm"], weights["15-20 cm"], weights["20-25 cm"]))) / sum(weights),
    FineSoilDensity_g_cm3 = sum(`FineSoilDensity_g/cm^3` * c(weights["0-5 cm"], weig
hts["5-10 cm"], weights["15-20 cm"], weights["20-25 cm"]))) / sum(weights)
  )

#////////////////////////////////////

#-----
# SoilC grassland Carbon %
#-----
library(tidyr)
# Filter for depths "0-10 cm" and "10-25 cm" and select specific columns
SoilC_grasslands_C <- SoilC_CP_grasslands %>%
  filter(Depth %in% c("0-10 cm", "10-25 cm")) %>%
  select(Site, Depth, `Carbon_%`)

# Pivot the data to create separate columns for Carbon_0-10cm and Carbon_10-25cm
Carbon_by_depth <- SoilC_grasslands_C %>%
  pivot_wider(
    names_from = Depth, #
    values_from = `Carbon_%`,
    names_prefix = "Carbon_"
  )
# Rename
Carbon_by_depth <- Carbon_by_depth %>%
  rename(
    Carbon_0_10cm = `Carbon_0-10 cm`,
    Carbon_10_25cm = `Carbon_10-25 cm`
  )

#-----
# SoilC grassland chemical properties (CP) 0-25cm
#-----
CP_Depths_0_to_25cm <- SoilC_CP_grasslands %>%

```

```

        filter(Depth %in% c("0-10 cm", "10-25 cm"))

View(CP_Depths_0_to_25cm)

# Define weights for each depth
weights <- c("0-10 cm" = 0.4, "10-25 cm" = 0.6)

# Calculate weighted averages and sums
Weighted_Chem_P_0_to_25cm <- CP_Depths_0_to_25cm %>%
  group_by(Site) %>%
  summarise(
    Depth = "0-25 cm", # Set a new depth Label
    `Carbon_%` = sum(`Carbon_%` * c(weights["0-10 cm"], weights["10-25 cm"])),
    `Nitrogen_%` = sum(`Nitrogen_%` * c(weights["0-10 cm"], weights["10-25 cm"])),
    `C/N Ratio` = sum(`C/N Ratio` * c(weights["0-10 cm"], weights["10-25 cm"])),
    `OrganicMatter_%` = sum(`OrganicMatter_%` * c(weights["0-10 cm"], weights["10-25
cm"])),
    TEC = sum(TEC * c(weights["0-10 cm"], weights["10-25 cm"])),
    pH = sum(pH * c(weights["0-10 cm"], weights["10-25 cm"])),
    Al_ppm = sum(Al_ppm * c(weights["0-10 cm"], weights["10-25 cm"])),
    B_ppm = sum(B_ppm * c(weights["0-10 cm"], weights["10-25 cm"])),
    Ca_ppm = sum(Ca_ppm * c(weights["0-10 cm"], weights["10-25 cm"])),
    Cu_ppm = sum(Cu_ppm * c(weights["0-10 cm"], weights["10-25 cm"])),
    Fe_ppm = sum(Fe_ppm * c(weights["0-10 cm"], weights["10-25 cm"])),
    K_ppm = sum(K_ppm * c(weights["0-10 cm"], weights["10-25 cm"])),
    Mg_ppm = sum(Mg_ppm * c(weights["0-10 cm"], weights["10-25 cm"]))
  )

# Prepare bulk density for 0-10 cm and 10-25 cm layers
BD_0_10 <- SoilC_BD_grasslands %>%
  filter(Depth %in% c("0-5 cm", "5-10 cm")) %>%
  group_by(Site) %>%
  summarise(BD_0_10 = mean(`Actual_BD_g/cm^3`, na.rm = TRUE))

BD_10_25 <- SoilC_BD_grasslands %>%
  filter(Depth %in% c("15-20 cm", "20-25 cm")) %>%
  group_by(Site) %>%
  summarise(BD_10_25 = mean(`Actual_BD_g/cm^3`, na.rm = TRUE))

# Assign layer depth in cm
CP_mass <- CP_Depths_0_to_25cm %>%
  mutate(Layer_cm = ifelse(Depth == "0-10 cm", 10, 15)) %>%
  left_join(BD_0_10, by = "Site") %>%
  left_join(BD_10_25, by = "Site") %>%
  mutate(
    BD = ifelse(Depth == "0-10 cm", BD_0_10, BD_10_25),
    LayerMass = BD * Layer_cm * 100 # g/cm³ × cm × 100 = Mg/ha
  )

# Now compute mass-weighted averages
Mass_Weighted_Chem_P_0_to_25cm <- CP_mass %>%
  group_by(Site) %>%
  summarise(
    Depth = "0-25 cm",
    TotalMass = sum(LayerMass),
    `Carbon_%` = sum(`Carbon_%` * LayerMass) / TotalMass,
    `Nitrogen_%` = sum(`Nitrogen_%` * LayerMass) / TotalMass,
    `C/N Ratio` = sum(`C/N Ratio` * LayerMass) / TotalMass,
    `OrganicMatter_%` = sum(`OrganicMatter_%` * LayerMass) / TotalMass,
    TEC = sum(TEC * LayerMass) / TotalMass,
    pH = sum(pH * LayerMass) / TotalMass, # Use with caution
    Al_ppm = sum(Al_ppm * LayerMass) / TotalMass,
    B_ppm = sum(B_ppm * LayerMass) / TotalMass,
    Ca_ppm = sum(Ca_ppm * LayerMass) / TotalMass,
    Cu_ppm = sum(Cu_ppm * LayerMass) / TotalMass,
    Fe_ppm = sum(Fe_ppm * LayerMass) / TotalMass,
    K_ppm = sum(K_ppm * LayerMass) / TotalMass,
    Mg_ppm = sum(Mg_ppm * LayerMass) / TotalMass
  )

```

```

#####

#-----
# SoilC grassland Soil Texture (ST) 0-25cm
#-----
# Calculate the mass for each site at the given depth.

### 0-10cm Dataframe
ST_Depths_0_to_10cm <- SoilC_ST_grasslands %>%
  filter(Depth %in% c("0-10 cm"))
ST_Depths_0_to_10cm$Depth <- 10
ST_Depths_0_to_10cm$Area <- 1.0

BD_0_to_10cm <- SoilC_BD_grasslands %>%
  filter(Depth %in% c("0-5 cm", "5-10 cm"))

# Group by Site and calculate the mean for each group
Mean_BD_0_to_10cm <- Depths_0_to_10cm %>%
  group_by(Site) %>%
  summarise(
    Depth = "0-10 cm", # Set a new depth Label
    Number_SampleRings = mean(Number_SampleRings),
    Apparent_BD_g_cm3 = mean(`Apparent_BD_g/cm^3`),
    Actual_BD_g_cm3 = mean(`Actual_BD_g/cm^3`),
    FineSoilDensity_g_cm3 = mean(`FineSoilDensity_g/cm^3`)
  )
ST_Depths_0_to_10cm$Bulk_Density <- Mean_BD_0_to_10cm$Actual_BD_g_cm3

ST_Depths_0_to_10cm$Mass <- ST_Depths_0_to_10cm$Depth*ST_Depths_0_to_10cm$Area*
  ST_Depths_0_to_10cm$Bulk_Density

### 10 to 25cm
ST_Depths_10_to_25cm <- SoilC_ST_grasslands %>%
  filter(Depth %in% c("10-25 cm"))
ST_Depths_10_to_25cm$Depth <- 15
ST_Depths_10_to_25cm$Area <- 1.0

BD_10_to_25cm <- SoilC_BD_grasslands %>%
  filter(Depth %in% c("15-20 cm", "20-25 cm"))

# Group by Site and calculate the mean for each group
Mean_BD_10_to_25cm <- BD_10_to_25cm %>%
  group_by(Site) %>%
  summarise(
    Depth = "10-25 cm", # Set a new depth Label
    Number_SampleRings = mean(Number_SampleRings),
    Apparent_BD_g_cm3 = mean(`Apparent_BD_g/cm^3`),
    Actual_BD_g_cm3 = mean(`Actual_BD_g/cm^3`),
    FineSoilDensity_g_cm3 = mean(`FineSoilDensity_g/cm^3`)
  )
ST_Depths_10_to_25cm$Bulk_Density <- Mean_BD_10_to_25cm$Actual_BD_g_cm3

ST_Depths_10_to_25cm$Mass <- ST_Depths_10_to_25cm$Depth*ST_Depths_10_to_25cm$Area*
  ST_Depths_10_to_25cm$Bulk_Density

# Total Mass
Total_Mass = ST_Depths_0_to_10cm$Mass + ST_Depths_10_to_25cm$Mass

ST_Depths_0_to_10cm$Total_Mass_0_25 <- Total_Mass
ST_Depths_10_to_25cm$Total_Mass_0_25 <- Total_Mass

# Mass weighing values (MW_values)
ST_Depths_0_to_10cm$MW_values <- ST_Depths_0_to_10cm$Mass/ST_Depths_0_to_10cm$Total_M
ass_0_25
ST_Depths_10_to_25cm$MW_values <- ST_Depths_10_to_25cm$Mass/ST_Depths_10_to_25cm$Tota
l_Mass_0_25

```

