Dynamics of soil organic matter in agricultural systems: Assessing the impact of bioenergy production, agri-environmental measures and climate at regional scales

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Summary

The stability and fertility of the Earth’s soil resources are highly dependent on soil organic matter (SOM), which is also the world’s largest terrestrial carbon reservoir. SOM controls a wide range of physical, chemical and biological processes that are fundamental to maintaining and improving soil-based ecosystem functions and services, including primary production, climate regulation, water quality, erosion control and soil biodiversity. Increasing SOM stocks is therefore recognised as a crucial element in addressing the challenges of global change and achieving the UN sustainability goals. Nevertheless, while the appropriate management of SOM can provide economic, environmental and social benefits, there are significant challenges to achieving long-term gains in SOM stocks on arable land. A multitude of drivers, operating at different scales, influence the SOM cycle of arable land. Some of these drivers act through feedback loops that affect SOM through changes in the agricultural system or environmental boundaries. Consequently, systems analysis and regional assessments of SOM dynamics are vital for informed decision-making and an increased understanding of the impact of different drivers and potential management options. Unfortunately, the scarcity of appropriate tools, approaches and data represents a considerable challenge.

Against this background, the present thesis aims to improve the regional perspective on SOM in agricultural systems, which is crucial for the development of future carbon management policies. Specifically, this doctoral thesis aimed to (1) clarify and quantify significant carbon and matter fluxes in agricultural systems, (2) conduct spatially distributed and integrated simulations of soil carbon and nitrogen dynamics at regional scales, (3) evaluate the impact of climate and best management practices on SOM stocks, and (4) find methods to operationalise SOM modelling for policy support.

In order to achieve these objectives, the thesis focused on a specific case study, namely the federal state of Saxony in Germany, and conducted three research studies that have been published in peer-reviewed academic journals. The first study presents a novel approach for investigating the impact of bioenergy production systems on regional soil carbon cycling. Through an ex-post analysis of biogas production in the agricultural landscapes of Saxony, novel insights into agricultural carbon and matter fluxes, as well as the regional area requirements of biogas production are provided. The second study demonstrated a newly developed ‘regional mode’ for the CANDY Carbon Balance model (CCB), which is capable of simulating regional trends in soil organic carbon (SOC) stocks and organic matter-related nitrogen fluxes. The novel CCB module enables the use of aggregated data on agricultural management and grid-based modelling units. Finally, the new capabilities of CCB’s regional mode are employed to conduct a scaling experiment across a series of administrative levels with the aim to enhance the applicability and comparability of regional SOC assessments. Here, the SOC dynamics in Saxony as well as the carbon sequestration potential of selected best management practices are simulated using simplified, upscaled modelling set-ups.

The results showed that biogas plants in Saxony can be operated sustainably in terms of SOC recycling, but this is highly dependent on the application of digestate and is associated with considerable land requirements. For each kilowatt of installed electrical capacity, 2.0 ha of agricultural land was required to supply the biogas plants and to dispose their digestate. Regional SOM stocks increased over most of Saxony's arable land between 1998 and 2014, but with distinct regional differences. Both the increase in soil carbon inputs and the decrease in carbon turnover rates had positive effects on the SOM storage of Saxony, with the latter being largely driven by the increased use of conservation tillage. Along with the increase in SOC, a significant amount of nitrogen was immobilised. This presents a considerable risk of nitrate leaching if the measures that promote SOM stocks are not maintained. The simulation of SOC dynamics at the scale of administrative units has proven to be feasible in practice and provides results that can be considered acceptable in terms of their scaling error. Furthermore, the methodology proves to be advantageous for model set-up and its application. In light of these findings, the new regional mode of CCB has demonstrated its potential to improve the applicability and comparability of SOM assessments and thus provide an important basis for political decision-making processes. Field grass, cover crops, and conservation tillage have been identified as promising strategies for carbon sequestration in Saxon arable soils.

Overall, the diversity, complexity and interconnectedness of the drivers of SOM dynamics in agricultural landscapes are considerable. In this dissertation, this complexity was analysed from different perspectives and by applying novel methodological approaches. It must be acknowledged that there are still considerable uncertainties and limitations in regional assessments. Nevertheless, this thesis has made a valuable contribution to capacity building and provided concrete recommendations on how to improve SOM management in the case study region of Saxony and beyond.

Keywords: Soil organic matter, carbon sequestration, CCB model, regional scale assessment, biogas production system, reduced tillage, field grass, cover crops, climate change mitigation, areal efficiency, Saxony, administrative regions

Zusammenfassung

Die Stabilität und Fruchtbarkeit der Bodenressourcen der Erde hängen in hohem Maße von der organischen Bodensubstanz ab, die zudem den weltweit größten terrestrischen Kohlenstoffspeicher darstellt. Humus ist an einer Vielzahl physikalischer, chemischer und biologischer Prozesse beteiligt, die für den Erhalt und die Verbesserung der Ökosystemfunktionen und -leistungen des Bodens von grundlegender Bedeutung sind. Dazu gehören die Primärproduktion, die Regulierung des Klimas, die Verbesserung der Wasserqualität, der Erosionsschutz sowie die Förderung der biologischen Vielfalt des Bodens. Die Erhöhung der organischen Bodensubstanz ist daher ein entscheidendes Element, um den Herausforderungen des Globalen Wandels zu begegnen und die Nachhaltigkeitsziele der Vereinten Nationen zu erreichen. Obgleich eine adäquate Bewirtschaftung der organischen Bodensubstanz ökonomische, ökologische und soziale Vorteile mit sich bringen kann, sind doch erhebliche Herausforderungen zu bewältigen, um die Humusvorräte auf Ackerflächen langfristig zu erhöhen. Der landwirtschaftliche Humuskreislauf unterliegt einer Vielzahl von Einflussfaktoren, die auf unterschiedlichen Ebenen wirken. Einige dieser Einflussfaktoren entfalten ihre Wirkung in Form von Rückkopplungseffekten, z.B. durch Veränderungen des landwirtschaftlichen Systems oder bestimmter Umweltparameter. Systemanalysen und regionale Bewertungen der Humusdynamik sind daher von entscheidender Bedeutung für eine fundierte politische Entscheidungsfindung und ein besseres Verständnis der Auswirkungen verschiedener Einflussfaktoren und möglicher Bewirtschaftungsoptionen. Leider stellt der Mangel an geeigneten Instrumenten, Ansätzen und Daten eine große Herausforderung dar.

Vor diesem Hintergrund zielte diese Arbeit darauf ab, das Verständnis der regionalen Humusdynamik in landwirtschaftlichen Systemen zu verbessern, was für die Entwicklung zukünftiger Kohlenstoffmanagementstrategien von entscheidender Bedeutung ist. Konkret verfolgte die Dissertation vier Ziele: (1) die Analyse und Quantifizierung signifikanter Kohlenstoffflüsse in landwirtschaftlichen Systemen, (2) die Durchführung großmaßstäblicher, räumlich verteilter und integrierter Simulationen der Humusdynamik, (3) die Bewertung der Auswirkungen des Klimas und empfohlener landwirtschaftlicher Maßnahmen und (4) die Entwicklung von Verfahren zur Operationalisierung der Bodenkohlenstoff-Modellierung auf verschiedenen Entscheidungsebenen.

Um die genannten Ziele zu erreichen, wurden drei Studien durchgeführt, deren Ergebnisse in wissenschaftlichen Fachzeitschriften publiziert wurden. Die Forschungsarbeiten fokussierten sich dabei auf eine spezifische Fallstudie, nämlich das Bundesland Sachsen in Deutschland. Im Rahmen der ersten Studie wurde ein innovativer Ansatz zur Analyse der Auswirkungen von Bioenergieproduktionssystemen auf den regionalen Kohlenstoffkreislauf im Boden entwickelt. Mit Hilfe einer Ex-post-Analyse der Biogaserzeugung in den Agrarlandschaften Sachsens werden neue Erkenntnisse über die landwirtschaftlichen Stoffflüsse sowie den

regionalen Flächenbedarf der Biogaserzeugung gewonnen. In der zweiten Studie wurde ein neu entwickelter ‘regionaler Modus‘ für das CANDY-Carbon-Balance Modell (CCB) demonstriert, welcher die Simulation der regionalen Bodenkohlenstoffdynamik sowie damit verbundener Stickstoffflüsse ermöglicht. Das neu entwickelte Modul ermöglicht dabei die Verwendung aggregierter Daten zur landwirtschaftlichen Bewirtschaftung sowie rasterbasierter Modellierungseinheiten. In einem letzten Schritt werden die neuen Möglichkeiten von CCBs regionalen Modus genutzt, um ein Skalierungsexperiment über mehrere administrative Ebenen durchzuführen, mit dem Ziel, die Anwendbarkeit und Vergleichbarkeit regionaler Bodenkohlenstoffstudien zu verbessern. Dazu erfolgt die Simulation der Bodenkohlenstoffdynamik in Sachsen und des CO_2 Sequestrierungspotenzial ausgewählter landwirtschaftlicher Maßnahmen unter Verwendung vereinfachter, hochskalierter Modellaufbauten.

Die Ergebnisse legen nahe, dass Biogasanlagen in Sachsen in Bezug auf den Humuskreislauf nachhaltig betrieben werden können. Dies ist jedoch in erheblichem Maße von der Ausbringung der Gärreste abhängig und geht mit einem umfangreichen Flächenbedarf einher. Pro Kilowatt installierter elektrischer Leistung wurden 2,0 ha landwirtschaftliche Fläche zur Versorgung der Biogasanlagen und zur Entsorgung der Gärreste benötigt. Die rasterbasierte Simulation der regionalen Humusvorräte in den sächsischen Ackerböden zeigt eine Zunahme zwischen 1998 und 2014, allerdings mit deutlichen regionalen Unterschieden. Sowohl die Zunahme der Kohlenstoffeinträge in den Boden als auch die Abnahme des Kohlenstoffumsätze wirkten sich positiv auf die Humusspeicher in Sachsen aus. Letzteres ist insbesondere auf den verstärkten Einsatz konservierender Bodenbearbeitung zurückzuführen. Im Kontext der Zunahme des Bodenkohlenstoffs ist zudem eine erhebliche Menge an Stickstoff immobilisiert worden, welches ein signifikantes Auswaschungsrisiko birgt, sofern die humusfördernden Maßnahmen nicht fortgeführt werden. Die Simulation der Bodenkohlenstoffdynamik auf der Skala von Verwaltungseinheiten hat sich in der Praxis als durchführbar erwiesen und liefert Ergebnisse, die hinsichtlich ihres Skalierungsfehlers als akzeptabel zu bewerten sind. Des Weiteren erweist sich die Methodik als vorteilhaft für den Modellaufbau und -anwendung. In Anbetracht dieser Ergebnisse hat der neue regionale Modus von CCB sein Potenzial unter Beweis gestellt, die Anwendbarkeit und Vergleichbarkeit von Bodenkohlenstoffstudien zu verbessern und somit eine wichtige Grundlage für politische Entscheidungsprozesse zu liefern. Feldgras, Zwischenfrüchte und konservierende Bodenbearbeitung wurden als vielversprechende Strategien zur Kohlenstoffbindung in sächsischen Ackerböden identifiziert.

Die Vielfalt und Vernetzung der Einflussfaktoren auf die Humusdynamik in Agrarlandschaften ist beträchtlich. In dieser Dissertation wurde diese Komplexität aus verschiedenen Blickwinkeln und mit neuen methodischen Ansätzen untersucht. Es bleiben erhebliche Unsicherheiten und Einschränkungen bei regionalen Bewertungen. Dennoch leistet diese Arbeit einen wertvollen Beitrag zum Aufbau von Kapazitäten und gibt konkrete Empfehlungen zur Verbesserung des Humusmanagements in der Fallstudienregion Sachsen und darüber hinaus.

Publications

This cumulative dissertation synthesises three scientific publications that were published in peer-reviewed journals in the fields of soil science, environmental management and agronomy. The first two papers are reprinted with permission from Geoderma (Elsevier) and Journal of Environmental Management (Elsevier), respectively. The third paper is published in an open-access journal and the authors retain the copyright.

Chapter 2 has been published as: **Witing, F.**, Prays, N., O'Keeffe, S., Gründling, R., Gebel, M., Kurzer, H.-J., Daniel-Gromke, J. & U. Franko (2018): Biogas production and changes in soil carbon input - A regional analysis. *Geoderma* 320: 105–114. https://doi.org/10.1016/j.geoderma.2018.01.030

Chapter 3 has been published as: **Witing, F.**, Gebel, M., Kurzer, H.-J., Friese, H. & U. Franko (2019): Large-scale integrated assessment of soil carbon and organic matter-related nitrogen fluxes in Saxony (Germany). *Journal of Environmental Management* 237: 272-280. https://doi.org/10.1016/j.jenvman.2019.02.036

Chapter 4 has been published as: **Witing, F.**, Volk, M. & U. Franko (2023): Modeling Soil Organic Carbon Dynamics of Arable Land across Scales: A Simplified Assessment of Alternative Management Practices on the Level of Administrative Units. *Agronomy* 13(4): 1159. https://doi.org/10.3390/agronomy13041159

The introduction (chapter 1) and discussion (chapter 5) of this doctoral thesis are partly inspired by the following co-authored book chapters and scientific journal article:

- Franko U., **Witing, F.** & M. Volk (2019): Climate Change Induced Carbon Competition: Bioenergy Versus Soil Organic Matter Reproduction. *In: Schröter M., Bonn A., Klotz S., Seppelt R. & C. Baessler (Eds), Atlas of Ecosystem Services: Drivers, Risks, and Societal Responses.* Springer International Publishing, Cham, pp. 257–262. https://doi.org/10.1007/978-3-319-96229-0_40
- Franko, U. & **F. Witing** (2020): Dynamics of Soil Organic Matter in Agricultural Landscapes. *In: Mirschel, W., Terleev, V. & K.-O. Wenkel (Eds.), Landscape Modelling and Decision Support. Innovations in Landscape Research.* Springer, Cham., pp 283-298. https://doi.org/10.1007/978-3-030-37421-1_14
- Schwengbeck, L., Hölting, L. & **F. Witing** (2023): Modeling Climate Regulation of Arable Soils in Northern Saxony under the Influence of Climate Change and Management Practices. *Sustainability* 15(14): 11128. https://doi.org/10.3390/su151411128

Author contributions summary

This dissertation was written by Felix Witing. However, it is important to recognise the contributions of the co-authors to the synthesised publications. The following authors' contributions are specified using the Contributor Role Taxonomy (CRediT) (Allen et al., 2014, 2019).

Witing et al. (2018), chapter 2: Conceptualisation, FW, NP, SOK, RG and UF; methodology, FW, NP, RG and UF; software, FW; validation, FW, NP, SOK, RG, UF and MG; formal analysis, FW and NP; investigation, FW, NP and SOK; resources, MG, HJK and JDG; data curation, FW and NP; writing — original draft, FW; writing — review & editing, FW, NP, SOK, RG, UF, MG and JDG; visualisation, FW; supervision, UF; project administration, FW and UF; funding acquisition, UF and MG.

Witing et al. (2019), chapter 3: Conceptualisation, FW, UF and MG; methodology, FW and UF; software, FW and UF; validation, FW, UF and MG; formal analysis, FW; investigation, FW; resources, MG and HJK; data curation, FW; writing — original draft, FW; writing — review & editing, FW, UF and MG; visualisation, FW; supervision, UF; project administration, FW, UF and MG; funding acquisition, UF and MG.