```

# Weight samples
Soil_Text_0_10cm_MW <- data.frame(Clay_MW = ST_Depths_0_to_10cm$`%_Clay`*ST_Depths_0_
to_10cm$MW_values,
                                Coarse_sand_MW = ST_Depths_0_to_10cm$`%_CoarseSand`*
                                Fine_sand_MW = ST_Depths_0_to_10cm$`%_FineSand`*ST_D
epths_0_to_10cm$MW_values,
                                Total_sand_MW = ST_Depths_0_to_10cm$`%_TotalSand`*ST
_Depths_0_to_10cm$MW_values,
                                Silt_MW = ST_Depths_0_to_10cm$`%_Silt`*ST_Depths_0_t
o_10cm$MW_values
                                )

Soil_Text_10_25cm_MW <- data.frame(Clay_MW = ST_Depths_10_to_25cm$`%_Clay`*ST_Depths_
10_to_25cm$MW_values,
                                Coarse_sand_MW = ST_Depths_10_to_25cm$`%_CoarseSan
d`*ST_Depths_10_to_25cm$MW_values,
                                Fine_sand_MW = ST_Depths_10_to_25cm$`%_FineSand`*S
T_Depths_10_to_25cm$MW_values,
                                Total_sand_MW = ST_Depths_10_to_25cm$`%_TotalSand`
*ST_Depths_10_to_25cm$MW_values,
                                Silt_MW = ST_Depths_10_to_25cm$`%_Silt`*ST_Depths_
10_to_25cm$MW_values)

# Sum values
Soil_Text_0_25cm_MW <- Soil_Text_0_10cm_MW + Soil_Text_10_25cm_MW

#####

#-----
# Calculating SOC stock by Layer
#-----
# To calculate SOC stock we need to do it by Layer which requires BD, Carbon (%) and
depth

# Gather all information into one dataframe
Carbon_and_BD_df <- Carbon_by_depth %>%
  left_join(Mean_BD_0_to_10cm, by = "Site")

Carbon_and_BD_df <- Carbon_and_BD_df %>%
  left_join(Mean_BD_15_to_25cm, by = "Site")
names(Mean_BD_15_to_25cm)

## [1] "Site" "Apparent_BD_15_25cm"
## [3] "Actual_BD_15_25cm" "FineSoilDensity_15_25cm"

# Calculate 0-10cm SOC stock
Carbon_and_BD_df <- Carbon_and_BD_df %>%
  mutate(Carbon_Stock_0_10cm = Carbon_0_10cm * Mean_BD_0_to_10cm$Actual_BD_g_cm3 * 10
)

# Calculate 10-25cm SOC stock
Carbon_and_BD_df <- Carbon_and_BD_df %>%
  mutate(Carbon_Stock_10_25cm = Carbon_10_25cm * Mean_BD_10_to_25cm$Actual_BD_g_cm3 *
15)

# Total SOC stock
Carbon_and_BD_df <- Carbon_and_BD_df %>%
  mutate(Carbon_Stock_0_25cm = Carbon_Stock_0_10cm + Carbon_Stock_10_25cm)
# View(Carbon_and_BD_df)

#####

#-----
# Easting and Northing converison
#-----
# SoilC provides easting and northing conversions. These need to be converted to lati
tude and longitude.

```

```

# install.packages("sf")
library(sf)

## Warning: package 'sf' was built under R version 4.3.3

## Linking to GEOS 3.11.2, GDAL 3.8.2, PROJ 9.3.1; sf_use_s2() is TRUE

grassland_coords <- data.frame(easting = SoilC_grassland$Easting_ING,
                               northing = SoilC_grassland$Northing_ING)

# Convert to an sf object with the Irish National Grid (ING) CRS
grassland_coords_sf <- st_as_sf(grassland_coords, coords = c("easting", "northing"),
                                crs = 29902) # EPSG:29902 for ING

# Transform to WGS84 (EPSG:4326)
grassland_coords_latlon <- st_transform(grassland_coords_sf, crs = 4326)

# Extract the Latitude and Longitude
latlon <- st_coordinates(grassland_coords_latlon)
latlon_df <- data.frame(Longitude = latlon[, 1], Latitude = latlon[, 2])

#####

#-----
# RothC model inputs
#-----
RothC_Inputs <- data.frame(ID = 1:length(SoilC_grassland$Site),
                           Site = SoilC_grassland$Site,
                           Location = SoilC_grassland$County,
                           Clay = round(Soil_Text_0_25cm_MW$Clay_MW,2),
                           SOC_stock = round(Carbon_and_BD_df$Carbon_Stock_0_25cm,2),
                           Latitude = latlon_df$Latitude,
                           Longitude = latlon_df$Longitude)

# print(RothC_Inputs)
# write.csv(RothC_Inputs, "SoilC_IMG_inputs.csv")

#####

#-----
# Other SoilC parameters
#-----
# Join all all parameters together (0 to 25cm)
combined_df <- SoilC_grassland %>%
  left_join(Carbon_and_BD_df, by = "Site")

combined_df <- combined_df %>%
  left_join(Weighted_Chem_P_0_to_25cm, by = "Site")

Soil_Text_0_25cm_MW$Site <- SoilC_grassland$Site
combined_df <- combined_df %>%
  left_join(Soil_Text_0_25cm_MW, by = "Site")

SoilC_Parameters_0_25cm <- combined_df
# write.csv(SoilC_Parameters_0_25cm, "SoilC_Parameters_0_25cm.csv")

#-----
# Overview table
#-----
Overview_table <- data.frame(Site = SoilC_grassland$Site,
                              Country = SoilC_grassland$County,
                              SoilType = SoilC_grassland$SoilType,
                              ParentMaterial = SoilC_grassland$ParentMaterial,
                              Elevation = SoilC_grassland$Elevation_GPS_m,
                              Clay = Soil_Text_0_25cm_MW$Clay_MW,
                              TotalSand = Soil_Text_0_25cm_MW$Total_sand_MW,
                              Silt = Soil_Text_0_25cm_MW$Silt_MW,
                              SOC = Carbon_and_BD_df$Carbon_Stock_0_25cm,

```

```

BulkDensity = Weighted_Mean_BD_0_to_25cm$Actual_BD_g_cm3
,
pH = Weighted_Chem_P_0_to_25cm$pH,
Organic_Matter = Weighted_Chem_P_0_to_25cm$`OrganicMatte
r_%`,
C_N_ratio = Weighted_Chem_P_0_to_25cm$`C/N Ratio`)
# write.csv(Overview_table, "Overview_table.csv")

#####

#-----
# C% added
#-----
Overview_table_Carbon <- data.frame(Site = SoilC_grassland$Site,
Country = SoilC_grassland$County,
SoilType = SoilC_grassland$SoilType,
ParentMaterial = SoilC_grassland$ParentMaterial,
Elevation = SoilC_grassland$Elevation_GPS_m,
Clay = Soil_Text_0_25cm_MW$Clay_MW,
TotalSand = Soil_Text_0_25cm_MW$Total_sand_MW,
Silt = Soil_Text_0_25cm_MW$Silt_MW,
SOC = Carbon_and_BD_df$Carbon_Stock_0_25cm,
BulkDensity = Weighted_Mean_BD_0_to_25cm$Actual_BD_g_cm3
,
pH = Weighted_Chem_P_0_to_25cm$pH,
Organic_Matter = Weighted_Chem_P_0_to_25cm$`OrganicMatte
r_%`,
C_N_ratio = Weighted_Chem_P_0_to_25cm$`C/N Ratio`,
Carbon = Weighted_Chem_P_0_to_25cm$`Carbon_%`)
# write.csv(Overview_table_Carbon, "Overview_table_Carbon.csv")

```

Appendix C.2

This appendix provides the user guide for the Mineral Grassland (MG) model. It describes the model's operation, the underlying assumptions made during SOC stock estimation, and the data requirements for its application. Using the input data outlined in Appendix C.1, the results presented in Chapter 6 can be fully replicated. The following presents the output from the corresponding R Markdown file.

Mineral Grassland (MG) Model - User Guide

2025-09-01

Introduction

The Mineral Grassland (MG) Model is a generic framework designed to estimate soil organic carbon (SOC) stocks in mineral grassland soils. Rather than being an entirely novel model, it integrates three established components into a unified system for estimating SOC stocks across multiple grassland sites using a standardised methodology. These components include:

1. **Climate Module** – This module utilises Network Common Data Form (NetCDF) files containing national gridded climate data. These files are processed using the R package `climate4R` (Iturbide *et al.*, 2019), which extracts site-specific information on temperature and precipitation based on latitude and longitude coordinates. The monthly mean temperature is then used to estimate evapotranspiration (ET) via the Thornthwaite (1948) method, implemented through the SPEI R package (Beguería *et al.*, 2014).
2. **Carbon (C) Input Model** - This component applies the Miami model of net primary production (NPP) (Lieth, 1973) to estimate NPP based on annual temperature and precipitation values. Carbon inputs are derived from NPP following the approach of Peralta *et al.* (2022), converting Miami NPP (Dry Matter; $\text{gm}^{-2} \text{yr}^{-1}$) to $\text{t C ha}^{-1} \text{yr}^{-1}$ for a grassland system.
3. **The RothC model** - The RothC model is a widely used SOC model that estimates SOC stocks at plot and regional scales (Coleman *et al.*, 1997; 2024). In this framework, the RothC model is implemented in R using the SoilR package (Sierra *et al.*, 2012) and is hereafter referred to as 'RothC_R'.

Each component is described in detail in its respective literature and user documentation. For further information, refer to:

- **climate4R**: Iturbide *et al.* (2019); <https://github.com/SantanderMetGroup/climate4R>.
- **Miami Model**: Lieth (1973); Peralta *et al.* (2022).
- **RothC Model**: Coleman *et al.* (1997, 2024); <https://www.rothamsted.ac.uk/rothamsted-carbon-model-rothc>.
- **SoilR Framework**: Sierra *et al.* (2012); <https://www.bgc-jena.mpg.de/TEE/software/soilr/>.

To avoid redundancy, this user guide focuses on the integration and methodology specific to the MG Model.

Our proposed framework is designed to be relatively simple and streamlined. This allows the MG Model to generate SOC stocks with minimal data requirements for almost any site. The data inputs required to operate this model are:

1. Latitude

2. Longitude
3. Clay (as %)
4. Known SOC stock measurement (Mg C ha^{-1})
5. Sampling depth (e.g., 10cm, 25cm, 30cm)

These inputs can be supplied via a comma-separated values (CSV) file to enable batch processing of multiple sites or entered directly in the R environment using an appropriately structured data frame.

MG Structure

The section outlines the functionality of each model component within the MG Model and describes its interactions.

Climate Module

The climate module is the initial step in the MG Model workflow. Upon providing the model with site latitude and longitude coordinates via a .csv file or manually, the climate4R framework retrieves monthly temperature and precipitation values for the specified location. The monthly average temperature estimates evapotranspiration (ET) using the Thornthwaite method (Thornthwaite, 1948), implemented via the SPEI R package. At this stage, the MG Model has generated climatic data for:

- Monthly temperature.
- Monthly precipitation.
- Monthly Thornthwaite ET, for the length of the desired simulation

Additionally, a long-term average (LTA) is calculated for the appropriate period, which is used in both the C Input Model and the RothC_R Model.

Carbon Input Model

The C input model utilises the Miami model of NPP (Lieth, 1973), a simple conceptual model that links the NPP to annual mean temperature and total precipitation (Grieser *et al.*, 2006). The Climate Module outputs supply the yearly mean temperature and total precipitation. A single NPP estimate is derived using the Miami Model with the LTA values, followed by annual NPP values from the remaining length of the model simulation. Carbon inputs are derived from Miami NPP values by the following equation: $C_{input_{Miami}} = Miami_{NPP} * 0.01 * 0.45 * CRC$.

Where $C_{input_{Miami}}$ are C input values derived from Miami NPP values ($Miami_{NPP}$) converted to t C ha^{-1} by 0.01, assuming a C content of plant biomass of 0.45% and an appropriate C input Reduction Coefficient (CRC). The Miami-derived C input values are often too large for the RothC; the purpose of the CRC is to reduce C input to more appropriate values. Two data frames of C input values are derived from the C input model

- A single C input estimate using the LTA climate data.

- Annual C input estimates for the remainder of the simulation

RothC_R Model

The final stage of the MG Model is the RothC_R model. The RothC_R requires the outputs from the Climate Module and C input model as inputs, clay content and a known SOC stock measurement supplied to the model. The known SOC stock measurement has two purposes:

- To estimate the size of the inert organic (IOM) pool.
- Required for measured versus modelled analysis.

The RothC_R is not an emulation of the RothC model. Rather, it provides a generalised matrix-based framework to replicate any SOC model of decomposition. Some notable differences between the original RothC Windows Model are:

- Different language architectures.
- RothC_R C inputs and SCF must be entered annually instead of the monthly values prescribed to the RothC Windows Model.
- RothC_R requires an SCF to amended to external environmental(xi) modifier.

Our RothC_R model has a 'spin-up' phase, followed by an annual simulation. The spin-up model determines the initial pool sizes of the active pools (e.g., DPM, RPM, BIO and HUM) by repeating LTA climatic and C input values. Once the initial pool sizes are determined, we can run this model forward for the desired length of the simulation. Operating the RothC_R model with annual C inputs is challenging, as C input vectors are handled as constants. For more detailed information on the SoilR C inputs, please visit the SoilR workflow packages: <https://www.bgc-jena.mpg.de/TEE/basics/2023/09/20/Input-Fluxes/>.

To circumvent this, we created a daisy chain of RothC_R models that operate on a 5-year basis, with the next consecutive model relying on the outputs of the previous model within the sequence. Once the RothC_R model is finished, we will have estimated the SOC stock for the desired period for the site. Now that we have a rudimentary understanding of the MG Model components and workflow structure, we can work through a practical example of the model in operation.

Input Data

The required R packages required to operate the MG Model and plot the results are:

```
# install.packages("") # if needed

library(readr)
library(devtools)
library(loader)
library(transformer)
library(downscaleR)
library(visualizeR)
library(tidyverse)
library(dplyr)
library(SPEI)
```

```
library(SoilR)
library(cowplot)
```

The climate4R packages can be challenging to install. Please check their official GitHub: <https://github.com/SantanderMetGroup/climate4R>, if this problem occurs.

For this practical example, we will utilise a publicly accessible Irish land-use-oriented SOC database called the ‘SoilC project’. This data set can be downloaded from <https://eparesearch.epa.ie/safer/iso19115/displayISO19115.jsp?isoID=107>. The relative file for this experiment is “Att 5 SoilC_FinalData_04-Sept-08”, but it must be formatted to create suitable RothC model inputs. The sampling campaign for the SoilC project was undertaken between May 2006 and February 2007. We can read in the amended database with the following code:

```
SoilC_MG <- read_csv("~/Chapter_6_Modelling_Irish_SOC/SoilC_data/SoilC_IMG_inputs.csv")
head(SoilC_MG)

## # A tibble: 6 × 8
##   ...1 ID Site Location Clay SOC_stock Latitude Longitude
##   <dbl> <dbl> <dbl> <chr>   <dbl>   <dbl>   <dbl>   <dbl>
## 1     1     1     68 Wexford  36.6     58.3     52.5    -6.29
## 2     2     2    126 Carlow   6       112.     52.9    -6.65
## 3     3     3    180 Tipperary 19.5     80.6     52.5    -7.77
## 4     4     4    268 Kildare  17.9     74.6     53.1    -6.72
## 5     5     5    355 Cork     7.46     77.9     51.8    -8.71
## 6     6     6    358 Cork     19.0     77.8     51.8    -8.28
```

For more information on the SoilC Project, please see Kiely *et al.* (2009). For demonstration purposes, we will select a single site; site 180 was chosen to run the MG Model. To select Site 180 from the list of sites, we can subset it:

```
SoilC_MG_inputs <- SoilC_MG[3,]
latitude <- SoilC_MG_inputs$Latitude
longitude <- SoilC_MG_inputs$Longitude
Site_clay <- SoilC_MG_inputs$Clay
SOC <- SoilC_MG_inputs$SOC_stock
Site_soil.thick = 25 # Soil thickness in cm
Site_ID <- SoilC_MG_inputs$Site

print(SoilC_MG_inputs)

## # A tibble: 1 × 8
##   ...1 ID Site Location Clay SOC_stock Latitude Longitude
##   <dbl> <dbl> <dbl> <chr>   <dbl>   <dbl>   <dbl>   <dbl>
## 1     3     3    180 Tipperary 19.5     80.6     52.5    -7.77
```

This process can be automated within the MG Model for a series of sites by incorporating a basic loop like this:

```
# SoilC_MG_inputs <- SoilC_MG
# for (i in 1:nrow(SoilC_MG)) {
#   SoilC_MG_inputs <- SoilC_IMG[i, ]
#
#   SoilC_MG_inputs <- SoilC_MG
#   SoilC_MG_inputs <- SoilC_MG_inputs[i,] # Change value to match site/row # of inte
rest.

# Latitude <- SoilC_MG_inputs$Latitude
# Longitude <- SoilC_MG_inputs$Longitude
# Site_clay <- SoilC_MG_inputs$Clay
# SOC <- SoilC_MG_inputs$SOC_stock
# Site_soil.thick = 25 # Soil thickness in cm
# Site_ID <- SoilC_MG_inputs$Site
```

```
# ..... Place closing bracket after the final line.....
# }
```

Some coefficients are required to ensure the RothC_R model remains faithful to the original and reduces the C input values. The original RothC model has a soil cover factor (SCF) to reduce decomposition rates by 0.60 if the soil is vegetated (Coleman *et al.*, 2024). However, RothC_R lacks SCF but can be easily amended into the environmental rate modifier. For now, you can define the SCF as:

```
SCF = 0.60 # Soil Cover Factor
```

Another coefficient that will need to be adjusted depending on the vegetation, location or climate is the CRC. This value is a simple adjustment coefficient to lower the C input values, which can be expressed as:

```
CRC = 0.72 # C input reduction coefficient
```

These coefficients and factors can be expressed anywhere in the MG Model. However, we decided to place them in the data inputs section as these values are subject to change depending on the management system, location, vegetation type, and coverage.

Climate Module

The Climate Module is predominantly based on the 'climate4R' package. The original developers, Iturbide *et al.* (2019), have already detailed the code utilised in this section. To understand the following code section, refer to Iturbide *et al.* (2019) and <https://github.com/SantanderMetGroup/climate4R>. The climate model is the initial component of the MG model and provides key climatic inputs for the C Input and RothC_R models. For the practical example, the NetCDF files are Met Eireann meteorological 1x1km Irish grid (TM65). This data set's temperature range is from 1951 to 2020, and rainfall ranges from 1961 to 2020. Therefore, we want a uniform meteorological range from 1961 to 2020.