Witing et al. (2023), chapter 4: Conceptualisation, FW, UF and MV; methodology, FW; software, FW and UF; validation, FW, UF and MV; formal analysis, FW; investigation, FW; data curation, FW; writing—original draft, FW; writing—review and editing, FW, UF and MV; visualisation, FW; supervision, UF and MV; project administration, FW; funding acquisition, FW, UF and MV.

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Thesis at a glance

Chapter 1: General introduction

The introduction provides an overview of the functions and dynamics of soil organic matter (SOM). It explains how models can be used to assess the effects of management and environmental changes on SOM. Recent challenges are discussed, including (1) SOM dynamics under changing climate, (2) agricultural practices in the carbon cycle, (3) diversity of drivers in agricultural landscapes and (4) challenges in SOM modelling for policy support. This leads to an outline of the specific and general aims of this thesis, namely the improvement of the landscape perspective on SOM in agricultural systems.

Chapter 2: Paper I

Aim: To analyse the area requirements of the biogas production system in Saxony together with potential changes in regional agricultural carbon fluxes to soils caused by the rise of the biogas sector.
Method: A regional spatial analysis was conducted based on the location, capacity and substrate mix of the Saxon biogas plants and a range of agricultural parameters. Carbon flux calculations were perfomed using the 'carbon reproduction flux' (C_{rep}) concept of the SOM models CANDY and CCB.
Conclusion: Biogas production in Saxony affects an area of 2.0 ha of agricultural land per kW of installed electrical capacity, including 0.4 ha for energy crops. Biogas plants with less than 500 kW capacity have the highest area requirements. The C_{rep} flux into the soils of Saxony increased by 2.8% within the observed time period. The areas affected by biogas production showed higher C_{rep} fluxes than the surrounding agricultural land, but this is highly dependent on the digestate recycling.

Chapter 3: Paper II

Aim: To conduct a large-scale, spatially distributed analysis of the soil carbon and nitrogen dynamics in Saxony and evaluate the impact of climate and best management practices on regional SOM stocks.
Method: The CCB model was adapted for large-scale simulations of SOM by linking spatial data on soils and climate with regional statistics on agricultural management. This new 'regional mode' of CCB was validated for different European locations and applied for the Saxon arable land (7345 km²).
Conclusion: Between 1998 and 2014, the SOC stocks of the arable soils in Saxony increased by 0.79 Mt C. The average net immobilisation of soil nitrogen was 7.5 kg N ha^{-1} a^{-1}, with considerable variations between years and subregions. Both the increase in carbon inputs to soil (+8%) and the reduction of carbon turnover rates (-10%) had positive effects on SOC storage. While the increased use of conservation tillage was the main driver for the overall increase in SOM storage in Saxony, climate variability, crop production and fertilisation had the largest effect on its annual dynamics.

Chapter 4: Paper III

Aim: To contribute to the operationalisation of regional SOM assessments for policy support by using a simplified modelling approach at the scale of administrative units, which often corresponds to the level of policy-making, data availability and communication.
Method: A scaling experiment was conducted, simulating the SOC dynamics of the arable soils of Saxony using upscaled CCB model set-ups at four different administrative levels: NUTS1, NUTS2, NUTS3, and LAU. The simulation results of the upscaled models were assessed against a 500 m grid-based reference model. The carbon sequestration potential of selected best management practices, such as field grass, cover crops, and conservation tillage, was determined across all of the five scales.
Conclusion: The upscaled model set-ups simulated the SOC trends of the Saxon arable land with an acceptable scaling error of 0.8-3.8%, while providing significant benefits for model application, data availability and runtime compared to the grid-based reference simulation. The carbon sequestration potential of the best management scenarios (1.33 Mt C by 2050) was slightly overestimated (+0.07-0.09 Mt C) by the upscaled model set-ups, mainly due to the aggregation of agricultural input data. The use of LAU and NUTS3 levels provides a balanced approach to quantifying SOC dynamics.

Chapter 5: General discussion and synthesis

The synthesis summarises the findings of the three articles and provides a discussion in the general context of the dissertation, along with recommendations for the case study Saxony. It highlights the need for a joint management of carbon and nitrogen pools in agriculture, as well and an increasing capacity to assess their stocks and fluxes on a regional scale. Furthermore, this chapter briefly outlines the limitations and main methodological challenges, along with future research prospects.

Contents

Abbreviations

Al	Aluminium
AMP	Alternative Management Practices
BAT	Biological Active Time
BAU	Business-As-Usual
BFA	Biogas Fingerprint Area
BMP	Best Management Practice
BPU	Biomass Providing Unit
C	Carbon
C:N	Carbon to Nitrogen ratio
Ca	Calcium
CANDY	Carbon And Nitrogen Dynamics model
CAP	Common Agricultural Policy
CCB	CANDY Carbon Balance model
CO_2	Carbon Dioxide
COP	Conference of the Parties
C_{rep}	Carbon reproduction flux
DM	Dry Matter
DNDC	DeNitrification-DeComposition model
FAT	Fine particle content
Fe	Iron
FM	Fresh Matter
FOM	Fresh Organic Matter
GhG	Greenhouse Gases
GIS	Geographic Information System
IACS	Integrated Administration and Control System
InVeKoS	Integriertes Verwaltungs- und KontrollSystem
IPCC	Intergovernmental Panel on Climate Change
LAU	Local Administrative Unit
LCA	Life Cycle Assessment
LUCAS	Land Use and Cover Area frame Survey’
MAE	Mean Absolute Error
ME	Mean Error

Mg	Magnesium
N	Nitrogen
N_2O	Nitrous oxide
NH_4^+	Ammonium
NUTS	Nomenclature d'Unités Territoriales Statistiques (Nomenclature of Territorial Units for Statistic)
OM	Organic Matter
P	Phosphorus
PBIAS	Percent bias
RMSE	Root-Mean-Square Error
Roth-C	Rothamsted Carbon model
UN	United Nations
SOC	Soil Organic Carbon
SOM	Soil Organic Matter

1. General introduction

1.1 Ecosystem functions of soil organic matter (SOM)

Human well-being and security depend on the Earth's soil resources, which require a sensitive balance of inputs and losses of carbon and nutrients in order to preserve their stability and fertility (Amundson et al., 2015). Soil organic matter (SOM) is the organic component of soil and consists of accumulated, mainly plant-based debris in various stages of decomposition (Hoffland et al., 2020). Soil microbes use enzymatic biochemical processes to break down organic compounds such as carbohydrates, fats, lignins and proteins to obtain energy and nutrients. Consequently, SOM is both a substrate for and a product of soil microorganisms, and microbial matter can be an important component of SOM (Hoffland et al., 2020; Kallenbach et al., 2016). It has been shown that fungal and bacterial necromass can account for more than half of the organic carbon in soils (SOC) (Liang et al., 2019; B. Wang et al., 2021).

Research on SOM has a long history and initially focused on fertility-related aspects as it was recognised as a key component of soil quality and productivity (Manlay et al., 2007). SOM is a source of nutrients (e.g. nitrogen, phosphorus) that are used for plant nutrition and increases the cation exchange capacity of soils. Yet, primary production is also influenced by the impact of SOM on soil structure, which affects soil aeration, aggregation, water infiltration and retention capacity (Wiesmeier et al., 2019). In recent decades, however, attention has shifted towards other soil functions and the awareness of the potential trade-offs between them has risen. It is now widely recognised that SOM controls a wide range of physical, chemical and biological processes that are fundamental to soil-based ecosystem functions and services (Smith et al., 2015). SOM is therefore recognised as an important component in addressing the challenges of global change and achieving the UN sustainability goals (Keesstra et al., 2016). According to Hoffland et al. (2020), the preservation of SOM is particularly relevant for erosion control, supporting soil biodiversity, regulating climate, retaining compounds for water quality improvements and, of course, maintaining primary production.

The climate-regulating function of SOM was widely and controversially discussed in recent years, as SOC can be an important sink in the global carbon cycle (Stockmann et al., 2013, 2015), but must be managed appropriately. Global SOC stocks have been estimated to contain three times as much carbon as all aboveground biomass and up to twice the size of the atmospheric carbon pool (Lal, 2004; Padarian et al., 2022; Scharlemann et al., 2014), underlining the potential of SOC management to mitigate climate change and hence global warming. However, the exclusive focus on climate may have counterproductive effects and several authors argue that the objective ought to be the restoration of all soil functions (Baveye et al., 2020). Soils play a crucial role in multiple global biogeochemical cycles, while being habitat for the greatest diversity of organisms on terrestrial land (Smith et al., 2015). Soil life itself is a promoter of plant health, NPS mineralisation and C sequestration. Furthermore, increasing SOM stocks can be beneficial for several physical, chemical and biological soil properties, resulting in enhanced water infiltration and retention capacity, increased resilience against droughts, and prevention of soil erosion and related nutrient losses (Lal, 2020; Wiesmeier et al., 2019). However, the value of organic matter stems from its dynamic nature. It is most useful when it decays, as an active soil biota leads to greater biological benefits. Consequently, the most common trade-off in SOM management is an apparent paradox (Janzen, 2006): to increase C sequestration, we may need to suppress microbial activity, which has negative implications for soil fertility (e.g. nutrient availability) and other soil-based ecosystem functions.

1.2 The dynamic equilibrium of SOM

When addressing SOM dynamics and both natural and anthropogenic disturbances that alter SOM stocks, it is essential to acknowledge that human land-use has significantly altered the terrestrial carbon balance. The conversion of land to agricultural use typically results in a decline in SOC stocks (Don et al., 2011; Guo & Gifford, 2002; Wei et al., 2014). Over the past 12,000 years, there has been a marked increase in the use of land, which corresponds to the trend in carbon loss from soils (Sanderman, Hengl, et al., 2017). This trend has accelerated significantly over the last 200 years. Meta-analytic studies have quantified a 26% reduction in topsoil SOC (median value for a depth of 0-30 cm) as a result of agricultural land-use conversion (Sanderman et al., 2018; Sanderman, Hengl, et al., 2017). Furthermore, these studies estimate a global soil carbon debt of 116 gigatons (Gt) C due to agriculture in the top two metres of soil. This is equivalent to an average of 17.7 t C ha^{-1}. The most significant losses of SOC were observed on arable land.

Despite these long-term trends and dynamics, SOM remains one of the most stable carbon pools in Earth's ecosystems, and its short-term changes are often small (Kuzyakov et al., 2018). The mean residence time of SOC is often used as an indicator of soil carbon stability. It can be understood as the average time between when a carbon atom enters the soil and when it leaves the soil (Luo et al., 2019). Plant residues are highly variable in their chemical composition (Johnson et al., 2007). Thus, the transformation of the different organic inputs in the soil during their decomposition occurs at very different rates (Semenov et al., 2019) and with changing communities of microbial decomposers (Bonanomi et al., 2019). During decomposition of the highly diverse plant material, some of the organic carbon is respired and leaves the soil as CO_2. The decreasing energy content of the remaining, more uniform residual material slows down further transformation and microbial assimilation. In addition, interactions with the soil environment can stabilise SOM and reduce its further decomposition (Kögel-Knabner & Rumpel, 2018). The association of SOM with soil mineral surfaces (e.g. clay surfaces and edges) is particularly important in this context, accounting for approximately

40-60% of SOC (Giannetta et al., 2018). However, occlusion of SOM in soil aggregates (G. Angst et al., 2017; Š. Angst et al., 2017) and the self-assembly of SOM compounds into larger structures also stabilise and protect SOM from decomposition (Sutton & Sposito, 2005).

In addition to soil properties (parent material, soil type, aggregation, silt/clay content, Al/Fe/Ca/Mg content), environmental conditions that affect microbial activity, such as soil moisture and temperature, are important factors that control the turnover time of carbon in soils (Chen et al., 2013; Luo et al., 2019). Under constant environmental conditions and input of fresh organic matter, carbon input and turnover will approach a dynamic equilibrium, resulting in a long-term steady state of SOC stocks (Wiesmeier, Mayer, Paul, et al., 2020). In reality, however, soils are rarely in a steady state due to environmental changes and management (e.g. land-use change, climate variability). These changes can affect both carbon input and its turnover conditions, altering the potential equilibrium state and resulting in gains or losses in SOC stocks. Another important factor that can affect SOM stocks in the long term is topography. SOM is involved in erosion processes and is therefore subject to spatial redistribution in a landscape (Doetterl et al., 2016).

1.3 Recent challenges in managing SOM on arable land

Achieving gains in SOM stocks on arable land will require changes in agricultural management. These changes can be associated with significant challenges, but they can also provide economic, ecological and social co-benefits (Tang et al., 2016). The following sections introduce some of these challenges and conflicts, as well as measures to enhance SOM stocks.

1.3.1 Agricultural practices and the carbon cycle

Cultivated crops leave organic residues in the soil, such as roots, stubble, litter, straw. Each of these sources contributes differently to the formation of new SOM, depending on the properties of the fresh materials (Gasser et al., 2022; Nguyen & Marschner, 2016; Shahbaz et al., 2017). The same applies to the application of organic amendments, including traditional forms such as animal excrements (manure, slurry) or compost, and new forms such as biogas digestate. The amount of plant-derived organic matter that enters the soil is partly dependent on crop yields, as more plant biomass often means more residues (Jacobs et al., 2020; Scarlat et al., 2019). Thus, any management activity that controls crop yield will affect the SOM dynamics. Obviously, this applies to both mineral and organic fertilisation of crops, but also to tillage and irrigation practices. Soil tillage and irrigation affect not only crop yields but also SOM turnover rates through their effects on soil structure, water retention capacity and content, and thus microbial activity (Bescansa et al., 2006; Ghezzehei et al., 2019; Védère et al., 2022).

Consequently, agricultural management is key to controlling the development of SOM stocks on arable land. Under defined site conditions, such as soil and climate, the build-up and breakdown of SOM is controlled by farm management decisions such as: cropping, fertilisation, tillage, and irrigation systems (Liu et al., 2006; Singh et al., 2018). However, agricultural systems undergo constant change. Alterations in cultivation patterns arise, for example, from changes in regulations (e.g. greening requirements), market situations (e.g. new dietary habits) and farm types (e.g. large and equipment-intensive farms vs. organic and community-supported agriculture). Furthermore, the agricultural system experiences new types of carbon fluxes, including those resulting from bioeconomy, which have long-term impacts on the SOC cycle (Andrade Díaz et al., 2024). It is therefore essential, but also challenging, to consider all these factors in adaptation strategies.

1.3.2 Soil nutrients associated with SOM

SOM contains essential soil nutrients, such as nitrogen and phosphorus, which play an important role in arable land management. Up to 95% of soil nitrogen is bound in organic matter, making it inaccessible to plants (Bingham & Cotrufo, 2016). Therefore, soil fertility is closely linked to SOM turnover. The process of SOM mineralisation converts SOC into CO_2 and organic nutrients into plant-available forms, such as ammonium (NH_4^+). The carbon to nitrogen (C:N) ratios of the different organic components involved are very important in this context. The C:N ratio of cropland SOM is typically around 10-12:1, which is relatively narrow (Poeplau et al., 2020; Sparks, 2003). In contrast, the C:N ratio of FOM varies widely, for example from 7:1 (cow slurry) to 300:1 (wheat straw). When FOM has a high C:N ratio, its decomposition to SOM can immobilise plant-available nitrogen and increase the need for mineral fertiliser. Different thresholds for C:N ratios have been reported in this context. For net N immobilisation, a FOM C:N ratio of about >25:1 has been observed, while a C:N ratio of about <15:1 is required for net N mineralisation (Kaleeem Abbasi et al., 2015; Nicolardot et al., 2001; van der Sloot et al., 2022). Proper SOM management should therefore always be accompanied by proper nutrient management. This principle applies not only to the management of residues with high C:N ratios, but also to organic fertilisers with low C:N ratios. Organic amendments from animal husbandry return carbon and nutrients back to the soil, which is desirable. However, areas with a high livestock densities and thus high application rates of organic excrements often have high nitrogen surpluses. This can lead to nitrate leaching into water bodies and ammonia emissions into the atmosphere (Ge et al., 2020; Leip et al., 2015; Möckel, 2019).