```
MEh_Temp = "~/Climate4R/Gridded_Weatherfiles/Unzipped/tas/tas"
list.files(MEh_Temp, recursive = T)

MEh_Rain = "~/Climate4R/Gridded_Weatherfiles/Unzipped/pr/pr"
list.files(MEh_Rain, recursive = T)

makeAggregatedDataset(source.dir = MEh_Temp, recursive = T, ncml.file = "MetEireann_Temp_hist.ncml")
makeAggregatedDataset(source.dir = MEh_Rain, recursive = T, ncml.file = "MetEireann_Rain_hist.ncml")

# Created ncml.files are used as a single access point to load data and to do the data inventory aswell:
di_Temp <- dataInventory("MetEireann_Temp_hist.ncml")
di_Rain <- dataInventory("MetEireann_Rain_hist.ncml")

# Latitude & Longitude range
lat_plus0.1 <- latitude + 0.1
lat_minus0.1 <- latitude - 0.1

lon_plus0.1 <- longitude + 0.1
lon_minus0.1 <- longitude - 0.1

lon <- c(lon_plus0.1, lon_minus0.1)
lat <- c(lat_plus0.1, lat_minus0.1)

# Loading Historical Monthly Temperature Data
```

```

MetEireann_Temp <- loadGridData(dataset = "MetEireann_Temp_hist.ncml",
                                var = "tas",
                                season = 1:12,
                                lonLim = lon,
                                latLim = lat,
                                years = 1961:2020,
                                aggr.m = "mean")

MetEireann_Rain <- loadGridData(dataset = "MetEireann_Rain_hist.ncml",
                                var = "pr",
                                season = 1:12,
                                lonLim = lon,
                                latLim = lat,
                                years = 1961:2020,
                                aggr.m = "sum")

MetEireann_Temp.annual <- aggregateGrid(MetEireann_Temp, aggr.m = list(FUN = "mean"))
MetEireann_Rain.annual <- aggregateGrid(MetEireann_Rain, aggr.m = list(FUN = "sum"))

# Obtaining temperature values for site of interest
S1_Temp_sm <- subsetSpatial(MetEireann_Temp, lonLim = longitude, latLim = latitude)
S1_Temp <- data.frame(S1_Temp_sm$Dates['start'], S1_Temp_sm$Data)
stno_S1_Temp <- data.frame(S1_Temp_sm$Dates['start'], S1_Temp_sm$Data)

# Obtaining rainfall values for site of interest
S1_Rain_sm <- subsetSpatial(MetEireann_Rain, lonLim = longitude, latLim = latitude)
S1_Rain <- data.frame(S1_Rain_sm$Dates['start'], S1_Rain_sm$Data)
stno_S1_Rain <- data.frame(S1_Rain_sm$Dates['start'], S1_Rain_sm$Data)

```

We can now estimate Thornthwaite evapotranspiration (ET) using the monthly temperature values derived from the climate4R processing. Thornthwaite is one of the simplest methods for estimating ET. However, it was selected based on two reasons:

- It only requires a monthly temperature, allowing it to be used at almost every site.
- Previous results have shown that the RothC model is relatively insensitive to different ET estimates (Maas and Lal, 2023), and preliminary testing demonstrated that Thornthwaite performed very well compared to other ET methods (see Chapter 5).

```

Thornthwaite <- thornthwaite(Tave = S1_Temp$S1_Temp_sm.Data, lat = latitude)

## [1] "Checking for missing values (`NA`): all the data must be complete. Input type
is vector. Assuming the data are monthly time series starting in January, all regular
(non-leap) years."

```

Now that the main climatic inputs are obtained, we can organise our climatic results into a data frame, which we can use to run the RothC_R model later and plot.

```

Climate_df <- data.frame(Date = stno_S1_Temp$start,
                        Temperature = stno_S1_Temp$S1_Temp_sm.Data,
                        Rainfall = stno_S1_Rain$S1_Rain_sm.Data,
                        ET = Thornthwaite)

Climate_df <- Climate_df %>%
  mutate(Month = format(as.Date(Date), "%m"),
         Year = format(as.Date(Date), "%Y"))

```

We must separate some outputs from this data frame to calculate the long-term average and annual climatic values for the RothC spin-up and annual RothC model simulations.

```

# Filter the first 10 years (1971-1980) for the LTA period
LTA_period <- Climate_df %>%

```

```

filter(Year >= 1961 & Year <= 1970)

LTA_Climate <- LTA_period %>%
  filter(Year >= 1961 & Year <= 1970) %>%
  group_by(Month) %>%
  summarise(
    Temperature = mean(Temperature, na.rm = TRUE),
    Rainfall = mean(Rainfall, na.rm = TRUE),
    Thornthwaite = mean(ET, na.rm = TRUE))

# Meteorological period (1981-2020)
Climate_period <- Climate_df %>%
  filter(Year >= 1971 & Year <= 2020)

```

This is the end of the Climate Module, in which the outputs are monthly temperature, rainfall and ET.

Carbon Input Model

The C input model relies on the climatic outputs of the Climate Module, as the Miami model of NPP requires annual temperature and rainfall. The Miami Model can be expressed as:

```

miami_npp <- function(T, P) {
  NPP_max <- 3000 # Maximum possible NPP in gC/m²/year
  NPP_T <- NPP_max * (1 - exp(-0.119 * (T - 3.98)))
  NPP_P <- NPP_max * (1 - exp(-0.000664 * P))
  NPP <- min(NPP_T, NPP_P)
  return(NPP)
}

```

To calculate the C input for the spin-up model, we can supply the Miami model with LTA for temperature and rainfall:

```

Annual_LTA <- LTA_Climate %>%
  summarise(
    Annual_LTA_Temp = mean(Temperature, na.rm = TRUE),
    Annual_LTA_Rain = sum(Rainfall, na.rm = TRUE))

Miami_LTA_Output <- mapply(miami_npp, Annual_LTA$Annual_LTA_Temp, Annual_LTA$Annual_LTA_Rain)

```

The Miami model output is not in t C ha⁻¹ and must be converted into an appropriate C input:

```

Miami_LTA_Cinput <- Miami_LTA_Output * 0.01 * 0.45
Miami_LTA_Cinput <- Miami_LTA_Cinput * CRC

```

Again, this process must be done to estimate C inputs for the annual RothC_R model simulations.

```

Annual_Met <- Climate_period %>%
  group_by(Year) %>%
  summarise(Annual_Met_Temp = mean(Temperature, na.rm = TRUE),
    Annual_Met_Rain = sum(Rainfall, na.rm = TRUE))

# Meteorological C input
Miami_Annual_Output <- mapply(miami_npp, Annual_Met$Annual_Met_Temp, Annual_Met$Annual_Met_Rain)
Miami_Annual_Cinput <- (Miami_Annual_Output * 0.01 * 0.45)
Miami_Annual_Cinput <- Miami_Annual_Cinput * CRC

```

The RothC_R daisy chain operates on a 5-year basis. We need to divide the C inputs accordingly:

```

Miami_Cinput_M1 <- mean(Miami_Annual_Cinput[1:5])
Miami_Cinput_M2 <- mean(Miami_Annual_Cinput[6:10])
Miami_Cinput_M3 <- mean(Miami_Annual_Cinput[11:15])
Miami_Cinput_M4 <- mean(Miami_Annual_Cinput[16:20])
Miami_Cinput_M5 <- mean(Miami_Annual_Cinput[21:25])

Miami_Cinput_M6 <- mean(Miami_Annual_Cinput[26:30])
Miami_Cinput_M7 <- mean(Miami_Annual_Cinput[31:35])
Miami_Cinput_M8 <- mean(Miami_Annual_Cinput[36:40])
Miami_Cinput_M9 <- mean(Miami_Annual_Cinput[41:45])
Miami_Cinput_M10 <- mean(Miami_Annual_Cinput[46:50])

```

RothC_R Model

The RothC_R requires known pool sizes for each pool to simulate the SOC stocks moving forward. To estimate the size of the Inert Organic Matter (IOM) pool, we use the pedo-transfer function (PTF) proposed by Falloon *et al.* (1998), which estimates the size of the IOM pool based on a known SOC stock measurement. It can be expressed as:

```
Falloon_IOM = 0.049*SOC^(1.139)
```

We conduct a spin-up run to determine the other four active RothC_R pool (e.g., DPM, RPM, BIO, and HUM) sizes. This involves running the model into equilibrium with repeated climatic, soil and management conditions. The RothC_R rate of decomposition is calculated in the xi. frame, this needs to be calculated before executing the spin-up run.

```

SpinUp_Years = seq(1/12, 500, by=1/12) # 500 year spin-up.
SpinUp_ft = ft.RothC(LTA_Climate$Temperature)
SpinUp_fw_THO = fw.RothC(P=(LTA_Climate$Rainfall),
                        E=(LTA_Climate$Thorntwaite),
                        S.Thick = Site_soil.thick, pClay = Site_clay,
                        pE = 1, bare = FALSE)$b

SpinUp_xi.frame_THO = data.frame(SpinUp_Years, rep(SpinUp_ft*SpinUp_fw_THO*SCF, length.
out=length(SpinUp_Years)))

```

Once the modifying rates are calculated, we can use the RothC_R function to calculate the other initial pool sizes. The spin-up model can be executed using the following code:

```

SpinUp_Model = RothCModel(
  t=SpinUp_Years,
  C0 = c(DPM=0,
        RPM=0,
        BIO=0,
        HUM=0,
        IOM=Falloon_IOM),
  In = Miami_LTA_Cinput, # Obtained from the C input model
  clay = Site_clay, # Obtained from the user
  xi = SpinUp_xi.frame_THO)

SpinUp_Ct = getC(SpinUp_Model)
SpinUp_Model_Pool = as.numeric(tail(SpinUp_Ct,1))
names(SpinUp_Model_Pool)<-c("DPM", "RPM", "BIO", "HUM", "IOM")

```

We need to determine the decomposition rate for the annual RothC_R simulation runs.