1.3.3 Soil carbon sequestration measures for arable land

In operational terms, net soil carbon sequestration is the difference between the uptake and release of CO_2 in a given environment (Henderson et al., 2022; Rees et al., 2005). There are various agricultural practices that can increase soil carbon sequestration. These practices can be broadly classified as (1) ‘best management practices’ (BMPs) or (2) ‘frontier technologies’ (National Academies of Sciences, Engineering, and Medicine, 2019). BMPs refer to ‘well-known' conservation management systems that are already being practiced and have the potential for widespread adoption. Frontier technologies may have a great potential for carbon sequestration, but they still face significant barriers, such as technological and economic challenges. As a result, they are rarely applied outside of experimental settings up to now. Table 1 presents an overview of some of the most relevant measures for increasing SOM stocks on arable land and their main principles for carbon sequestration, either by increasing the FOM flux into the soil or by reducing carbon decomposition. In addition, some of the measures also reduce the risk of soil erosion and associated SOM losses from fields.

Table 1: Selection of measures for increasing soil carbon storage on arable land (own compilation based on: Freibauer et al., 2004; Henderson et al., 2022; Paustian et al., 2019). * Refers to measures that can be classified as 'frontier technologies'.

Measure category	Measure	Increased C input to soil	Reduced turnover of SOC	Prevent erosion losses of SOC
Improved rotations	Crop rotation design (selection of main crops)	✓		(✓)
	Catch crops (as a cover crop that is grown between two main crops)	✓		✓
	Intercropping (or undersown crops)	✓		✓
	*New crop varieties (e.g. annuals bred to develop deeper and larger root systems)	✓		(✓)
	*Perennial (grain) crops	✓	(✓)	(✓)
Land-use change (conversion of arable land)	Conversion to grassland (perennial grasses and legumes)	✓	✓	✓
	Conversion to mixed systems like agroforestry	✓	(✓)	✓
Organic resource management	Crop residues retention (incl. high-residues crops)	✓		✓
	Reduced removal of by-products (e.g. straw, beet leaves)	✓		✓
	Organic matter application (manure, slurry, compost, digestate, sewage sludge)	✓		
	Relocation of organic amendments (e.g. to low-turnover soils)		✓	
	*Biochar additions	✓	✓	
Tillage, water and nutrient management	Reduced tillage and other forms of conservation tillage		✓	✓
	Optimised nutrient and pH management	✓	(✓)	
	Optimised soil water management	✓	(✓)	
	Rewetting of organic soils		✓	

A large number of existing measures are related to the improvement of cropping choices, as these can be very effective in increasing the carbon input to soil and often contribute to erosion prevention at the same time. Due to the high relevance of cover crops, there have been several meta-analytical studies in recent years showing their strong positive effect on SOC stocks, with an overall average SOC increase of about 15% (Jian et al., 2020; McClelland et al., 2021; Poeplau & Don, 2015). However, enhancing the crop rotation design can also increase average annual C inputs, especially when increasing the number of main crops in the rotation that provide high amounts of residues (Triberti et al., 2016; West & Post, 2002; Zani et al., 2023). The same principles apply to the different types of changes in land-use, such as the conversion of arable land to grassland (Conant et al., 2017). In addition to an increase in FOM fluxes into the soil, such conversions often reduce SOM turnover due to the cessation of tillage.

On-farm organic matter management also affects soil carbon inputs, but it is necessary to distinguish between two categories: (1) the reduced removal of organic resources from the field (e.g. by-products such as straw) and (2) the addition of organic matter to the field (e.g. slurry). A reduced in-field removal rate may clearly contribute to net carbon sequestration, but this is not always the case for organic matter additions. The application of organic substances obviously adds carbon to the soil, but it may not results in a net removal of CO_2, particularly if the amendment originates from an off-site location (Paustian et al., 2019). To determine the leakage effects and net CO_2 removal potential in such cases, a full life cycle assessment approach is necessary, which includes both on-farm and off-farm GhG emissions and savings. However, organic amendments also contribute indirectly to carbon sequestration by improving soil physical properties and nutrient availability (Paustian et al., 1997). This, in turn, enhances crop productivity and residue inputs.

Advances in tillage, fertilisation and irrigation technologies allow farmers to reduce soil disturbance and optimise the amount of water and nutrients applied. Reduced tillage and no-tillage practices significantly enhance aggregation and aggregate stability and have been identified as one of the most important measures to increase topsoil carbon storage (Lal et al., 2003). On the other hand, the effects of no-till farming on deeper soil layers have been debated in the literature, but with no clear conclusion to date (Baker et al., 2007; Dimassi et al., 2014; Du et al., 2017; Minasny et al., 2017; Syswerda et al., 2011).

When aiming to increase SOM stocks, it is crucial to consider all soil functions, as discussed in section 1.1. All of the measures presented in Table 1 also provide benefits for other soil functions. For example, catch crops not only increase carbon input into the soil but also reduce nutrient losses and the risk of soil erosion. Despite this, trade-offs are also common. For instance, in agricultural practice, no-tillage often requires the use of herbicides, which negatively impacts soil biodiversity (Alletto et al., 2010). Finally, it is important to bear in mind that SOM is subject to continuous microbial turnover and carbon sequestration is usually reversible. Therefore, it is necessary to constantly maintain a new equilibrium level of SOM to avoid a subsequent release of CO_2 (Paul et al., 2023).

1.3.4 Targets for soil carbon sequestration in light of increased turnover rates

SOM affects the exchange of greenhouse gases (GhG) between the biosphere and the atmosphere at both global and local scales (Franko & Witing, 2020). Locally, SOM affects the water and nutrient retention capacity of soils, as well as soil temperature. This, in turn, affects plant growth, which has feedback loops with the carbon inputs to SOM. Globally, SOM can make a significant contribution to climate change mitigation. At the 2015 United Nations Climate Change Conference in Paris (COP21), the '4 per 1000' initiative was launched with the aim of increasing SOC stocks by 4‰ per year to offset anthropogenic greenhouse gas emissions (Lal, 2016; Minasny et al., 2017). However, achieving the target is difficult to track as SOC is often a blind spot in European national GhG inventories and the accuracy of reported values is estimated to be low, especially for croplands (Bellassen et al., 2022). Furthermore, climate trends pose a significant obstacle to the '4 per mille' target. Climate change is expected to increase the turnover rates of soil carbon in many regions due to increased temperatures and microbial activity. This implies that either an increased amount of carbon input or measures to reduce OM turnover will be required to prevent declines in SOC stocks (Franko et al., 2015).

Agricultural areas, in particular, have a high need, but also a high potential for adaptation, due to their high level of management and the availability of various measures (Table 1), some of which are well researched. Nevertheless, there are many associated challenges that need to be addressed. These include, for example, the up-scaling of measures and concepts, as their effectiveness varies between regions (Bamière et al., 2021; Freibauer et al., 2004; Govaerts et al., 2009; Henderson et al., 2022). Furthermore, it is important to consider feedback loops and potential environmental burdens when setting carbon sequestration targets. For instance, the increased emissions of nitrous oxide (N_2O) (Guenet et al., 2021) and the accumulation of soil nutrient stocks may reduce the benefits of increased SOC storage.

1.3.5 Considering landscape-scale heterogeneity and a diversity of drivers

Most of the studies on the impact of anthropogenic factors on SOM pools and fluxes have been conducted at the point or pedon scale. However, SOM concentrations exhibit significant spatial heterogeneity within and across agricultural landscapes (Aksoy et al., 2016; de Brogniez et al., 2015; Lugato et al., 2014; Rial et al., 2017). In order to develop effective management strategies for agricultural regions, it is necessary to assess the impact of management options on SOM and ecosystem services at the farm, landscape and watershed scale (Lal, 2009). This requires considering heterogeneity and a variety of drivers at different scales (Figure 1), some of which act through feedback loops that affect SOM (in the long term) through changes in the agricultural system or environmental boundaries.

Soil properties, such as parent material and texture, and climatic conditions form the basis for the regional heterogeneity in SOM stocks (Wiesmeier et al., 2019). Yet, these two drivers tend to change rather slowly, e.g. due to soil formation processes, erosion or climate change. On the other hand, land-use and management practices are often highly dynamic. These practices have a significant impact on the amount of carbon that enters the soil. Land management also affects soil microbial activity and thus the conditions for turnover of organic matter (e.g. via tillage and irrigation systems) (Guo & Gifford, 2002; Jarecki & Lal, 2003; Poeplau et al., 2011). Policy, market and historical conditions drive decisions about field and farm management (e.g. farm types), as well as interactions and hence carbon flows between farms (e.g. organic fertilisers) (Zhao et al., 2018). All of these drivers arise from different scales, but strongly modify the cycle of organic matter in agricultural landscapes, resulting in a heterogeneous pattern of field-scale SOM concentrations and trends.

Furthermore, a driver may not only have a direct impact on SOM, but also strong interactions with other drivers (Beillouin et al., 2022). For instance, policies can have both rather direct effects, such as regulations on the use of organic fertilisers, and indirect effects on SOM. Indirect effects of policies result from feedback loops that can be either short-term, such as changes in farming systems, or long-term, such as effects on climate change. The same applies to land management, which can affect soil properties in the longer term. Additionally, SOM has a 'slow' responsiveness (long time to reach a steady state) and the current levels in agricultural soils are a complex result of historical transformations in agriculture, climate and soils that have occurred over millennia.

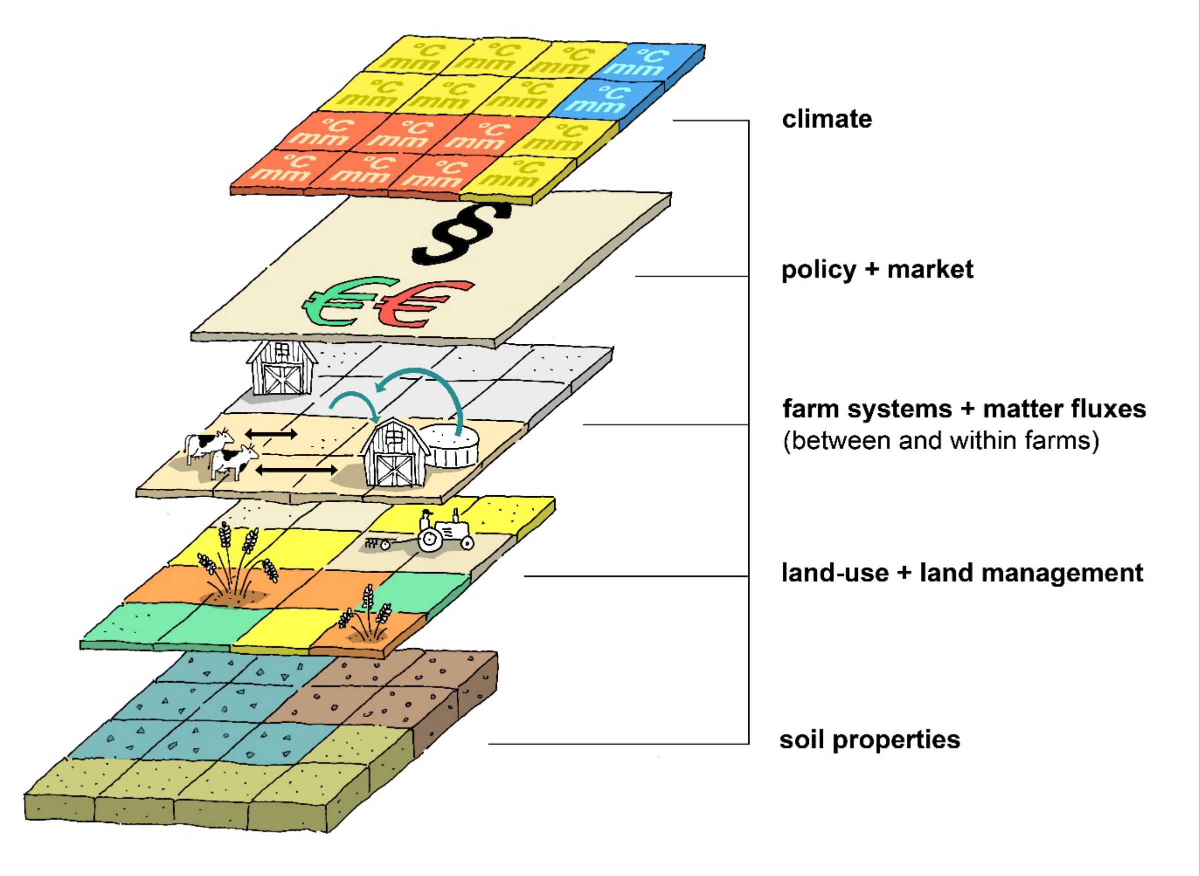

Figure 1: Selected drivers of SOM dynamics in agricultural landscapes (based on Franko and Witing, 2020)

Direct spatial fluxes of SOM are primarily associated with soil erosion (Wiesmeier et al., 2019). However, SOM dynamics are also influenced by spatial fluxes of carbon sources within the agricultural system and related markets (Andrade Díaz et al., 2024). Traditionally, the local agricultural biomass cycle was relatively closed, with the exception of agricultural products brought to market, such as food and fibres. A significant portion of the biomass removed from fields was returned to agricultural soils (e.g. as excrements) on the same farm that produced the feed and bedding for the barn (Franko & Witing, 2020). This cycle, however, has become increasingly complex. Additional carbon sources are imported from outside the regional agricultural system, such as soya used as animal feed, and organic matter is often transferred between different specialised farms. The demand and diversity of uses for agricultural carbon has grown (e.g. biogas production from animal excrements). This may on one side reduce the return of agricultural biomass to the soil, but on the other side has also led to new types of carbon fluxes in the agricultural system (e.g. digestate residues as organic amendments) (Baştabak & Koçar, 2020; Czekała et al., 2022).

The market for agricultural products and the demands placed on agricultural production, as well as societal attitudes, are constantly changing, with indirect effects on SOM. For example, changes in dietary habits, such as reduced meat consumption, can lead to changes in cropping patterns and in the availability and use of organic fertilisers. Increasing demand for products from organic farming or community-supported agriculture can lead to changes in farm types and matter fluxes (Egli et al., 2023; Wellner, 2017). Policies such as the Common Agricultural Policy (CAP) and regional subsidy schemes aim to encourage the adoption of sustainable management practices. Nevertheless, an increasing number of farmers are also adopting these practices for other reasons (Piñeiro et al., 2020). These include a better understanding and evidence of the benefits of sustainable practices (e.g. improving and protecting agricultural soils), their own innovation and curiosity, but also social pressure from local communities.

Overall, agricultural landscapes are highly dynamic and subject to various political, societal, and environmental factors that affect their soil-related matter flows. To develop and evaluate potential management strategies that benefit SOM stocks and their functions, it is necessary to take a broader view of agricultural systems at different scales.

1.4 Modelling SOM dynamics

As shown in the sections above, the dynamics of SOM are becoming an increasingly important factor in many areas of research and policy. There is a need to evaluate the effects of changing environmental boundaries, such as climate change, on SOM dynamics and the potential of management actions and strategies to sequester soil carbon. Direct measurements of SOM alone can only partly support such efforts (Dungait et al., 2012; Murindangabo et al., 2023). Simulation models are therefore an indispensable component of SOM research. They provide a mathematical framework for integrating, exploring, and testing our understanding and hypotheses of SOM dynamics (Campbell & Paustian, 2015). Furthermore, simulation models are increasingly being used to assess the impact of human interventions and to test the effects of management options on various ecosystem functions of SOM.

Approaches for SOM modelling are constantly evolving, but according to Stockmann et al. (2013) there are two main philosophies: process-oriented and organism-oriented models. Organism-oriented models, such as food web models, simulate SOM dynamics through different pools of soil biota. In contrast, process-oriented SOM models use different conceptual pools of carbon with comparable chemical and physical properties, yet varying decomposition rates and stabilisation mechanisms. Thus, most process-oriented models represent soil biota only in the form of microbial biomass.

Process-oriented models such as CANDY (Franko, 1996), CCB (Franko et al., 2011), CENTURY (Parton et al., 1987), DAISY (Hansen et al., 1990), DNDC (C. Li et al., 1992) and Roth-C (Coleman & Jenkinson, 1996) are dominant in the scientific literature to study the effects of management practices on SOM (Stockmann et al., 2013). The models have been developed and tested using datasets from long-term field experiments (e.g. Franko et al., 2007, 1997) and have demonstrated a good ability to predict SOM dynamics across a range of soil-climatic regions and scales. However, independent validation data, particularly observation time series, are often scarce (Le Noë et al., 2023). A key consideration in model selection is the scale of both the model hypotheses and the model use (e.g. microsite, ecosystem, global), as each scale imposes distinct limitations (Campbell & Paustian, 2015; Manzoni & Porporato, 2009).

Many of the existing process-oriented SOM models divide the non-living SOM into at least three carbon pools: an active, a stabilised and a passive pool (Campbell & Paustian, 2015). Figure 2 illustrates this principle using CANDY Carbon Balance (CCB) model as an example. CCB is based on the CANDY (Carbon And Nitrogen DYnamics) model and has been simplified to work with limited input data, thus making it more suitable for answering practice-oriented research questions (Franko et al., 2011). The model simulates the SOM dynamics in the top 30 cm of soil and was validated for various site conditions in Central Europe (Franko et al., 2011) and applied in several case studies (e.g. Franko et al., 2022; Franko and Spiegel, 2016; Spiegel et al., 2018).

The SOM pools are defined according to their biological stability, decomposition rate and turnover time. Consequently, these SOM pools are largely conceptual and cannot be measured directly. However, they are used to simplify the various states of decay and stability, and this approach has been shown to be useful for long-term SOM modelling (Campbell & Paustian, 2015; Paustian, 1994). The turnover rates of the active pool are typically described in years, while those of the stabilised/slow pool are described in decades. The passive or long-term stabilised pool is often considered to be background SOM, with minimal decomposition and turnover rates spanning several centuries to millennia (Trumbore, 2009). In addition, several pools of fresh organic matter (FOM) are commonly considered to represent the input flux to

SOM. These FOM pools are distinguished, for example in the case of CCB, by the origin and quality of the organic matter, including crop by-products (e.g. straw), crop residues (e.g. roots, stubble) and organic fertilisers (e.g. slurry). (Franko et al., 2011, 2017).

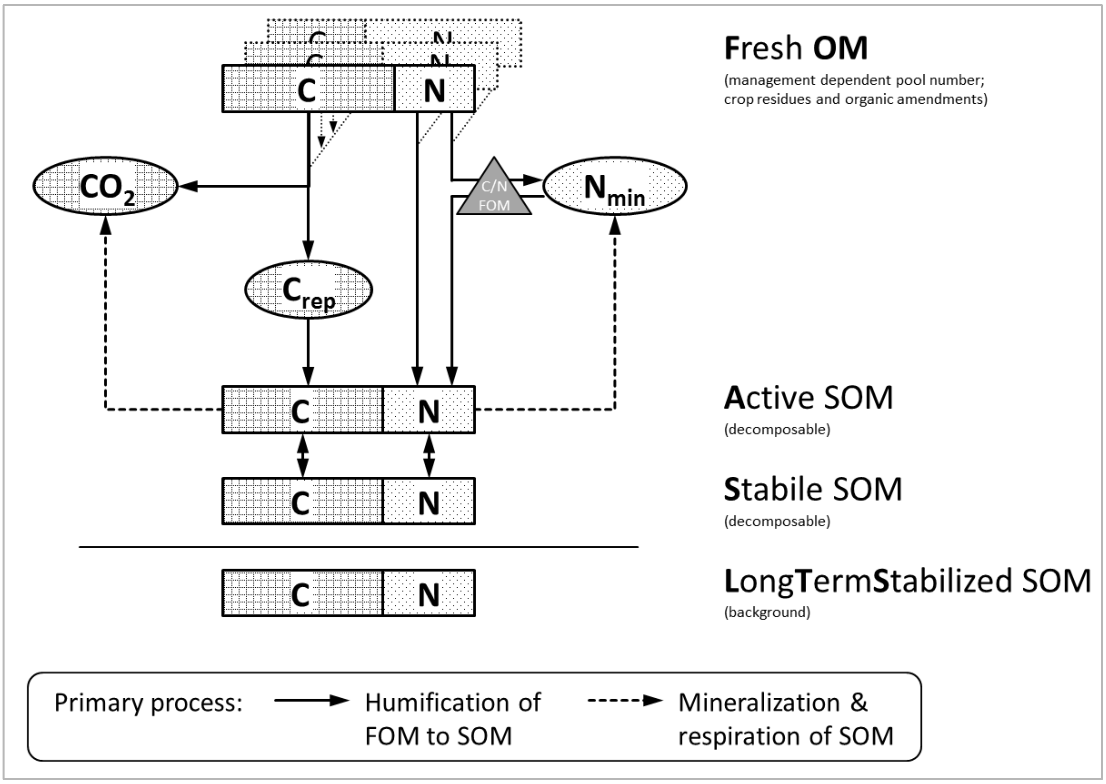

Figure 2: Simplified overview of pools (blocks) and fluxes (arrows) in the CCB model. C_{rep}: carbon reproduction flux from fresh organic matter (FOM) to soil organic matter (SOM). CO_2: release of carbon dioxide. N_{min}: external pool of mineral nitrogen (modified from Franko et al., 2016, 2011).

The turnover or mean residence time of carbon within SOM is a commonly used metric to assess the persistence of SOM and its carbon pools (Derrien & Amelung, 2011; Lehmann & Joseph, 2015). Although the use of these terms as a measure of persistence has been criticised (Sierra et al., 2018), they still remain important in modelling approaches. The turnover and mass loss of FOM and SOM pools over time is often modelled using first-order decay kinetics (Campbell & Paustian, 2015), which means that the decay of material is linearly related to the pool size. Turnover coefficients, which describe the resistance of the material to microbial breakdown, are used to calibrate the decomposition rates (day^{-1}) of organic matter in the FOM and SOM pools. In CCB, carbon turnover is modelled using first-order kinetics with the time variable ‘Biological Active Time’ (BAT), following the concept used in CANDY (Franko et al., 1995; Franko & Oelschlägel, 1995). BAT is an indicator on the number of days per year on which microbial activity occurs, and is calculated based on site-specific environmental conditions, such as air temperature, water availability (precipitation, irrigation), soil texture and tillage system.

Changes in SOM turnover and storage can affect the release of nitrogen from the organic pools, impacting both nitrogen availability and the risk of nitrate leaching (Bingham & Cotrufo, 2016). Consequently, some SOM models, including CCB, simulate both organic carbon and organic nitrogen pools and cycles. In these models, the simulation of nitrogen mobilisation and immobilisation involves fluxes with an 'external' pool of mineral nitrogen (N_{min}). The turnover of organic nitrogen is controlled by the dynamics and the carbon to nitrogen (C:N) ratios of the different FOM and SOM pools (e.g. Franko et al., 2011, 1995).

1.4.1 SOM modelling for policy support

All models need to balance the conceptual understanding of the system they represent with the available data to inform and evaluate their functions and outputs. Policy-driven modelling applications and decision support for land management face challenges when the required data is unavailable at the scale of the decision-making (Jones et al., 2005). With regard to SOM modelling, the need for large-scale assessments to inform policy advice is clear, as SOM is critical for a wide range of challenges, particularly in agricultural systems, but also beyond. Several studies have performed large-scale, spatially distributed estimates of the amount of SOC stored in soils now (e.g. for Europe: (de Brogniez et al., 2015; Lugato et al., 2014; Yigini & Panagos, 2016), for example by using data from the 'Land Use and Cover Area frame Survey' (LUCAS) (Tóth et al., 2013). These studies are valuable for creating inventories of the status quo and for understanding the regional distribution of SOC stocks. However, the existing approaches are partially difficult to use for quantifying the impact of management strategies on SOM on a large scale. Consequently, the number of regional to large-scale scenario applications is rather limited, particularly in the agricultural context. In order to use process-oriented SOM models for developing management strategies for agricultural regions at the landscape or watershed scale (Lal, 2009), these models must be used in conjunction with geographic information systems (GIS). This task involves collecting and managing a multitude of input data for these heterogeneous study areas. Thus, the model structure and process representation must be suitable for the chosen scale (Manzoni & Porporato, 2009). To account for the different feedback loops within agricultural systems, the modelling framework must be capable of considering different objectives (e.g. carbon, nitrogen), as well as options in the decision space (e.g. management variables). For instance, there are only a few models that can account for changes in management factors, such as tillage systems (Murindangabo et al., 2023). Another very common challenge and source of projection uncertainty in regional to large-scale model applications is the limited availability of measured SOM data, both in terms of quality and quantity. These data are required to initialise SOC levels and the initial distribution of carbon between the model pools (Dimassi et al., 2018; Foereid et al., 2012), which can have a profound impact on the simulated trends in carbon and nitrogen storage.

1.5 Objectives, research questions and structure of this doctoral thesis

SOM stocks are in a constant state of flux and, as shown above, their integrated management is crucial for maintaining soil fertility to produce food for a growing human population, mitigating and adapting to climate change, and supporting all other SOM-related soil functions such as clean water and habitat. The overarching objective of this dissertation is *to improve the landscape perspective on SOM in agricultural systems, which is crucial for the development of future carbon management policies* and has several research gaps that need to be addressed. Specifically, this doctoral thesis aimed to (1) clarify and quantify significant carbon and matter fluxes in agricultural systems, (2) conduct large-scale, spatially distributed and integrated simulations of soil carbon and nitrogen dynamics, (3) evaluate the impact of climate and best management practices on SOM stocks, and (4) find methods to operationalise SOM modelling for policy support at larger scales. The dissertation focuses on a specific case study - the federal state of Saxony in Germany - and conducts three research studies (Figure 3) to address specific challenges of SOM management on arable land outlined in **Chapter 1**.

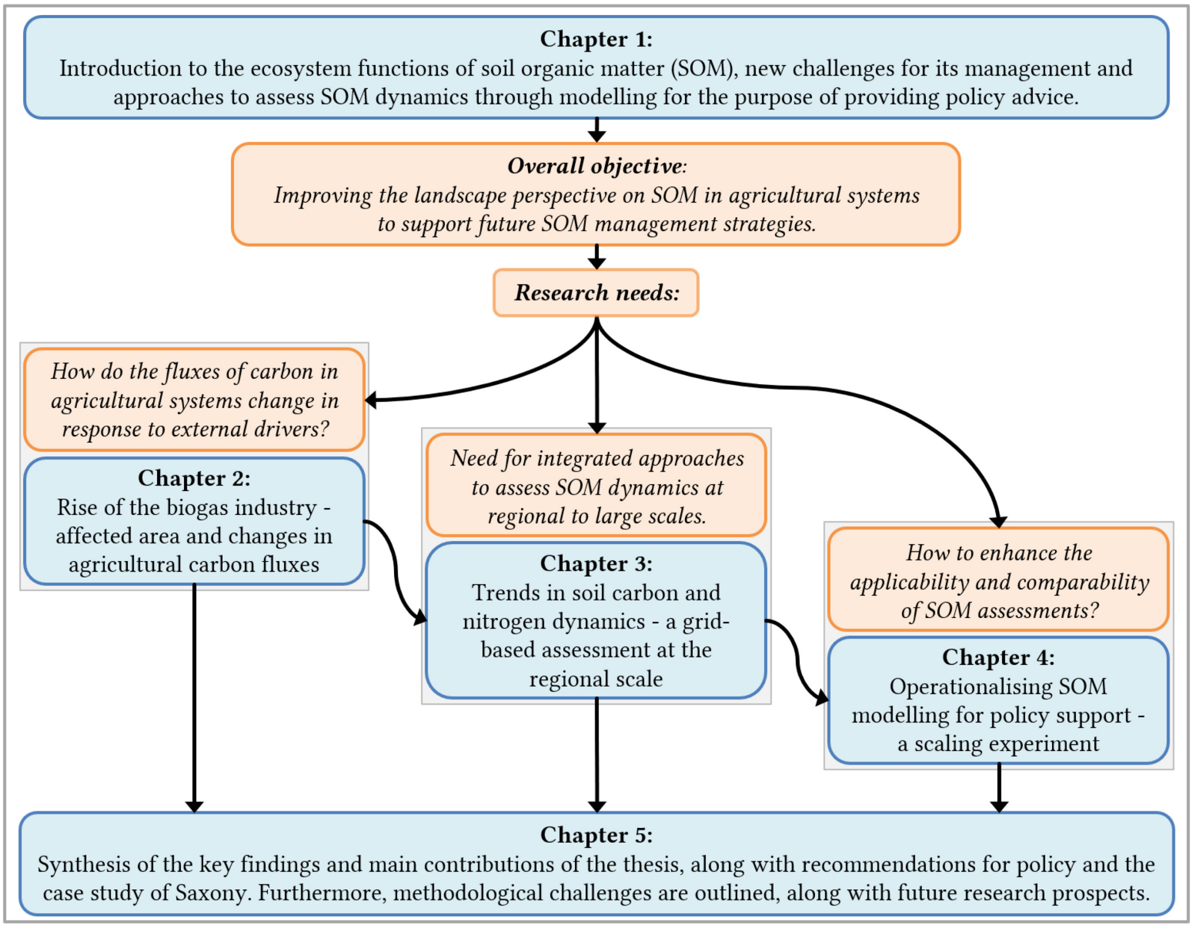

Figure 3: Overview of the structure of this dissertation.

In order to **contribute to an increased understanding of the carbon fluxes in agricultural systems**, the **first research study** analyses recent changes in agricultural carbon fluxes at the example of the policy-driven rise of the biogas industry (Britz & Delzeit, 2013; Purkus et al., 2018). The Renewable Energy Sources Act in 2000 and the amendments to the Renewable Energies Act in 2004 and 2009, led to a significant change in the carbon dynamics of the German agricultural system. Specific tariffs for electricity generated from renewable sources were guaranteed to energy supply companies, and strong incentives were created for the cultivation of energy crops (Theuerl et al., 2019). Between 2000 and 2016, the number of biogas plants in Germany increased by more than eightfold (Daniel-Gromke et al., 2018), resulting in significant changes in crop cultivation patterns (Theuerl et al., 2019) and the utilization of substantial quantities of agricultural livestock excrements as a biogas feedstock (Daniel-Gromke et al., 2018). These changes in matter fluxes affected the in-field SOM balance, resulting in a reduced return flux of traditional agricultural carbon sources to the field, but also to a new type of carbon source, biogas digestate, which has the potential to be more stable. Accordingly, there has been and still is a strong debate on the sustainability and carbon benefits, as well as the area efficiency of this technology (Emmann et al., 2013; Hansjürgens et al., 2017; Priefer & Meyer, 2019; Rantala et al., 2020; Sterner & Fritsche, 2011; Thrän et al., 2020). In this context, **Chapter 2** of this doctoral thesis presents a novel regional analysis of the biogas production system in Saxony. In particular, the study addresses the following research question and hypotheses:

- *What are the area requirements of biogas production systems and their impact on carbon fluxes to soils in the agricultural landscapes of Saxony?*

Hypotheses: Each biogas plant has a unique 'fingerprint' that is defined by its location, installed electrical capacity and substrate mix. This fingerprint can be characterised in terms of its spatial extent, in particular the area of agricultural land required for substrate production and biogas residue application, and typical soil carbon fluxes.