```

Years = seq(1/12, 50, by=1/12) # The remaining of the simulation.
Annual_ft = ft.RothC(Climate_period$Temperature)

```



```

Annual_fw_THO = fw.RothC(P=(Climate_period$Rainfall),
                        E=(Climate_period$ET),
                        S.Thick = Site_soil.thick, pClay = Site_clay,
                        pE = 1, bare = FALSE)$b
Annual_xi.frame_THO = data.frame(Years,rep(Annual_ft*Annual_fw_THO*SCF,length.out=length(Years)))

```

As mentioned, we are operating the RothC_R model on a 5-year basis over 50 years. We achieve this by creating a daisy chain of 10 RothC_R models. Each 5-year RothC_R model has unique decomposition rates and a single C input value. We must divide our annual xi. frame to match this time interval. This can be done using the following code:

```

# Five-year sections
years5 <- seq(1/12, 5, by=1/12)

Annual_xi.frame_THO_M1 = data.frame(years5,rep(Annual_ft[1:60]*Annual_fw_THO[1:60]*SCF,length.out=length(years5)))
Annual_xi.frame_THO_M2 = data.frame(years5,rep(Annual_ft[61:120]*Annual_fw_THO[61:120]*SCF,length.out=length(years5)))
Annual_xi.frame_THO_M3 = data.frame(years5,rep(Annual_ft[121:180]*Annual_fw_THO[121:180]*SCF,length.out=length(years5)))
Annual_xi.frame_THO_M4 = data.frame(years5,rep(Annual_ft[181:240]*Annual_fw_THO[181:240]*SCF,length.out=length(years5)))
Annual_xi.frame_THO_M5 = data.frame(years5,rep(Annual_ft[241:300]*Annual_fw_THO[241:300]*SCF,length.out=length(years5)))

Annual_xi.frame_THO_M6 = data.frame(years5,rep(Annual_ft[301:360]*Annual_fw_THO[301:360]*SCF,length.out=length(years5)))
Annual_xi.frame_THO_M7 = data.frame(years5,rep(Annual_ft[361:420]*Annual_fw_THO[361:420]*SCF,length.out=length(years5)))
Annual_xi.frame_THO_M8 = data.frame(years5,rep(Annual_ft[421:480]*Annual_fw_THO[421:480]*SCF,length.out=length(years5)))
Annual_xi.frame_THO_M9 = data.frame(years5,rep(Annual_ft[481:540]*Annual_fw_THO[481:540]*SCF,length.out=length(years5)))
Annual_xi.frame_THO_M10 = data.frame(years5,rep(Annual_ft[541:600]*Annual_fw_THO[541:600]*SCF,length.out=length(years5)))

```

Now that we have pre-defined our 5-year section, we create our RothC_R daisy chain with ten RothC_R models that are linked together:

```

# Model 1:
Annual_M1 = RothCModel(
  t=years5,
  C0 = c(DPM = tail(SpinUp_Model_Pool["DPM"],1),
        RPM = tail(SpinUp_Model_Pool["RPM"],1),
        BIO = tail(SpinUp_Model_Pool["BIO"],1),
        HUM = tail(SpinUp_Model_Pool["HUM"],1),
        IOM = Falloon_IOM),
  In = Miami_Cinput_M1,
  clay = Site_clay,
  xi = Annual_xi.frame_THO_M1)
Annual_Ct_M1 = getC(Annual_M1)
Annual_Ct_M1 <- data.frame(Annual_Ct_M1)

# Model 2:
Annual_M2 = RothCModel(
  t=years5,
  C0 = c(DPM = tail(Annual_Ct_M1$X1,1),
        RPM = tail(Annual_Ct_M1$X2,1),
        BIO = tail(Annual_Ct_M1$X3,1),
        HUM = tail(Annual_Ct_M1$X4,1),
        IOM = Falloon_IOM),
  In = Miami_Cinput_M2,
  clay = Site_clay,
  xi = Annual_xi.frame_THO_M2)
Annual_Ct_M2 = getC(Annual_M2)

```



```

Annual_Ct_M2 <- data.frame(Annual_Ct_M2)

# Model 3:
Annual_M3 = RothCModel(
  t=years5,
  C0 = c(DPM = tail(Annual_Ct_M2$X1,1),
          RPM = tail(Annual_Ct_M2$X2,1),
          BIO = tail(Annual_Ct_M2$X3,1),
          HUM = tail(Annual_Ct_M2$X4,1),
          IOM = Falloon_IOM),
  In = Miami_Cinput_M3,
  clay = Site_clay,
  xi = Annual_xi.frame_THO_M3)
Annual_Ct_M3 = getC(Annual_M3)
Annual_Ct_M3 <- data.frame(Annual_Ct_M3)

# Model 4:
Annual_M4 = RothCModel(
  t=years5,
  C0 = c(DPM = tail(Annual_Ct_M3$X1,1),
          RPM = tail(Annual_Ct_M3$X2,1),
          BIO = tail(Annual_Ct_M3$X3,1),
          HUM = tail(Annual_Ct_M3$X4,1),
          IOM = Falloon_IOM),
  In = Miami_Cinput_M4,
  clay = Site_clay,
  xi = Annual_xi.frame_THO_M4)
Annual_Ct_M4 = getC(Annual_M4)
Annual_Ct_M4 <- data.frame(Annual_Ct_M4)

# Model 5:
Annual_M5 = RothCModel(
  t=years5,
  C0 = c(DPM = tail(Annual_Ct_M4$X1,1),
          RPM = tail(Annual_Ct_M4$X2,1),
          BIO = tail(Annual_Ct_M4$X3,1),
          HUM = tail(Annual_Ct_M4$X4,1),
          IOM = Falloon_IOM),
  In = Miami_Cinput_M5,
  clay = Site_clay,
  xi = Annual_xi.frame_THO_M5)
Annual_Ct_M5 = getC(Annual_M5)
Annual_Ct_M5 <- data.frame(Annual_Ct_M5)

# Model 6:
Annual_M6 = RothCModel(
  t=years5,
  C0 = c(DPM = tail(Annual_Ct_M5$X1,1),
          RPM = tail(Annual_Ct_M5$X2,1),
          BIO = tail(Annual_Ct_M5$X3,1),
          HUM = tail(Annual_Ct_M5$X4,1),
          IOM = Falloon_IOM),
  In = Miami_Cinput_M6,
  clay = Site_clay,
  xi = Annual_xi.frame_THO_M6)
Annual_Ct_M6 = getC(Annual_M6)
Annual_Ct_M6 <- data.frame(Annual_Ct_M6)

# Model 7:
Annual_M7 = RothCModel(
  t=years5,
  C0 = c(DPM = tail(Annual_Ct_M6$X1,1),
          RPM = tail(Annual_Ct_M6$X2,1),
          BIO = tail(Annual_Ct_M6$X3,1),
          HUM = tail(Annual_Ct_M6$X4,1),
          IOM = Falloon_IOM),
  In = Miami_Cinput_M7,
  clay = Site_clay,
  xi = Annual_xi.frame_THO_M7)

```

```

Annual_Ct_M7 = getC(Annual_M7)
Annual_Ct_M7 <- data.frame(Annual_Ct_M7)

# Model 8:
Annual_M8 = RothCModel(
  t=years5,
  C0 = c(DPM = tail(Annual_Ct_M7$X1,1),
          RPM = tail(Annual_Ct_M7$X2,1),
          BIO = tail(Annual_Ct_M7$X3,1),
          HUM = tail(Annual_Ct_M7$X4,1),
          IOM = Falloon_IOM),
  In = Miami_Cinput_M8,
  clay = Site_clay,
  xi = Annual_xi.frame_THO_M8)
Annual_Ct_M8 = getC(Annual_M8)
Annual_Ct_M8 <- data.frame(Annual_Ct_M8)

# Model 9:
Annual_M9 = RothCModel(
  t=years5,
  C0 = c(DPM = tail(Annual_Ct_M8$X1,1),
          RPM = tail(Annual_Ct_M8$X2,1),
          BIO = tail(Annual_Ct_M8$X3,1),
          HUM = tail(Annual_Ct_M8$X4,1),
          IOM = Falloon_IOM),
  In = Miami_Cinput_M9,
  clay = Site_clay,
  xi = Annual_xi.frame_THO_M9)
Annual_Ct_M9 = getC(Annual_M9)
Annual_Ct_M9 <- data.frame(Annual_Ct_M9)

# Model 10:
Annual_M10 = RothCModel(
  t=years5,
  C0 = c(DPM = tail(Annual_Ct_M9$X1,1),
          RPM = tail(Annual_Ct_M9$X2,1),
          BIO = tail(Annual_Ct_M9$X3,1),
          HUM = tail(Annual_Ct_M9$X4,1),
          IOM = Falloon_IOM),
  In = Miami_Cinput_M10,
  clay = Site_clay,
  xi = Annual_xi.frame_THO_M10)
Annual_Ct_M10 = getC(Annual_M10)
Annual_Ct_M10 <- data.frame(Annual_Ct_M10)

```

As each model produces its subset of results, we must combine all the model outputs.