The soil carbon cycle is closely linked to the soil nitrogen cycle (Batlle-Aguilar et al., 2011; Manzoni & Porporato, 2009; Porporato et al., 2003). The decomposition of organic matter releases nitrogen, which is then accessible for plant uptake. In turn, the availability of nitrogen affects the rate of organic matter decomposition (Averill & Waring, 2018). Processes of enrichment and depletion of carbon and nitrogen in SOM can thus significantly affect the preservation of soil fertility and have side effects on nitrogen leaching. The **second research study** of this thesis therefore conducts an **integrated assessment of both soil carbon and nitrogen dynamics at a regional scale** to investigate ongoing trends, potential side effects and the role of climate and management. To avoid and mitigate trade-offs between the need for increased agricultural production and the efficient use of resources, it is essential to assess the impacts of agricultural activities and alternative land management strategies at larger scales. **Chapter 3** of this dissertation presents a novel approach for assessing regional-scale SOM dynamics using the CCB model with innovative model adjustments. In particular, the study addresses the following research question and hypotheses:

- *How can regional SOM dynamics be simulated for the entire arable land of Saxony (7,345 km²) and what is the contribution of different drivers to the regional trends in SOC and related organic nitrogen stocks?*

Hypotheses: The CCB model has the potential to simulate regional soil carbon and nitrogen dynamics at a grid level, provided that it is extended to accommodate aggregated input data and new types of spatial modelling units that integrate over several management units.

Carbon storage in agricultural soils is influenced by a multitude of political, socio-economic, and environmental factors, each with its own scale of origin and impact. In order to develop effective strategies for managing and promoting SOC storage, it is essential to comprehensively evaluate the impacts of drivers and agricultural measures across different scales. This will enable the prioritisation and adaptation of specific targets or measures at the relevant levels. Simplified methods for modelling SOC dynamics that are scaled to the level of administrative units could help to **operationalise SOM modelling for policy support**, as this aligns with the level of policy-making and data availability. However, there is a potential for systematic errors in such scaling operations, which was addressed in the **third research study**. Accordingly, **Chapter 4** of this doctoral thesis presents an innovative scaling experiment that addresses the following research question and hypotheses:

- *Is it possible and reasonable to model the dynamics of SOM at the level of large spatial units relevant to policy and environmental management, such as administrative units, and can such a simplified assessment be used to quantify the carbon sequestration potential of best management practices across different scales?*

Hypotheses: The carbon sequestration potential of alternative management practices can be quantified at the scale of administrative units using the novel 'regional mode' of the CCB model presented in Chapter 3, while maintaining an acceptable scaling error and being advantageous in terms of model application, data availability and run time.

The following Chapters 2-4 constitute the core of this dissertation and present the three articles published in international, peer-reviewed scientific journals. **Chapter 5** presents the final synthesis of the thesis, providing a summary of the key findings and a discussion within the broader scope of the thesis. The chapter demonstrates how the work presented contributes to improving the landscape perspective on SOM in agricultural systems, which is the overall aim of this thesis, and supports the development of future carbon management policies. In addition, the synthesis chapter offers a concise overview of the main methodological challenges and limitations encountered during the research process, along with perspectives for future research.

2. Biogas production and changes in soil carbon input - a regional analysis[*]

2.1 Chapter summary (abstract)

The inclusion of biogas production into the agricultural system has modified crop management and as a result the soil organic carbon (SOC) cycle of the agricultural landscape. To evaluate the effects for the German federal state of Saxony, this study determines: (1) the share of agricultural land required for biogas production, (2) the change in regional carbon input fluxes to soil during the time of the establishment of the biogas production considering also the quality of sources of different fresh organic matter (FOM) for the formation of SOC and (3) the differences in carbon input to SOC between the area influenced by biogas production (here 'biogas fingerprint area' (BFA)) and the surrounding arable land. Based on the location of biogas plants the region was subdivided into biomass providing units (BPUs) where a part of the arable land was considered as affected by biogas production (BFA). We hypothesised that each biogas plant uses a specific substrate mix according to its capacity. The carbon fluxes for each BPU were estimated for the years 2000 (without biogas plants) and 2011 (with biogas plants). For the year 2011, the analysis included the area demand for production of biogas feedstock and digestate recycling. On average 17.6% of the BPU agricultural land was required to supply the biogas plants and dispose of their digestate. Per kilowatt installed electrical capacity this equates to 2.0 ha, including inter alia 0.4 ha for energy crops. Highest area requirements have been observed for biogas plants with less than 500 kW installed capacity. Between 2000 and 2011 the total carbon flux into soil increased by 2.1%. When considering the quality of different FOM sources the gain in carbon input was 2.8%. The BFAs showed higher carbon input to soil than the surrounding agricultural land due to high contributions from digestate and crop residues (esp. agricultural grass). This compensated the low carbon input from crop by-products (e.g. straw).

2.2 Introduction

Soil is one of the most important and most complex natural resources and is an essential contributor to the global ecosystem, providing a regulatory system that supports a multitude of ecosystem functions and services (Adhikari & Hartemink, 2016; Garrigues et al., 2012; Podmanicky et al., 2011). Soil organic matter (SOM) and its major component soil organic carbon

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[*] Published as: **Witing, F.**, Prays, N., O'Keeffe, S., Gründling, R., Gebel, M., Kurzer, H.-J., Daniel-Gromke, J. & U. Franko (2018): Biogas production and changes in soil carbon input - A regional analysis. *Geoderma* 320: 105–114. https://doi.org/10.1016/j.geoderma.2018.01.030

(SOC) are fundamental to soil and its ecosystem functions in particular the sequestration of carbon (Campbell & Paustian, 2015; Podmanicky et al., 2011; Yigini & Panagos, 2016)

Biogas production within conventional agricultural systems has been promoted as an integrated approach to support nutrient cycling, while mitigating greenhouse gases emissions from conventional fossil energy production. Germany is the largest biogas producer in the European Union, with almost 8,700 biogas plants installed in 2016 (Daniel-Gromke, Rensberg, Denysenko, Stinner, et al., 2017; Daniel-Gromke, Rensberg, Denysenko, Trommler, et al., 2017). A previous study by Franko et al. (2015), for the region of Central Germany, identified a number of hot spots where the usage of carbon may raise a conflict between sustaining SOC and producing bioenergy. The expansion of the agricultural system to include bioenergy production has resulted in an adaption of the agricultural management (e.g. cultivated crops, digestate application instead of slurry), which in turn has changed the carbon input to soil within these agricultural landscapes. At the same time biogas production is heavily influenced by the regional availability and variability of feedstock.

To date, no general approach has been developed to understand the potential influence of bioenergy production on regional soil carbon cycling. It is a challenge to tackle the additional complexity that biogas production can introduce into agricultural systems (Arthurson, 2009; Barbosa et al., 2014; Möller & Müller, 2012). Therefore, the aim of this study was an ex-post evaluation of the biogas production within the agricultural landscape of a case study region. For each biogas plant within the federal state of Saxony we estimated the agricultural area required for the provision of biogas feedstock and recycling of digestate, proposing the combination of this as ‘biogas fingerprint area’ (BFA) of a biogas plant. The carbon input to arable soil has been estimated for two separate years 2000 (without biogas production) and 2011 (with biogas production). Here also the quality of different sources of fresh organic matter (FOM) regarding the formation of new SOC was considered. Furthermore, for the year 2011 we compared the carbon input on the BFAs and the arable land not affected by biogas production.

2.3 Materials and Methods

2.3.1 Spatial units of investigation

The federal state of Saxony in East Germany was used as the study region. During the last decade a rapid development of the biogas industry has been observed in this area (Grunewald, 2012). For regional subdivision of Saxony and main spatial element of the study, we used ‘biomass providing units’ (BPU), which separate catchment areas (i.e. for agricultural substrates) from competing biogas plants, as defined by Franko et al. (2015). The location and capacity of the biogas plants within Saxony were determined by Das et al. (2012). Relevant cropping and livestock data were aggregated to the BPU level.

We assumed that every BPU had a closed matter cycle regarding agricultural substrates in the context of biogas production. The feedstock demand of a biogas plant was supplied by the agricultural area within the associated BPU, with the biogas digestate being returned to the same area. The agricultural land required for the production of biogas feedstock and disposal of digestate was defined as 'biogas fingerprint area' (BFA) of a BPU (section 2.3.4). The soil related carbon flows within the BFAs are assumed to differ from the surrounding agricultural land (section 2.3.5). It was hypothesised that depending on the installed electrical capacity and the feedstock mix of the biogas plant, as well as the regional agricultural parameters (e.g. crop mix and yields, livestock mix, management of the arable land), every biogas plant will have its own unique BFA.

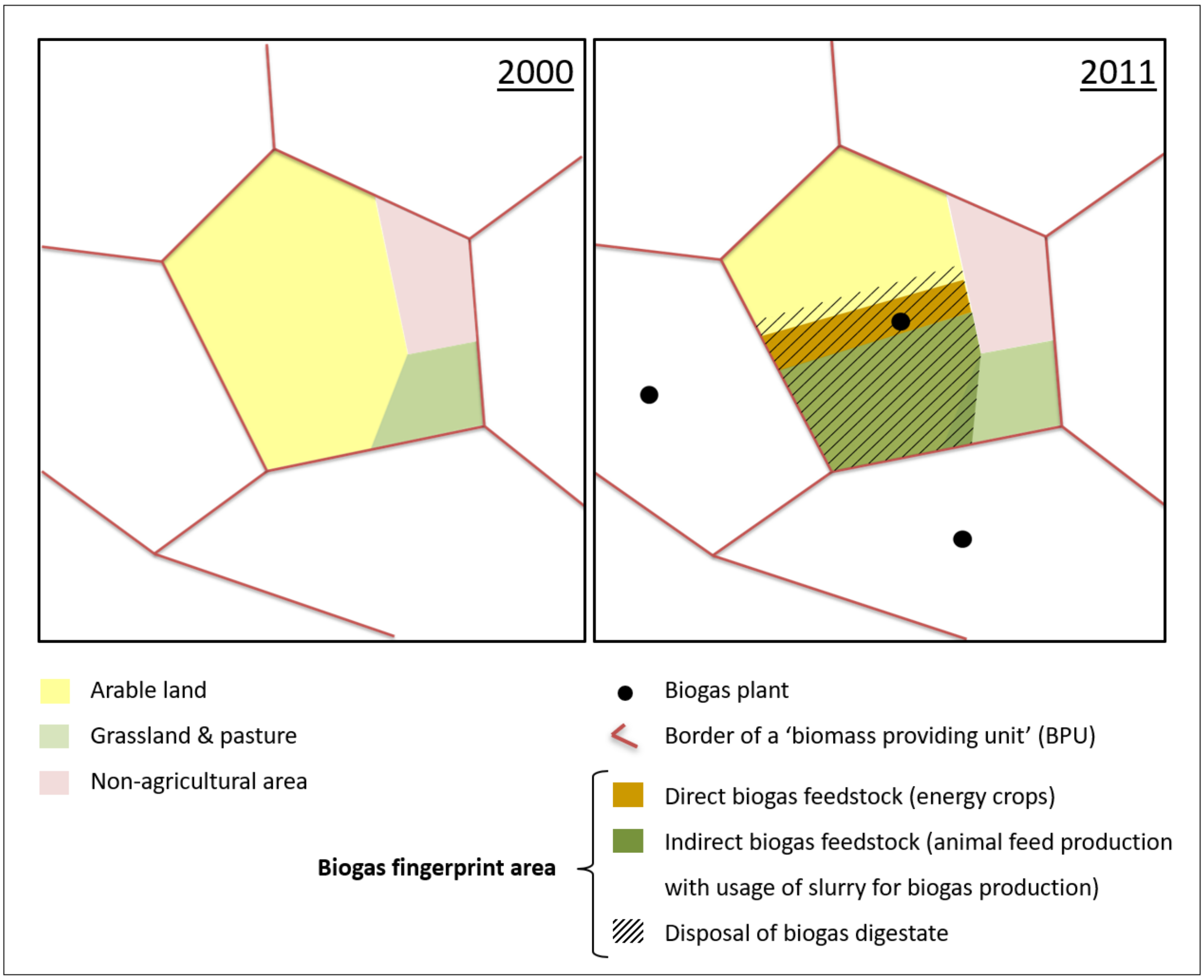

Figure 4: Graphical representation of a 'biomass providing unit' (BPU) and its associated land use categories for the base year of 2000 (without a biogas plant) and the year 2011 (with a biogas plant). For the 2011 time step a 'biogas fingerprint area' (BFA) is shown, to denote the area where the cycling of agricultural matter and the input of carbon to SOM is influenced by biogas production.

For each BPU the associated land use considerations are shown in Figure 4. The crop mix of the BFA corresponds to the direct and indirect demands for biogas feedstock. Depending on the fertilisation intensity, the agricultural area needed for the application of digestate may be smaller or larger than the area for production of biogas feedstock. If the area needed is larger, an additional area for the application of biogas digestate was considered to be necessary. Prior to the implementation of biogas production, livestock excrements were applied to all arable land (year 2000). However, with the installation of biogas plants (year 2011), it was assumed that excrement not used for biogas production were applied only to the BPU area outside of the BFA.

2.3.2 Regional agricultural parameters

Land use and agro-economic regions

The federal state of Saxony (approx. 18,400 km²) is dominated by arable land-use (Figure 5). Due to the very fertile loess soils, which cover a large part of the study area, 52% of the region is used for agricultural purposes. Saxony can be subdivided into three main 'agro-economic regions', based on characteristics of soil, landscape characteristics and their associated agricultural activities (LfL, 1999). These include: (1) Saxon heath and pond landscape, (2) Saxon loess region, (3) Saxon low mountain range and foreland. Supplementary material on these 'agro-economic regions' is provided in the appendix (section 6.1, Table A1).

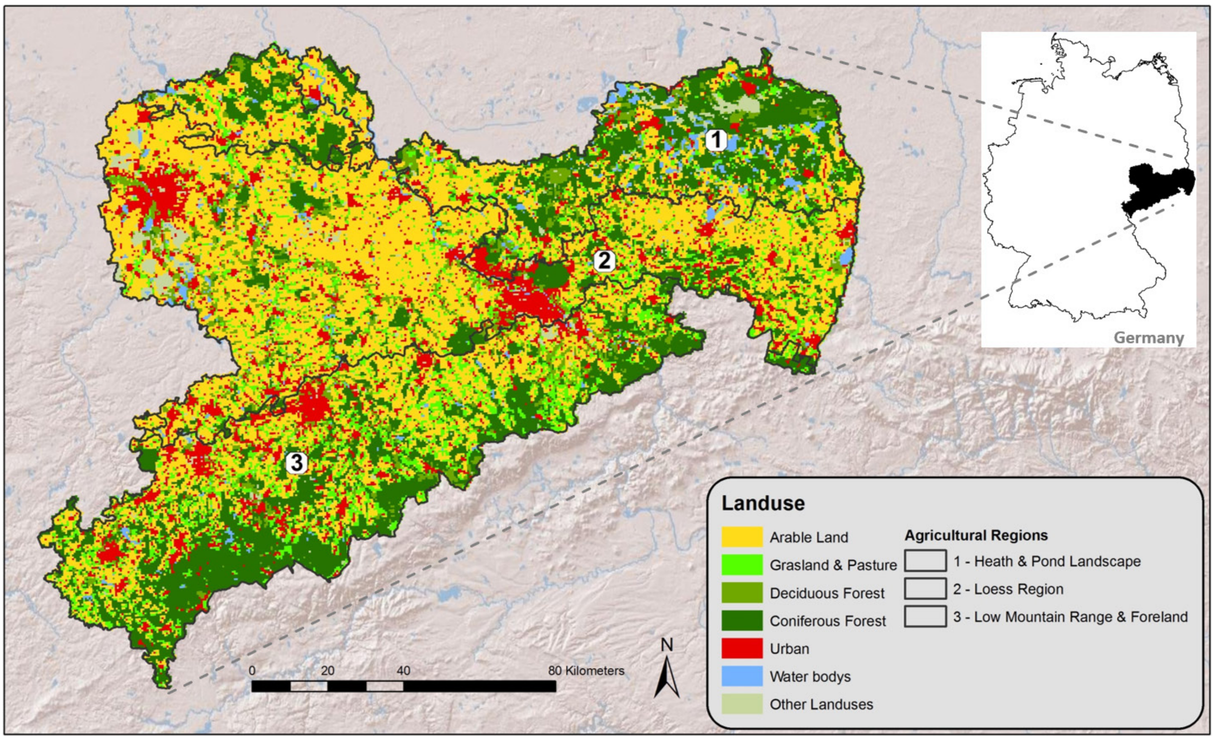

Figure 5: Location in Germany, land-use and the agro-economic regions of Saxony.

Crop harvest areas and yield

Data on crop harvest areas and crop yield for 20 different crops as well as catch crops have been provided by the 'State Agency for the Environment, Nature Conservation and Geology of Saxony' (LfULG). Crop harvest areas are derived from statistics on municipality level (year 2000) and InVeKoS data (Integriertes Verwaltungs- und Kontrollsystem) for the year 2011. Crop yield data was based on analysis of the software BEFU, a fertilisation advisory system used by Saxon farmers (Förster, 2013). Essential crops included in the analysis, as well as their average areal share and yield for the period 2000-2011 are shown in Table 2. For these years, cereals were found to be the dominant crops (58%) in Saxony, followed by winter rape (15%) and maize for silage (9%).

Non-harvested biomass was characterised into two groups, crop residues and crop by-products, -based on the potential usage of the material (see also section 2.3.5). While residues like crop roots and stubble were assumed to be left on the field, the fate of by-products depends on farmers decision: by-products (i.e. straw) can be left on the field or carried away to be used as litter for the livestock stable or sold on the market. Based on expert knowledge, at the state agency LfULG, it was assumed that by-products of relevant crops were removed from approx. 20% of the arable area.

Table 2: Average crop shares and crop yields within the agro-economic regions of Saxony for the period 2000-2011.

	Heath & Pond Landscape		**Loess Region**		**Low Mountain Range & Foreland**	
	Share [%]	**Yield** [t ha^{-1}]	**Share** [%]	**Yield** [t ha^{-1}]	**Share** [%]	**Yield** [t ha^{-1}]
Winter Wheat *(Triticum aestivum)*	13.7	6.4	31.9	7.2	15.5	6.5
Winter Barley *(Hordeum vulgare)*	13.0	5.9	14.5	6.9	11.8	60.0
Winter Rye & Triticale *(Secale cereal & Triticosecale)*	26.1	5.0	6.8	6.2	8.3	5.5
Spring Cereals *(Hordeum vulgare & Triticum aestivum)*	4.0	4.4	5.2	5.0	19.8	4.7
Winter Rape *(Brassica napus)*	12.2	3.4	16.9	3.9	14.3	3.8
Maize for Silage *(Zea mays)*	9.7	42.4	7.7	46.7	10.5	44.0
Field Grass *(Lolium multiflorum & Lolium perenne)*	2.5	30.9	1.6	38.5	5.4	39.0
Clover Grass *(Trifolium pretense & Lolium multiflorum)*	1.3	38.7	1.3	39.7	6.5	38.0
Other[1]	17.4		14.0		8.1	

[1] fallow, sugar beet *(Beta vulgaris)*, grain maize *(Zea mays)*, vegetables, legumes, sunflower *(Helianthus annuus)*, potatoes *(Solanum tuberosum)*

Excrement

We calculated the amount of excrement available for field application or biogas production ($excr_{av}$ in t a^{-1}) based on livestock statistics on district and municipality levels (StLa, 2016b, 2016a). Therefore the total amount of excrement produced from all livestock was corrected for the amount that is left on pasture during grazing (StLa, 2012b). For each animal group i the specific average annual amount of excrement ($excr_i$ in t a^{-1}; (LfULG, 2015)), the share of grazing time within one year (*grzt* [-]) and the number of individuals within this group (*n*) was used to calculate the amount of excrement which we assumed to be slurry:

$$excr_{av} = \sum_{i} \left(n_i \cdot excr_i \cdot (1 - grzt_i) \right) \tag{1}$$

The data was aggregated from municipality level to BPU level using the areal share of municipalities in the BPUs. Within the BPUs the excrement not used for the production of biogas was assumed to be equally distributed on arable land outside of the BFA.

2.3.3 Profile of regional biogas plants

Deriving representative feedstock mixes

The substrate mix used for the production of biogas can vary widely between individual biogas plants making it difficult to parameterise in large scale assessments. Therefore, the demand for biomass substrate was estimated using the approaches outlined in O'Keeffe et al. (2016) in collaboration with the DBFZ (Deutsches Biomasseforschungszentrum) (Ponitka et al., 2015). Six biogas clusters with representative feedstock profiles for agricultural biogas plants were identified for the federal state of Saxony (Table 3). The biogas clusters were differentiated by installed capacity and for the capacity class 151-500 kW also by agro-economic region. For the other capacity classes, a regional differentiation was not possible due to data limitations. The representative feedstock profiles for each biogas cluster were used to generate the appropriate feedstock demand for each biogas plant based on their individual installed electrical capacities (kW_{el}). Manure and slurry have been merged to the feedstock class 'animal excrement' using the differences in dry matter and carbon content of dry matter to be consistent with the calculation of available excrement.

Table 3: Profiles of representative feedstock demand (in tons of fresh matter) for 1 kW installed electrical capacity (tFM kW_{el}^{-1})

Power category [kW_{el}]	**<150**	**150-500**			**500-1000**	**>1000**
Associated sub-region[1]		HPL	LR	LMRF		
	Feedstock demand [tFM kW_{el}^{-1}]					
Animal slurry	43.4	22.9	54.6	77.9	43.8	5.9
Animal manure	2.8	3.3	1.9	0.6	1.0	6.4
Maize silage	6.43	6.72	6.78	2.03	5.31	14.81
Cereals[2]	2.95	1.76	0.88	0.57	1.84	0.85
Grass silage	-	3.30	1.27	3.29	1.36	0.23

[1]HPL=Heath & Pond Landscape; LR=Loess region; LMRF= Low Mountain Range & Foreland

[2]Cereals is a grouping referring to the following crops: rye, barely, triticale

Indirect feedstock requirements

Beside direct area requirements for the production of energy crops, the use of animal excrement for biogas production implicates an indirect land use, in relation to the fodder crops used for livestock production (i.e. the original carbon sources for the animal excrement). We determined the livestock associated with a biogas plant from the relation between the required amount of excrement of the biogas plant ($excr_{bg}$ in t a^{-1}) and the available excrement within a BPU, assuming that this relationship describes the proportion of animals associated with biogas production (N_i):

$$N_i = n_i \cdot \frac{excr_{bg}}{excr_{av}} \tag{2}$$

The total fodder amount of type k (tfd_k in t a^{-1}) necessary to feed the animals associated with a biogas plant was calculated, based on the typical daily fodder demand of type k ($dfd_{i,k}$ in t d^{-1}) and the total number of animals associated with biogas production:

$$tfd_k = \sum_i \left(N_i \cdot 365 \cdot dfd_{i,k}\right) \tag{3}$$

The diet for dairy cows and cattle was assumed to be a silage mix from grass and maize of 25% and 75% respectively, with a cereals diet assumed for pigs (Table 4) (L. Gruber et al., 2004, 2006). Additionally, it was assumed that only a basic diet is produced on the farm and concentrates were imported. Therefore, these were not considered for the calculation of the BFA (see section 2.3.4).

Table 4: Daily fodder demand of cows, cattle (elder than one year), brood sows and other pigs used for the calculation of indirect feedstock requirements. Calves and piglets are not considered. DM = dry matter; FM = fresh matter

		Dairy cows	Cattle	Brood sows	Other pigs
Total forage intake	[kg DM d^{-1}]	18,4	10,7	6,5	2
Basic diet		70%	70%	80%	80%
Maize silage	[kg FM d^{-1}]	36	21	-	-
Cereals	[kg FM d^{-1}]	-	-	6	1,8
Grass silage	[kg FM d^{-1}]	14	8	-	-

Biogas digestate

The amount of biogas digestate (BGD in t a^{-1}) produced and available for field application was estimated using equation (4).

$$BGD = \sum_x (FM_x - BG_x - L_x) \tag{4}$$

Where FM is the quantity of required substrate (t a^{-1}), BG is the amount of produced biogas (t a^{-1}), L is the amount of losses during the fermentation process (t a^{-1}) and x are the substrates listed in Table 5. According to (Vogt, 2008), the carbon flows in the biogas were assumed to consist of the sum of CH_4 and CO_2. The amount of biogas (t DM a^{-1}) was calculated with:

$$BG_x = FM_x \cdot DM_x \cdot oDM_x \cdot \frac{\alpha_x}{1000} \cdot \rho_x \tag{5}$$

Where *DM* is the substrate specific matter content (% FM), *oDM* is organic dry matter content (% DM), α is a substrate specific conversion factor for biogas (l kg^{-1} oDM^{-1}) and ρ is the substrate specific biogas density. Additionally, the nitrogen (N) content of the biogas was assumed to be insignificant. The carbon content of the biogas was determined from the share of CH_4 and CO_2 according to the specific substrate mix of the cluster.

Table 5: Substrate parameters used for biogas production calculations. DM = dry matter, oDM = organic dry matter content, biogas yield = substrate specific conversion factor for biogas (α), biogas density = substrate specific biogas density (ρ), losses = ensiling losses for silages (L_s), CH_4 = methane share in produced biogas.

Substrate	DM[1] [%]	oDM[1] [%]	C cont. [%]	N cont.[1] [%]	losses[3] [%]	CH_4 [3] [%]	Biogas yield[3] [l kg^{-1} oDM^{-1}]	Biogas density [kg m^{-3}]
Animal slurry	10	80	35[1]	4.67	0	55	380	1.28
Maize silage	28	95	45[2]	0.38	12	52	650	1.32
Cereals	86	97	45[2]	1.96	0	52	730	1.32
Grass silage	20	90	45[2]	0.38	12	53	600	1.31

[1] from CANDY database (Franko, 1996), [2] from Schilling (2000), [3] from KTBL (2012)

Losses during the fermentation process (*L*) were estimated using equation (6) and based on the assumption of 10% N losses during digestion (Vogt, 2008). *N* is the substrate specific N content (%).

$$L = \sum_x (FM_x \cdot DM_x \cdot N_x \cdot 0.1) \tag{6}$$

Consequently, the N content of the biogas digestate (N_{BGD}) is also based on the N content of the biogas substrate and was estimated using the following equation:

$$N_{BGD} = \sum_x (FM_x \cdot DM_x \cdot N_x) - Lf \tag{7}$$

2.3.4 Estimation of the biogas fingerprint area

The BFA corresponds either to the area which is needed for the production of the biogas feedstock (A_{pr} in ha) or to the area needed for returning the digestate (A_{rc} in ha) when it exceeds the fertiliser demand of A_{pr}:

$$BFA = max(A_{pr}, A_{rc}) \tag{8}$$

A_{pr} is calculated from the direct and indirect feedstock requirements of a biogas plant, considering typical ensiling losses Ls (Table 5) and the BPU specific yield Y (t ha^{-1}) of the relevant crops (x):

$$A_{pr} = \sum_{x} \left(\frac{(1 + Ls_x) \cdot FM_x}{Y_x} \right) \tag{9}$$

FM_x (in t) represents the feedstock requirement of energy crops or fodder crops. Grass silage demand is primarily provided by temporal grass crops and later by permanent grassland, if more substrate is required.

The area needed to recycle the digestate of a biogas plant (A_{rc} in ha) depends on the total N content of the digestate (N_{BGD} in t N) and application rates of N on arable land. We assume that the total amount of digestate-N applicable on A_{pr} (N_{pr} in t N) (1) compensates N offtake with harvested crops while (2) taking into account an application limit of 0.17 t N per ha given by legislation (Düngeverordnung - DüV, 2017). If N_{BGD} exceeds N_{pr} the application area has to be extended by an additional area (A_{ex} in ha) for the disposal of the excess N (N_{ex} in t N):

$$A_{rc} = A_{pr} + A_{ex} \tag{10}$$

$$N_{ex} = N_{BGD} - N_{pr} \tag{11}$$

with:

$$N_{pr} = min\left\{0.17 \cdot A_{pr}, \sum\nolimits_{x} (1 + Ls_x) \cdot FM_x \cdot Nc_x \right\} \tag{12}$$

where Nc_x is the N content in the fresh matter of the harvested yield of crop x.

If N_{BGD} is less than N_{pr} (N_{ex}<0), N_{BGD} will be evenly distributed on A_{pr}. If an additional area is required for digestate disposal (N_{ex} > 0), it is related to the average N removal by crop yield from the BPU area surrounding A_{pr} (N_{rem} in t N):

$$A_{ex} = \frac{N_{ex}}{N_{rem}} \tag{13}$$

BPUs where the local cultivation characteristics could not completely cover the feedstock demand of the corresponding biogas plants with respect to every type of substrate were excluded from the analysis. For example, some biogas plants at the Saxony border would require additional substrate from outside of the study region. This reduced the number of biogas plants included in the study from 183 to 121.

2.3.5 Carbon flows into soil

To characterise the impact of different land management systems on SOC we consider: (1) the total carbon flux from FOM into the soil as well as (2) the quality of different sources of FOM regarding the formation of new SOC. To assess the quality of the carbon flux from FOM to SOC, we use the 'carbon reproduction flux' (C_{rep}), an indicator that aggregates the effect of different carbon sources on SOC storage (Brock et al., 2013; Franko et al., 2011; Kolbe, 2010; Küstermann et al., 2008).

The total carbon input from FOM, as well as the C_{rep} flux into soil were calculated in accordance with the approach of the carbon turnover models in CANDY (Franko et al., 1995) and CCB (Franko et al., 2011). In this approach the turnover of several FOM pools (C_{FOM}) results in a carbon flux to the atmosphere (mineralisation) and a C_{rep} flux into the SOM pool. We calculated C_{FOM} and C_{rep} (in kg ha^{-1}) for different types of arable carbon sources: organic amendments (excrement, digestate), crop residues (roots and stubble) and crop by-products (straw and beat leaves) (Figure 6).