```

# Combine all outputs
Annual_Ct <- rbind(Annual_Ct_M1, Annual_Ct_M2, Annual_Ct_M3, Annual_Ct_M4, Annual_Ct_
M5,
                  Annual_Ct_M6, Annual_Ct_M7, Annual_Ct_M8, Annual_Ct_M9, Annual_Ct_
M10)
Annual_Ct$Total <- rowSums(Annual_Ct[,1:5])

```

This is effectively the end of the MG Model. The following sections will discuss the model outputs, how the MG Model saves the outputs and how to evaluate the MG Model against multiple sites.

Site Graphs

The main outputs from the MG model are the climatic variables and SOC stock estimates. We can create the estimated SOC stock graphs with the following code:

```

date_sequence <- seq.Date(from = as.Date("1971-01-01"),
                          to = as.Date("2020-12-01"),

```

```

        by = "month")

SOC_df <- data.frame(Date = date_sequence ,
                    Estimate = Annual_Ct$Total)

SOC_graph <- ggplot(SOC_df, aes(x = Date, y = Estimate)) +
  geom_line() +
  labs(title = paste(Site_ID), x = "", y = "SOC stock (Mg C/ha)") +
  theme_minimal()

```

A similar process can be done to create a boxplot for the main climatic variables of temperature, rainfall and ET:

```

Climate_df$Month <- month.abb

# Temperature boxplot
Temp_Boxplot <- ggplot(Climate_df, aes(x = Month, y = Temperature, colour = Month)) +
  geom_boxplot() +
  scale_x_discrete(limits = month.abb) +
  labs(title = paste(Site_ID),
        x = "",
        y = expression("Temperature (~degree*C)")) +
  theme_minimal() +
  theme(axis.text.x = element_text(angle = 45, hjust = 1),
        legend.position = "none")

# Rainfall boxplot
Rain_Boxplot <- ggplot(Climate_df, aes(x = Month, y = Rainfall, colour = Month)) +
  geom_boxplot() +
  scale_x_discrete(limits = month.abb) +
  labs(title = paste(Site_ID),
        x = "",
        y = "Rainfall (mm)") +
  theme_minimal() +
  theme(axis.text.x = element_text(angle = 45, hjust = 1),
        legend.position = "none")

# Thornthwaite boxplot
ET_Boxplot <- ggplot(Climate_df, aes(x = Month, y = ET, colour = Month)) +
  geom_boxplot() +
  scale_x_discrete(limits = month.abb) +
  labs(title = paste(Site_ID),
        x = "",
        y = "ET (mm)") +
  theme_minimal() +
  theme(axis.text.x = element_text(angle = 45, hjust = 1),
        legend.position = "none")

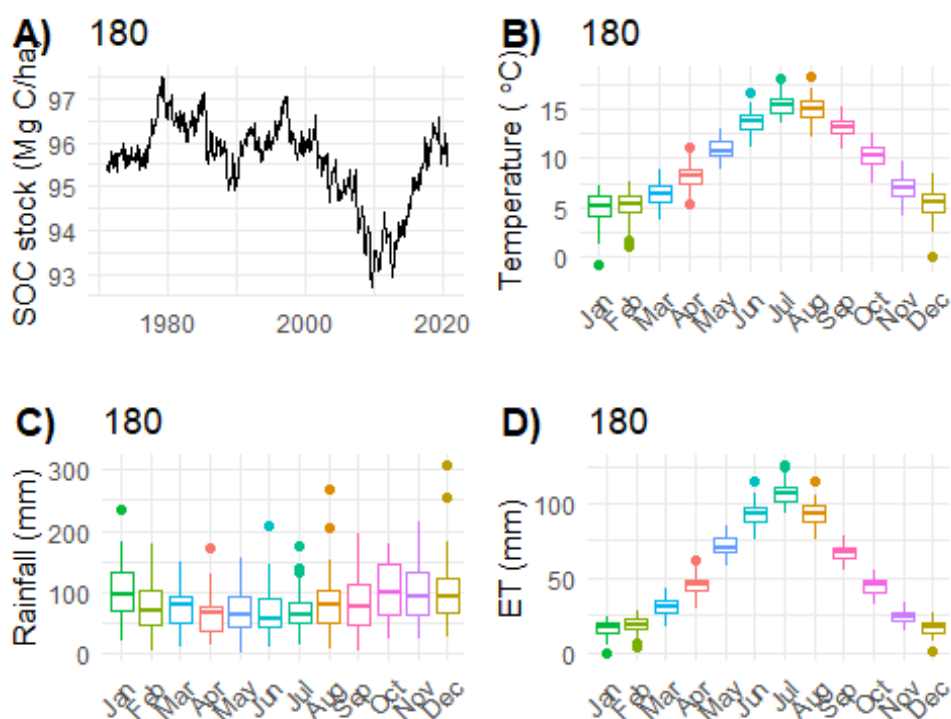
```

To view the climate box plots and the SOC stock estimation graph, we can arrange and plot them together:

```

SOC_climate_graph <- plot_grid(
  SOC_graph, Temp_Boxplot,
  Rain_Boxplot, ET_Boxplot,
  labels = c("A", "B", "C", "D"),
  ncol = 2)
print(SOC_climate_graph)

```



Summary Table

In addition to the site characteristics graphs, we can organise important site characteristics that are unsuitable for plotting into a summary table.

We can calculate the annual climatic variables from the MG Model to:

```
Climate_variables <- Climate_df %>%
  filter(Year >= 1961 & Year <= 2007)

Climate_summary <- Climate_variables %>%
  group_by(Year) %>%
  summarise(
    Temperature_Mean = mean(Temperature, na.rm = TRUE),
    Rainfall_Sum = sum(Rainfall, na.rm = TRUE),
    Thornthwaite_Sum = sum(ET, na.rm = TRUE))

Annual_Temp <- mean(Climate_summary$Temperature_Mean)
Annual_Rain <- mean(Climate_summary$Rainfall_Sum)
Annual_ET <- mean(Climate_summary$Thornthwaite_Sum)
```

Other important variables include the average C input and estimated SOC stock values for the year of interest and 10-year average to ensure the selected site is representative of the simulation for statistical analyses.

```
Mean_Cinput <- mean(Miami_Cinput_M1, Miami_Cinput_M2, Miami_Cinput_M3, Miami_Cinput_M4, Miami_Cinput_M5,
  Miami_Cinput_M6, Miami_Cinput_M7, Miami_Cinput_M8, Miami_Cinput_M9, Miami_Cinput_M10)

Estimated_SOC <- SOC_df %>% filter(Date == "2007-02-01") # SoilC samples were collected from May 2006 to February 2007.

SOC_10yr_avg <- SOC_df %>%
  filter(Date >= as.Date("1997-02-01") & Date <= as.Date("2007-02-01")) %>%
  summarise(Average_Estimated_SOC = mean(Estimate, na.rm = TRUE))

SOC_30yr_avg <- SOC_df %>%
```

```
filter(Date >= as.Date("1977-02-01") & Date <= as.Date("2007-02-01")) %>%
summarise(Average_Estimated_SOC = mean(Estimate, na.rm = TRUE))
```

Now, we create a summary table of the MG Model outputs and site characteristics provided by the user:

```
Summary_table <- data.frame(Site = Site_ID,
  Latitude = latitude,
  Longitude = longitude,
  Temperature = Annual_Temp,
  Rainfall = Annual_Rain,
  ET = Annual_ET,
  Clay = Site_clay,
  Cinput = Mean_Cinput,
  IOM = Falloon_IOM,
  Estimated_SOC = Estimated_SOC$Estimate,
  Measured_SOC = SOC,
  SOC_10yr = SOC_10yr_avg$Average_Estimated_SOC,
  SOC_30yr = SOC_30yr_avg$Average_Estimated_SOC)

print(Summary_table)
```

	Site	Latitude	Longitude	Temperature	Rainfall	ET	Clay	Cinput	IOM
## 1	180	52.47577	-7.765219	9.516469	977.6702	618.9645	19.5	4.2231	7.26962
			Estimated_SOC	Measured_SOC	SOC_10yr	SOC_30yr			
## 1		94.95851	80.6	95.61502	96.00426				

Exporting

The site graphs and summary table can be saved and exported for data analysis, graphing or collaboration. We employ a dynamic naming method to enable the MG Model to run multiple sites with the same code. We use the paste0 function to create unique names for each simulation. Each exported item will be saved as the Site ID, followed by the output title. Since this is site 180, all the associated files will be saved as "Site_ID_180...". You must create folders to save the individual simulations from the MG Model.

Once a folder is created to store the MG Model outputs, the site climatic and SOC stock graph can be saved with the following code:

```
setwd("~/Mineral_Grassland_Model/MG_results/MG_graphs") # Where we are storing our graph outputs
graph_filename <- paste0("Site_ID_", Site_ID, "Graphs.JPG")
ggsave(graph_filename, SOC_climate_graph, width = 10, height = 12, dpi = 300)
```

The summary table can be saved with the following code:

```
setwd("~/Mineral_Grassland_Model/MG_results/Summary_output") # Where we are storing our summary tables
output_name <- paste0("Site_ID_", Site_ID, "_summary.csv")
write.csv(Summary_table, output_name)
```

Other data frames, such as the SOC stock estimates and climatic values, can also be extracted to aid data visualisation and produce a paper trail of finished simulations.

```
SOC_estimate <- data.frame(Site = Site_ID,
  Date = SOC_df$Date,
  SOC_estimate = SOC_df$Estimate)
SOC_name <- paste0("Site_ID_", Site_ID, "_SOC_estimate.csv")

setwd("~/Mineral_Grassland_Model/MG_results/SOC_output")
write.csv(SOC_estimate, SOC_name)

Climate_df$Site <- Site_ID
```

```
Climate_file_name <- paste0("Site_ID_", Site_ID, "_climate_estimate.csv")
setwd("~/Mineral_Grassland_Model/MG_results/Climate_output")
write.csv(Climate_df, Climate_file_name)
```

Multiple Sites

If the MG Model is run for multiple sites, all outputs will be saved in the predefined folder. We can read multiple exported CSV files simultaneously, depending on what we want to graph. We can read the summary table to provide key values to aid graphs:

```
Site_Summary_List <- list.files(path = "~/Mineral_Grassland_Model/MG_results/Summary_
output",
                                pattern = "*.csv", full.names = TRUE)

Site_Summary <- lapply(Site_Summary_List, read.csv)
Site_Summary_df <- do.call(rbind, Site_Summary)

Site_Summary_df <- data.frame(Site = Site_Summary_df$Site,
                             Latitude = Site_Summary_df$Latitude,
                             Longitude = Site_Summary_df$Longitude,
                             Temperature = round(Site_Summary_df$Temperature,2),
                             Rainfall = round(Site_Summary_df$Rainfall,2),
                             ET = round(Site_Summary_df$ET,2),
                             Clay = Site_Summary_df$Clay,
                             IOM = round(Site_Summary_df$IOM,2),
                             Cinput = round(Site_Summary_df$Cinput,2),
                             Measured_SOC = round(Site_Summary_df$Measured_SOC),
                             Estimated_SOC = round(Site_Summary_df$Estimated_SOC,2),
                             SOC_10yr = round(Site_Summary_df$SOC_10yr,2),
                             SOC_30yr = round(Site_Summary_df$SOC_30yr,2))

Site_Summary_df <- Site_Summary_df[order(Site_Summary_df$Site), ]
```

We can analyse all the SOC stock estimates from the saved output folder to graph individual SOC stock simulations for the range of sites. The following code can do this:

```
# Read all CSV files and bind them together
Site_SOC_estimate <- list.files(path = "~/Mineral_Grassland_Model/MG_results/SOC_outp
ut",
                                pattern = "*.csv", full.names = TRUE)

Site_SOC_df <- Site_SOC_estimate %>%
  lapply(read.csv) %>%
  bind_rows()

Site_SOC_df <- Site_SOC_df %>%
  mutate(Date = as.Date(Date, format="%Y-%m-%d"))
```

We also need the measured SOC stock values for these sites obtained from the summary table:

```
# Measured SOC data frame
Site_Measured_SOC <- data.frame(Site = Site_Summary_df$Site,
                                Date = as.Date("2007-02-01"),
                                Measured_SOC = Site_Summary_df$Measured_SOC)
```

Now, we can create a plot for the measured and modelled SOC stock values for all the individual sites that the MG Model simulated for:

```
SoilC_Site_Simulations <- ggplot() +
  geom_line(data = Site_SOC_df,
            aes(x = Date, y = SOC_estimate, group = Site),
            color = "black", linewidth = 0.8) +
```

```

geom_point(data = Site_Measured_SOC,
           aes(x = Date, y = Measured_SOC, group = Site),
           color = "red", size = 2, shape = 16) +

facet_wrap(~ Site, scales = "fixed", ncol = 4) +
scale_y_continuous(breaks = function(x) pretty(x, n = 4)) +
labs(title = "",
     x = "",
     y = expression("SOC stock (Mg C ha-1)")) +
theme_minimal() +
theme(
  strip.background = element_rect(fill = "white", color = "dimgray", linewidth = 0.
5), # Border around site names
  strip.text = element_text(size = 10),
  panel.border = element_rect(color = "dimgray", fill = NA, linewidth = 0.5), # Bo
rder around graphs
  axis.text.x = element_text(angle = 45, hjust = 1),
  axis.text.y = element_text(size = 10),
  text = element_text(size = 10))

print(SoilC_Site_Simulations)

```

To evaluate the performance of the MG Model for selecting SoilC sites, we calculate the root mean square error (RMSE) with an RMSE of zero, indicating a perfect match.

```

# Calculate RMSE
Meas_v_Mod_RMSE <- sqrt(mean((Site_Summary_df$Measured_SOC - Site_Summary_df$Estimate
d_SOC)^2))

# Calculate %RMSE relative to the mean of observed values
observed_mean <- mean(Site_Summary_df$Measured_SOC, na.rm = TRUE)
percent_RMSE <- (Meas_v_Mod_RMSE / observed_mean) * 100

```

We can also graph the measured versus modelled analysis for all the sites and graph them with the total RMSE values.

```

# Create the Measured vs Modelled plot
Performance_plot <- ggplot(Site_Summary_df, aes(x = Measured_SOC, y = Estimated_SOC))
+
  geom_point(size = 3) +
  geom_smooth(data = Site_Summary_df, aes(x = Measured_SOC, y = Estimated_SOC),
             method = "lm", linetype = "solid", color = "blue", linewidth = 0.8, se
= FALSE) +
  geom_abline(slope = 1, intercept = 0, linetype = "dotted") +
  ylim(0, 170) +
  xlim(0, 170) +
  theme_minimal() +
  labs(
    title = "",
    x = expression("Measured SOC (Mg C ha-1)"),
    y = expression("Modelled SOC (Mg C ha-1)")
  ) +
  geom_smooth(method = "lm", linetype = "solid", color = "black", linewidth = 0.5, se
= FALSE) +
  annotate("text", x = 0, y = 150, label = paste("RMSE =", round(Meas_v_Mod_RMSE, 1))
,
         color = "red", size = 4, hjust = 0) +
  annotate("text", x = 0, y = 140, label = paste("%RMSE =", round(percent_RMSE, 1)),
         color = "red", size = 4, hjust = 0)

print(Performance_plot)

```

From the selection of sites, we simulated with the MG Model, resulting in an RMSE of 22.7 Mg C ha⁻¹. Overall, this result is poor; however, it displays great potential as

we utilise a fundamental framework. With further improvements via calibration or additional modifications, the MG Model could be more accurate.

Limitations

The primary limitation of our proposed MG Model framework lies in the carbon (C) input model. The methodology currently employed does not incorporate land-use management practices, thereby overlooking their influence on SOC dynamics. However, the MG Model is designed as a modular framework, allowing for future enhancements or replacements of individual components. Users can substitute the C input model with an alternative approach that better reflects the quality and availability of site or region-specific data.

Another potential drawback is the daisy-chaining of RothC_R model runs. While functional, this linear approach could be replaced with a more complex looping process to improve computational efficiency and enable the model to operate with annual C inputs rather than five-year averages. Although averaging over five years may obscure interannual variability, it should still provide a reliable representation of long-term SOC stock trends. Furthermore, the impact of this computational inefficiency is likely negligible when applying the MG Model to a relatively small number of sites (e.g., <50).

Appendix C.3

This appendix contains the ICBM extension of the MG model. The model ensemble combining RothC_R with alternative C and ET input methods is fully documented in the accompanying R Markdown file. Code and outputs are included here to ensure transparency and allow independent replication of the results presented in Chapter 5. The following presents the output from this R Markdown file.

Mineral Grassland Model - ICBM Configuration

2025-09-01

Introduction

One of the greatest strengths of the Mineral Grassland (MG) model is its transparency and flexibility. The MG model is designed to be modular, allowing for both minor and significant changes to the climate, carbon (C) input, and soil organic carbon (SOC) modules. We have already validated, verified, and evaluated the RothC model approach within the MG framework. In this document, we will demonstrate how to implement an alternative SOC model, the Introductory Carbon Balance Model (ICBM). This can allow the MG model to contain a suite of different SOC models to prevent over-calibration of a single approach.

Climate and C input Module

The climate and C input modules are the same as the original approach and are discussed in Appendix C.2. To avoid redundancy, this section will focus on the differences.

ICBM

The ICBM and RothC models are both process-based models used to simulate SOC dynamics. However, they differ significantly in complexity and structure. The ICBM is a simpler, semi-empirical model consisting of just two SOC pools: a young (Y) pool and an old (O) pool. One of the key differences between the two models is how they incorporate climate effects. In ICBM, the influence of climate is indirectly represented through the r coefficient, which governs the partitioning of carbon inputs between the two pools. In contrast, RothC applies climate modifiers (temperature, moisture, and cover) directly to decomposition rates. This ICBM was first described by Andrén and Kätterer (1997) and further developed in Kätterer and Andrén (2001). This implementation follows the formulation outlined by Sierra *et al.* (2012) using the default parameter values from earlier studies (Andrén and Kätterer, 1997; Kätterer and Andrén, 2001).

Similar to most SOC models, the initial pool sizes were determined by a model spin-up.