C_{FOM} flows were estimated using BPU specific yield data for each crop and application rates for organic amendments, as described in the previous sections. Parameterisation of the different carbon sources and crops was taken from the CCB database. For the conventional agricultural carbon flows (residues, by-products, excrement) a more in-depth description is given by (Franko et al., 2011). Regarding the matter flows from biogas digestate, equation (14) was used to calculate the carbon amount ($C_{FOM_{BDG}}$).

$$C_{FOM_{BDG}} = C_{FM} - C_{BG} \tag{14}$$

Here C_{BG} is the carbon equivalent of the produced biogas and C_{FM} is the total carbon amount of the biogas feedstock according to the material properties:

$$C_{FM} = \sum_x (FM_x \cdot DM_x \cdot C_x) \tag{15}$$

The carbon equivalent of the biogas C_{BG} was calculated using the molar volume of an ideal gas at 1 atmosphere of pressure V_m=22.42 l mol^{-1}, amount of biogas (BG_x), molar mass of carbon (M_C) in V_m depending on the methane share, biogas density ρ_x (kg m^{-3}) as sum over all added substrates x:

$$C_{BG} = \sum_x \left(\frac{BG_x * M_C}{\rho_x * V_m * 1000} \right) \tag{16}$$

For the calculations of C_{rep} every source of FOM has its specific substrate use efficiency parameter (η) characterising the potential quality of the substrate for the formation of new SOC

(Franko et al., 2011). The substrate use efficiency of biogas digestate was determined according to Prays et al. (2017).

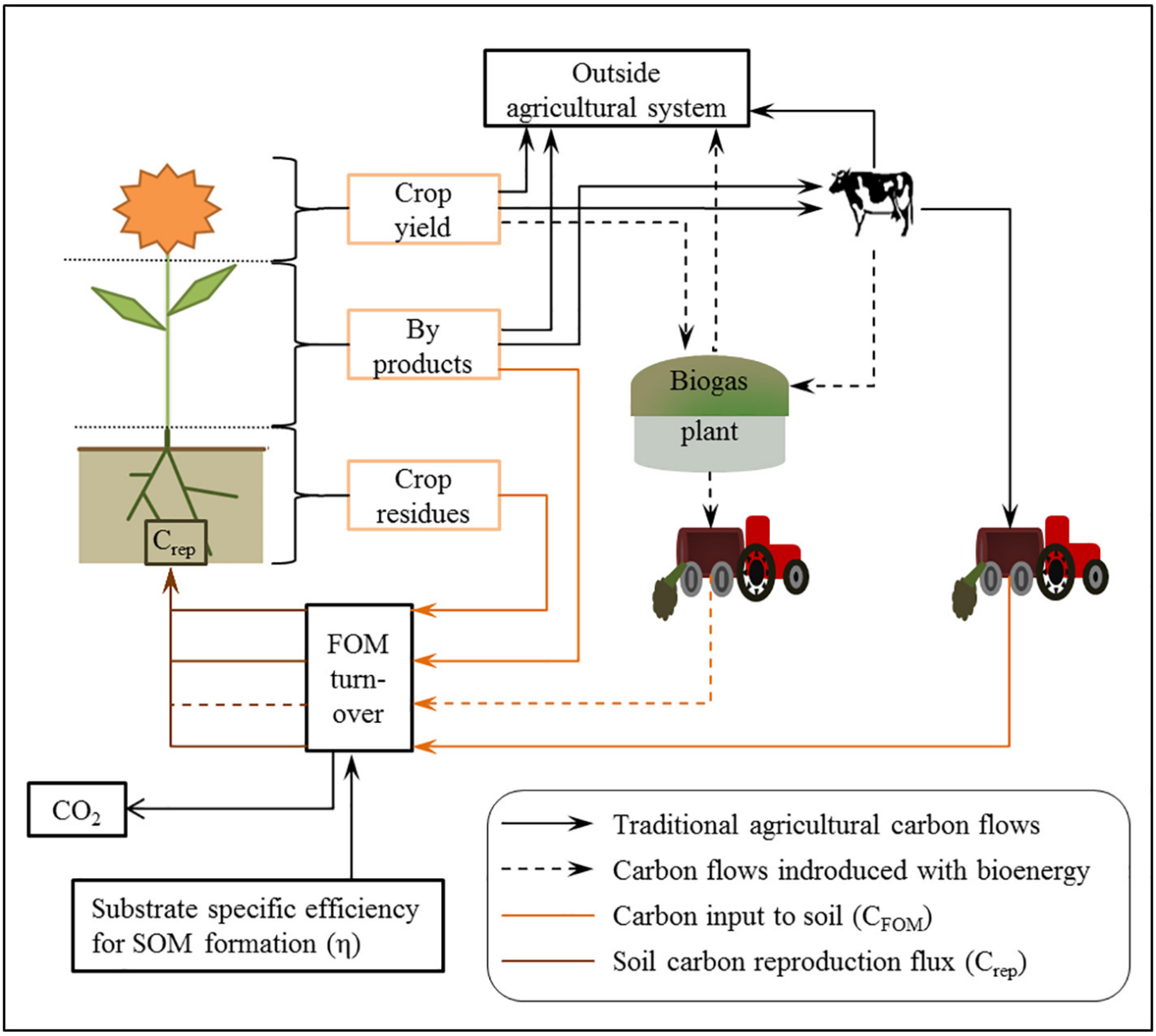

Figure 6: Carbon flows considered within the regional cycling of agricultural matter related to biogas production. Different pools of fresh organic matter (FOM) contribute to the total carbon flux to soil (C_{FOM}): crop residues, crop by-products, biogas digestate and livestock excrement. All sources of FOM have a different quality for the formation of new SOC. The C_{rep} flux is aggregating these differences and can be used as an indicator in a given environment to characterise the land use regarding SOC storage.

For the calculation of C_{FOM} and C_{rep} only arable land has been considered and permanent grassland has been left out. All carbon flows were calculated for two time steps, 2000 (without biogas) and 2011 (with biogas) for each BPU. For the year 2011, an additional analysis was performed for the BFA and for the area not affected by biogas production (see also section 2.3.1).

2.4 Results

2.4.1 Regional areal requirements of biogas production

BFAs and associated land use categories

The results of the model indicated that in 2011, the provision of biogas feedstock and distribution of digestate on average, affected 20.8% of the arable land within the BPUs. When considering the total agricultural land in Saxony (including permanent grassland) the BFA of the biogas plants covered 17.6% (Figure 7). Over 10% of all BPUs, were found to have a fingerprint area exceeding 40% of their BPU arable area.

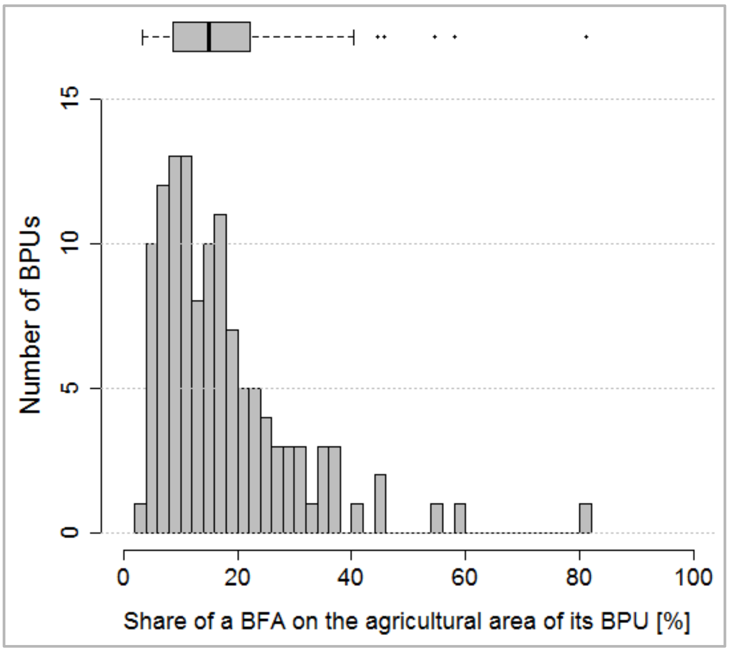

Figure 7: Share of the agricultural land of the BPUs in Saxony that is needed for the provision of biogas feedstock as well as for the distribution of digestate (BFA) in the year 2011.

The land use within BFAs was dominated by fodder crops on arable land (57.9%). The primary use of these areas is the production of meat and milk. The use of the livestock excrement for the production of biogas is a secondary and indirect use of these areas. The cultivation of energy crops on arable land covered 19.8% of the average BFA in Saxony and 7.1% was covered by permanent grassland. For most of the BFAs an additional area for the application of digestate was necessary. Digestate application to additional land outside the feedstock catchment accounted for 15.2% of an average BFA in Saxony.

Relationship between BFA and installed capacities

Relating the BFA to the installed electrical capacity of its biogas plant allows the different biogas systems to be compared with respect to the areal demand and hence areal efficiency per electrical energy output (ha kW_{el}^{-1}). On average for Saxony 2.0±0.4 ha kW_{el}^{-1} (± is the standard deviation) agricultural land was found to be influenced by biogas production. However, only 0.4±0.1 ha kW_{el}^{-1} from that was related to the cultivation of energy crops on arable land. The major part of the land demand consisted of fodder crops on arable land (1.2±0.3 ha kW_{el}^{-1}) for cattle supply, but also the additional area for digestate disposal was covering 0.3±0.3 ha kW_{el}^{-1}. To fulfil the demand for grass silage 0.1±0.1 ha kW_{el}^{-1} of permanent grassland was needed next to the use of field grass from arable land. Between individual BFAs the results differed due to regional differences in crop yields and livestock mix, as well as parameters of the specific biogas plant (e.g. installed capacity, feedstock mix).

The Saxon heath & pond landscape (1.8±0.3 ha kW_{el}^{-1}) as well as the loess region (1.9±0.2 ha kW_{el}^{-1}) showed significantly smaller area requirements than the low mountain range and foreland (2.6±0.4 ha kW_{el}^{-1}). Next to regional differences in crop yield this is a result of the greater number of smaller biogas plants in the low mountain range.

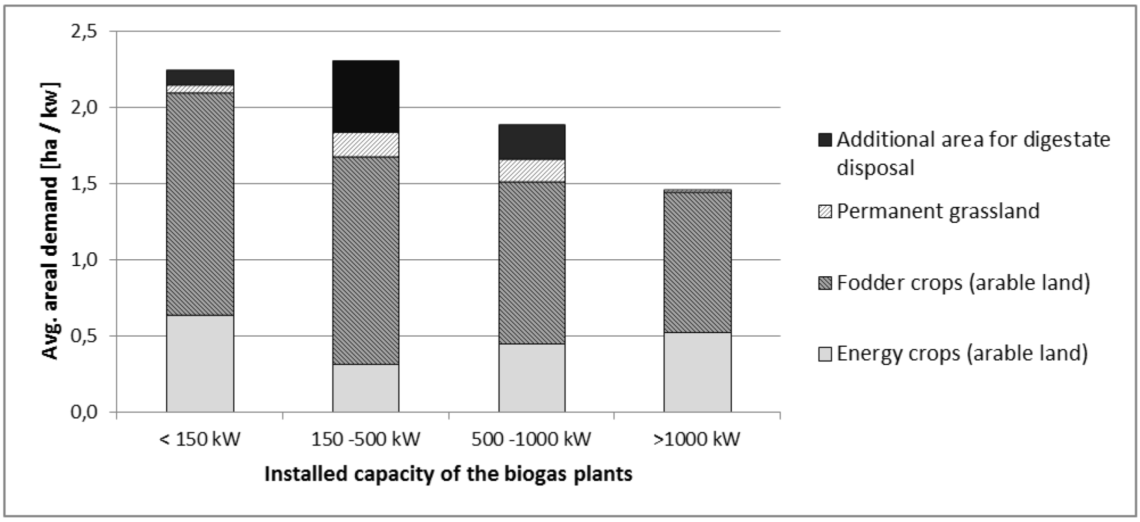

Figure 8: Average area demand (ha) per kilowatt installed electrical capacity of the biogas plants in Saxony. Biogas plants are differentiated by size classes. Area demand is separated by land use categories within a BFA.

Depending on the size classes of the biogas plants, major differences in the total area demand and its composition have been observed (Figure 8). A constant decrease in the area requirements for the provision of biogas feedstock was found with increasing classes of plant size. While biogas plants with installed capacity < 150 kW_{el} typically needed 2.1±0.3 ha kW_{el}^{-1} for feedstock supply, plants > 1000 kW_{el} only needed 1.5±0.1 ha kW_{el}^{-1}. This pattern was primarily caused by lower indirect feedstock requirements in the feedstock mix of larger biogas plants. However, also the location distribution of the biogas plants and the subsequent agricultural yields are important factors. The area demand for the cultivation of direct feedstock requirements (energy crops) was lowest (0.3±0.1 ha kW_{el}^{-1}) for biogas plants in the size class 150-500 kW_{el}. However, biogas plants in this capacity range showed the highest total areal demand per kW_{el} due to large requirements regarding additional area for digestate disposal

(0.5±0.3 ha kW^{-1}). Input from energy crop cultivation was especially high within BPUs containing plants in the size classes <150 kW_{el} and >1000 kW_{el}. This was most of all due to a high share of energy crops (>1000 kW_{el}) and especially cereals (<150 kW_{el}) in the feedstock mix.

2.4.2 Regional carbon input to soil before and after implementation of biogas plants

The average carbon input into the arable soil of the Saxon BPUs was 2,905 kg C ha^{-1} in the year 2000 and increased slightly to 2,965 kg C ha^{-1} (+2.1%) in the year 2011, after the implementation of biogas plants. When considering the quality of different sources of FOM for the formation of SOC by using the indicator C_{rep} we observed an even higher increase of 2.8% (2000: 1,524 kg C_{rep} ha^{-1}; 2011: 1,567 kg C_{rep} ha^{-1}). Within the individual BPUs the changes between 2000 and 2011 are much more apparent, ranging from -388 kg C ha^{-1} to +576 Kg C ha^{-1} or -119 kg C_{rep} ha^{-1} to +297 kg C_{rep} ha^{-1} respectively.

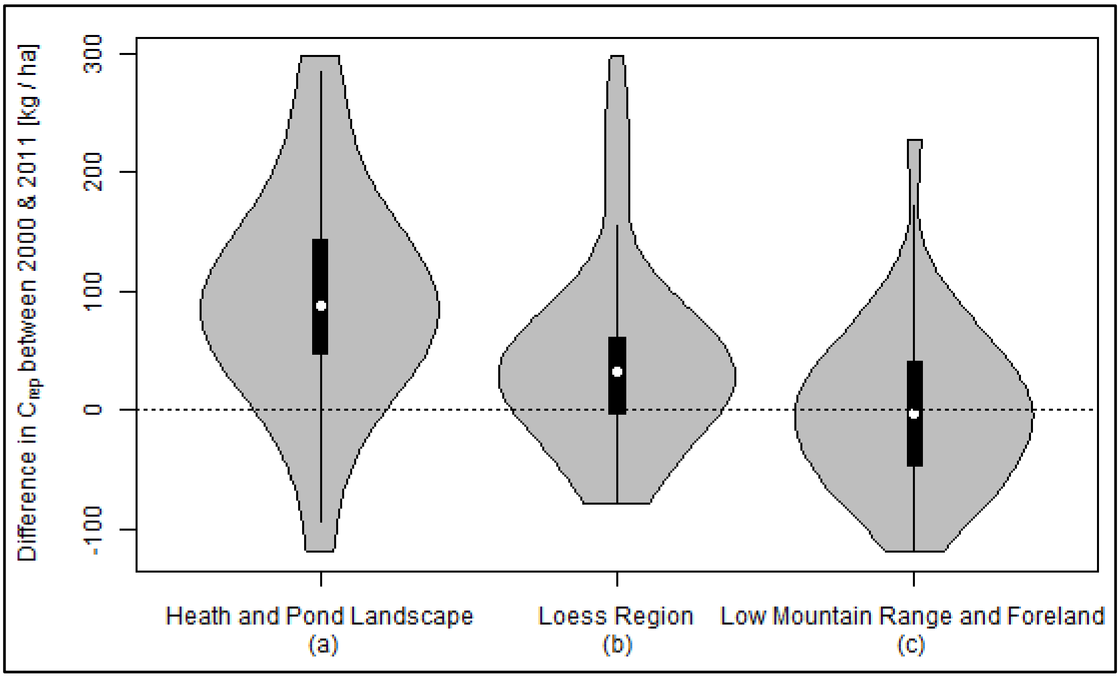

Figure 9: Violin plot showing the difference in C_{rep} between 2000 and 2011 on BPU-level, differentiated into the agro-economic regions within Saxony. The difference between the regions is significant (Welch t-test p-values: (a)-(b) 0.027, (a)-(c) <0.001, (b)-(c) 0.007). The Violin plot is combining a boxplot with a density plot.