```
SpinUp_Years = seq(1/12, 500, by=1/12)

SpinUp_Model = ICBMModel(t = SpinUp_Years,
  ks = c(k1=0.8, k2=0.00605),
  h = 0.13,
  r = 1.32,
  c0 = c(Y0=0.0, O0=0.0),
  In = Miami_LTA_Cinput)

SpinUp_Ct = getC(SpinUp_Model)
SpinUp_Model_Pool = as.numeric(tail(SpinUp_Ct,1))
names(SpinUp_Model_Pool) <- c("Y", "O")
```

Once the initial pool sizes are determined, we can start our daisy-chain of ICBM models that operate at a 5-year time interval:

```
Years5 <- seq(1/12, 5, by=1/12)

# Model 1:
Annual_M1 = ICBMModel(t = Years5,
  ks = c(k1=0.8, k2=0.00605),
  h = 0.13,
  r = 1.32,
  c0 = c(Y0 = SpinUp_Model_Pool["Y"], O0 = SpinUp_Model_Pool["O"])
,
  In = Miami_Cinput_M1)

Annual_Ct_M1 = getC(Annual_M1)
Annual_Ct_M1 <- data.frame(Annual_Ct_M1)
names(Annual_Ct_M1) <- c("Y", "O")

# Model 2:
Annual_M2 = ICBMModel(t = Years5,
  ks = c(k1=0.8, k2=0.00605),
  h = 0.13,
  r = 1.32,
  c0 = c(Y0 = tail(Annual_Ct_M1$Y, 1),
```

```

        O0 = tail(Annual_Ct_M1$O, 1)),
        In = Miami_Cinput_M2)

Annual_Ct_M2 = getC(Annual_M2)
Annual_Ct_M2 <- data.frame(Annual_Ct_M2)
names(Annual_Ct_M2) <- c("Y", "O")

# Model 3:
Annual_M3 = ICBMModel(t = Years5,
                      ks = c(k1=0.8, k2=0.00605),
                      h = 0.13,
                      r = 1.32,
                      c0 = c(Y0 = tail(Annual_Ct_M2$Y, 1),
                             O0 = tail(Annual_Ct_M2$O, 1)),
                      In = Miami_Cinput_M3)

Annual_Ct_M3 = getC(Annual_M3)
Annual_Ct_M3 <- data.frame(Annual_Ct_M3)
names(Annual_Ct_M3) <- c("Y", "O")

# Model 4:
Annual_M4 = ICBMModel(t = Years5,
                      ks = c(k1=0.8, k2=0.00605),
                      h = 0.13,
                      r = 1.32,
                      c0 = c(Y0 = tail(Annual_Ct_M3$Y, 1),
                             O0 = tail(Annual_Ct_M3$O, 1)),
                      In = Miami_Cinput_M4)

Annual_Ct_M4 = getC(Annual_M4)
Annual_Ct_M4 <- data.frame(Annual_Ct_M4)
names(Annual_Ct_M4) <- c("Y", "O")

# Model 5:
Annual_M5 = ICBMModel(t = Years5,
                      ks = c(k1=0.8, k2=0.00605),
                      h = 0.13,
                      r = 1.32,
                      c0 = c(Y0 = tail(Annual_Ct_M4$Y, 1),
                             O0 = tail(Annual_Ct_M4$O, 1)),
                      In = Miami_Cinput_M5)

Annual_Ct_M5 = getC(Annual_M5)
Annual_Ct_M5 <- data.frame(Annual_Ct_M5)
names(Annual_Ct_M5) <- c("Y", "O")

# Model 6:
Annual_M6 = ICBMModel(t = Years5,
                      ks = c(k1=0.8, k2=0.00605),
                      h = 0.13,
                      r = 1.32,
                      c0 = c(Y0 = tail(Annual_Ct_M5$Y, 1),
                             O0 = tail(Annual_Ct_M5$O, 1)),
                      In = Miami_Cinput_M6)

Annual_Ct_M6 = getC(Annual_M6)
Annual_Ct_M6 <- data.frame(Annual_Ct_M6)
names(Annual_Ct_M6) <- c("Y", "O")

# Model 7:
Annual_M7 = ICBMModel(t = Years5,
                      ks = c(k1=0.8, k2=0.00605),
                      h = 0.13,
                      r = 1.32,
                      c0 = c(Y0 = tail(Annual_Ct_M6$Y, 1),
                             O0 = tail(Annual_Ct_M6$O, 1)),
                      In = Miami_Cinput_M7)

Annual_Ct_M7 = getC(Annual_M7)

```

```

Annual_Ct_M7 <- data.frame(Annual_Ct_M7)
names(Annual_Ct_M7) <- c("Y", "O")

# Model 8:
Annual_M8 = ICBMModel(t = Years5,
                      ks = c(k1=0.8, k2=0.00605),
                      h = 0.13,
                      r = 1.32,
                      c0 = c(Y0 = tail(Annual_Ct_M7$Y, 1),
                              O0 = tail(Annual_Ct_M7$O, 1)),
                      In = Miami_Cinput_M8)

Annual_Ct_M8 = getC(Annual_M8)
Annual_Ct_M8 <- data.frame(Annual_Ct_M8)
names(Annual_Ct_M8) <- c("Y", "O")

# Model 9:
Annual_M9 = ICBMModel(t = Years5,
                      ks = c(k1=0.8, k2=0.00605),
                      h = 0.13,
                      r = 1.32,
                      c0 = c(Y0 = tail(Annual_Ct_M8$Y, 1),
                              O0 = tail(Annual_Ct_M8$O, 1)),
                      In = Miami_Cinput_M9)

Annual_Ct_M9 = getC(Annual_M9)
Annual_Ct_M9 <- data.frame(Annual_Ct_M9)
names(Annual_Ct_M9) <- c("Y", "O")

# Model 10:
Annual_M10 = ICBMModel(t = Years5,
                      ks = c(k1=0.8, k2=0.00605),
                      h = 0.13,
                      r = 1.32,
                      c0 = c(Y0 = tail(Annual_Ct_M9$Y, 1),
                              O0 = tail(Annual_Ct_M9$O, 1)),
                      In = Miami_Cinput_M10)

Annual_Ct_M10 = getC(Annual_M10)
Annual_Ct_M10 <- data.frame(Annual_Ct_M10)
names(Annual_Ct_M10) <- c("Y", "O")

```

The outputs from the individual models can be joined into a singular data frame, and a new column can be created summing the two pools together:

```

# Combine all outputs
Annual_Ct <- rbind(Annual_Ct_M1, Annual_Ct_M2, Annual_Ct_M3, Annual_Ct_M4, Annual_Ct_M5,
                  Annual_Ct_M6, Annual_Ct_M7, Annual_Ct_M8, Annual_Ct_M9, Annual_Ct_M10)
Annual_Ct$Total <- rowSums(Annual_Ct[,1:2])

```

Graph sites and exporting

The MG model produces SOC stock, monthly temperature, monthly rainfall, and monthly evapotranspiration estimates. Graphing and exporting them was already discussed in the MG User guide in Appendix B.2. To avoid redundancy, this section will focus on the differences.

Model performance

Using the same 28 mineral grassland sites from the SoilC database, we conducted a comparison between measured and modelled SOC values. This analysis allows for a

direct evaluation of the ICBM model's performance and enables comparison with our earlier results using the RothC model.

```
setwd("~/Mineral_Grassland_Model/MG_ICBM_Adaption/MG_ICBM_Evaluation")

# Read in MG model (ICBM configuration) outputs
Site_Summary_List <- list.files(path = "~/Mineral_Grassland_Model/MG_ICBM_Adaption/MG_ICBM_Results/Summary_output",
                                pattern = "*.csv", full.names = TRUE)

Site_Summary <- lapply(Site_Summary_List, read.csv)
Site_Summary_df <- do.call(rbind, Site_Summary)

Site_Summary_df <- data.frame(Site = Site_Summary_df$Site,
                              Latitude = Site_Summary_df$Latitude,
                              Longitude = Site_Summary_df$Longitude,
                              Temperature = round(Site_Summary_df$Temperature,2),
                              Rainfall = round(Site_Summary_df$Rainfall,2),
                              ET = round(Site_Summary_df$ET,2),
                              Clay = Site_Summary_df$Clay,
                              Cinput = round(Site_Summary_df$Cinput,2),
                              Measured_SOC = round(Site_Summary_df$Measured_SOC),
                              Estimated_SOC = round(Site_Summary_df$Estimated_SOC,2),
                              SOC_10yr = round(Site_Summary_df$SOC_10yr,2),
                              SOC_30yr = round(Site_Summary_df$SOC_30yr,2))

Site_Summary_df <- Site_Summary_df[order(Site_Summary_df$Site), ]

# Graphing results
Meas_v_Mod_RMSE <- sqrt(mean((Site_Summary_df$Measured_SOC - Site_Summary_df$Estimated_SOC)^2)) # Calculate RMSE

Meas_v_Mod_plot <- ggplot(Site_Summary_df, aes(x=Measured_SOC, y=Estimated_SOC)) +
  geom_point(size = 3.5) +
  geom_abline(slope = 1, intercept = 0, linetype = "dotted") +
  ylim(0,170) +
  xlim(0,170) +
  theme_minimal() +
  labs(
    title = "ICBM",
    x = expression("Measured SOC (Mg C ha-1)"),
    y = expression("Modelled SOC (Mg C ha-1)") +
    geom_smooth(method = "lm", linetype = "solid", color = "blue", li
newwidth = 0.8, se = FALSE) +
    annotate("text", x = 0, y = 150, label = paste("RMSE =", round(Me
as_v_Mod_RMSE, 1)), color = "red", size = 5, hjust = 0) +
    theme(
      plot.title = element_text(size = 16, hjust = 0.5),
      axis.title = element_text(size = 16),
      axis.text = element_text(size = 16)
    )

print(Meas_v_Mod_plot)

## `geom_smooth()` using formula = 'y ~ x'
```

The measured versus modelled analysis revealed a root-mean-square error (RMSE) of 29.4 Mg C ha⁻¹, indicating a poor fit between observed and estimated SOC values.

Limitations

It is important to note that this analysis may not accurately reflect the actual performance of the ICBM. The implementation presented here was not directly cross-referenced with the original ICBM formulations, making it uncertain how faithfully the model has been replicated. Moreover, the use of default parameter

values may not be appropriate for mineral temperate grasslands. Therefore, further research is necessary to validate this implementation against the original ICBM and to calibrate model parameters to represent site-specific conditions better.

References

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