The differences between individual BPUs were partly affected by their geographic location. On the level of agro-economic regions (Figure 9) significant differences in the temporal development of SOC input can be observed (ANOVA p-value: <0.001). Only limited statistical relationship between biogas plants capacity and SOC input have been found. BPUs having biogas plants in the power category 150-500 kW_{el} (+1.4% C_{rep}) contributed significantly less to the increase C_{rep} fluxes than the BPUs having biogas plants in all the other power categories (+4.0% C_{rep}) (Welch t-test p-value: 0.013).

2.4.3 Changes in carbon sources

SOC input from arable crops

The total crop-based C flux into soil from all analysed BPUs displayed a moderate increase (+5.8%) between 2000 (1,453 × 10^3 t C) and 2011 (1,538 × 10^3 t C). At the same time the contribution of the different cultivated crops changed greatly. Table 6 summarises the quality adjusted C input (C_{rep}) from individual arable crops for the two time steps, 2000 and 2011. Winter rape, maize, winter wheat and sugar beet showed a high total increase in C_{rep}. A decline in C_{rep} contribution was observed for all cereals other than winter wheat. The contribution from fallow land was also seen to drop remarkably, as these areas went back into cultivation. The shift in C input to SOM of different crops is primarily caused by changes in cultivated area and less by changes in yield.

Table 6: Total soil carbon reproduction flux (C_{rep}) from the cultivation of different arable crops for the two years 2000 and 2011. C_{rep} is aggregating the carbon input to soil considering also the quality of different sources of FOM for the formation of SOC. Altering C_{rep} flows are caused by changes in the crop specific cultivated area and crop specific yields between the two time steps 2000 and 2011.

	Total C_{rep}		**Differences between 2000 & 2011**	
	2000 [10^3 t C]	**2011** [10^3 t C]	**Cultivated area** [%]	**Yield per area unit** [%]
Winter Wheat	235.6	268.1 (+14%)	+13.8	+0.1
Winter Barley	121.0	103.4 (-15%)	-16.0	+2.4
Winter Rye & Triticale	98.1	62.4 (-36%)	-32.3	-4.4
Spring Cereals	49.3	45.5 (-8%)	-12.4	+7.0
Winter Rape	81.9	127.0 (+55%)	+43.7	+9.1
Maize for Silage	26.8	43.2 (+61%)	+61.4	-0.4
Grain Maize	12.2	21.7 (+78%)	+63.9	+12.2
Field Grass	21.7	26.4 (+22%)	+28.5	-9.9
Clover Grass	16.3	15.2 (-7%)	-6.2	-4.2
Sugar Beet	22.1	32.3 (+46%)	+23.4	+18.3
Other[1]	52.2	27.2 (-48%)	-32.2	-

[1] Fallow, vegetables, legumes, sunflower, potatoes, catch crops

SOC input from organic amendments

Our results indicate that major shifts in C flows on arable soils between 2000 and 2011 were associated with the type and contribution of organic fertilisers (i.e. animal excrement and biogas digestate). The total amount of regionally available C from livestock excrement declined from 295.8 × 10^3 t in 2000 to 259.0 × 10^3 t in 2011 (-12.4%) due to a reduction of livestock numbers. In the year 2000 all excrements were assumed to be applied to arable land, whereas in 2011 only 65% (167.2 × 10^3 t) of the potential available C from livestock excrement could be used for this purpose. This was because the remaining part of livestock excrement (91.8 × 10^3

t C) was used for the production of biogas. However, due to the usage of plant material (additional to the excrement) for biogas production, the C input to soil from biogas digestate (80.3×10^3 t) compensates the livestock related C that was taken out of the traditional matter cycling. When considering the different quality of excrement and digestate for the formation of SOC the total contribution of organic amendments to C_{rep} fluxes decreased by only 5.1% in the period under study (2000: 180.4×10^3 t C_{rep}; 2011: 171.1×10^3 t C_{rep}) despite the reduction in livestock (-12.4%).

2.4.4 Carbon fluxes in- and outside of the BFA

Both C_{FOM} and C_{rep} were found to be lower on the arable land not needed for the provision of biogas feedstock and distribution of digestate (C_{FOM}: 2,956 kg ha^{-1}; C_{rep}: 1,518 kg ha^{-1}) than on the fingerprint areas of the biogas plants (C_{FOM}: 3,008 kg ha^{-1}; C_{rep}: 1,814 kg ha^{-1}). Indeed, the C_{rep} fluxes were significantly different (-16.3%; Welch t-test p-value: <0.001).

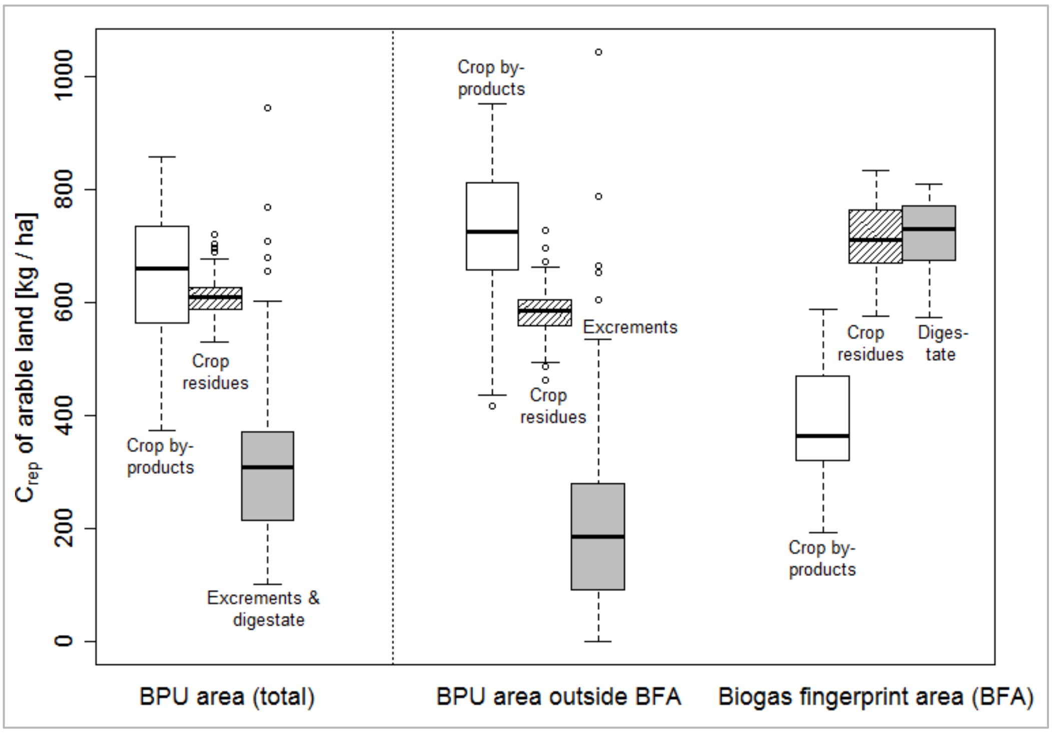

Figure 10: Soil-carbon reproduction fluxes (C_{rep}) of arable land for the year 2011 and with respect to different sources of carbon. C_{rep} aggregates the carbon input to soil considering also the quality of different sources of FOM for the formation of SOC. Regional basis are biomass providing units (BPU) as well as the two areal categories within a BPU: (1) biogas fingerprint area (BFA) and (2) BPU arable land outside of the BFA.

When analysing the different carbon sources, the BFAs showed a high carbon input to soil from crop residues and digestate application (Figure 10). The first is mainly due to a comparatively high share of agricultural grassland within the BFA which typically has higher amounts of residues (e.g. roots). The second is mainly due to the extensive application of digestate up to the limitation for organic N application. Furthermore, within the BFAs the amount of C from crop by-products (e.g. straw) is reduced, due to a lower share in cereal cultivation. In total the C_{rep} provision by arable crops (crop residues and crop by-products) is lower in the BFAs than in the surrounding BPU area.

2.5 Discussion

2.5.1 Influence of biogas production on land use

We developed a new approach of a 'biogas fingerprint area’ to determine and characterise the agricultural areas affected by biogas production, due to their feedstock requirements and digestate recycling. This is in contrast to the concept of the ‘ecological footprint’ (Wackernagel & Rees, 1997). We deal only with the direct land area requirement for the production of biogas and disposal of digestate and within this, only the associated direct soil carbon fluxes. The BFA aggregates effects of location (e.g. crop yields) and management (e.g. feedstock mix of the biogas plant, fertilisation practices). Therefore, the relationships between (1) the BFA and the total agricultural land of its BPU, as well as between (2) the BFA and the installed electrical capacity of its biogas plant are two valuable indicators for the analysis and differentiation of bioenergy production systems on larger scales. In this study the application of our methodology was successfully demonstrated for Saxony.

The need to establish a greater understanding of the relationship between power supply and area requirements of different renewable energy sources has already been identified (Evans et al., 2009; Lechon et al., 2011; Popp et al., 2014; Scheidel & Sorman, 2012; H. Wüstemann et al., 2017). Therefore, the results of this study contribute to a better understanding of this in relation to biogas production on the regional scale. We found that biogas production consumed the harvested crop yield from 4.1% of the BPUs arable land due to their direct feedstock requirements. This corresponds to on average 0.4 ha of energy crops from arable land per kW_{el} installed capacity of an average biogas plant in Saxony. A similar range has been discussed in other studies analysing the area demand of biogas plants in German study regions (Delzeit et al., 2011; Hartmann, 2008). However, we also showed that the total area requirements of the biogas production systems in Saxony, including indirect feedstock requirements and the area needed for disposal of excess digestate, are many times larger than the area strictly dedicated to energy crop cultivation. Within the study period considered, the harvest areas of the different cultivated crops changed considerably. While for the majority of crops, the increase in cultivated area may have been influenced by bioenergy production, the observed changes are also influenced by general changes in agricultural management (e.g. rotations).

Soil, climate and agricultural structure are important factors, which distinguish the agro-economic regions in Saxony (StLa, 2004, 2012a) and effected the management (e.g. feedstock mix) and area requirements of the biogas plants. For example, a large variability has been found with respect to the area needed for the disposal of digestate. But the regional properties (e.g.

livestock numbers, yield potential) also affect the biogas plants themselves, e.g. with respect to the choice of power category that has been build. Other studies have shown, that there is an incentive to build larger biogas plants in areas having high yield expectations as this limits transportation distance and costs (Delzeit et al., 2009, 2012). It is important to understand these relations to be able to give scientifically substantiated recommendations on how to improve the management of those complex agricultural systems. The indicators developed in this study can help to identify critical hot-spots, where an increased competition for agricultural area and harvested crop yield may occur on one side between neighbouring biogas plants, but also between biogas production and food production.

2.5.2 Biogas driven modifications in SOC input

The approach presented in this study can show the differences in carbon fluxes into soil between conventional agricultural systems and those with integrated biogas production. This is important, as the effects of bioenergy feedstock cultivation on SOC storage is a key factor in determining the sustainability of bioenergy (Anderson-Teixeira et al., 2009; Schrama et al., 2016; Tiemann & Grandy, 2015). Our results indicate that biogas production can be a win-win strategy that substitutes fossil fuel and leads to a positive effect on regional SOC input in Saxony. This also applies when considering the quality of the different sources of FOM for the formation of SOC.

The observed temporal shifts in carbon fluxes cannot be used to predict changes in long term SOC stocks, as they also depend on regional turnover conditions and the historical SOC development of the site. Large scale detailed monitoring data of SOC stocks in agricultural soils would allow quantifying actual changes in SOC storage. However, this kind of monitoring for the whole Saxon study region has yet to be conducted. For future studies it may be an option to initialise regional SOC levels based on interpolation of available site measurements (Y. Li, 2010; Mishra et al., 2010; Schloeder et al., 2001).

We propose to use the difference between the carbon input fluxes inside and outside of the BFA as indicator to characterise the sustainability of biogas production in terms of SOC storage. In Saxony average C fluxes to soil have been higher in the BFAs than in the arable land outside the BFAs. However, BFAs had a very low carbon input to soil from crop by-products (e.g. straw), due to a low share in cereal cultivation. The BFAs benefited from the extensive application of digestate, as well as from a high area share of agricultural grassland which typically has higher amounts of residues (e.g. roots). The effect of feedstock mix on the sustainability of biogas production has already been recognised by policy measures (Erneuerbare-Energien-Gesetz vom 21. Juli 2014 (BGBl. I S. 1066), das zuletzt durch Artikel 2 des Gesetzes vom 22. Dezember 2016 (BGBl. I S. 3106) geändert worden ist., 2017). Policy measures addressing the feedstock mix can effectively control the use of substrates and would affect the area of crop cultivation (Britz & Delzeit, 2013).

The calculated amounts of organic fertilisers applied on arable land (excrement and digestate) are about 3% lower than reported in official statistics on the application of organic amendments in Saxony (StLa, 2011), but are within a reasonable range (9.6×10^6 t compared to 9.9×10^6 t). For all BPUs analysed, the carbon input from organic fertilisers changed considerably within the observation time. While the application of livestock excrement on arable land was strongly reduced due to the use for biogas production and the reduction in livestock numbers, the application of digestate could almost completely compensate this. Here the higher quality of digestate for the formation of SOC is important. The digestate based carbon is essential to compensate the low crop-based carbon fluxes within the BFAs. Most of the biogas plants needed more area for the application of digestate than for feedstock supply. More practical field research is required to determine the effects of applying digestate, as of yet this knowledge base is sadly lagging behind what is known about application of animal slurries.

It must be pointed out that the analysis focused only on the biogas catchments and does not consider any indirect effects on SOC outside of Saxony due to imported fodder. But for this study these possible drawbacks are quite low as the rate of internal fodder production in Germany kept at about 90% between 2000 and 2011 (Deutscher Bundestag, 2012). Another uncertainty is the exact regional distribution of the livestock related organic fertilisers due to the spatial resolution of the initial data. However, the assumptions were consistent across the entire region and suitable for a relative comparison across the region.

2.5.3 Conclusions

The proposed modelling approach outlined in this paper has the benefit to provide better insight into agricultural carbon and matter fluxes, as well as regional area requirements related to biogas production. It is an attempt to understand the complexity of this system. It was shown that in the study region Saxony biogas plants can be operated sustainably with regard to SOC recycling. The total carbon flux into soil kept stable, with a slight tendency for an increase during the time period of the establishment of the biogas industry. On average, 17.6% of the agricultural land in Saxony was determined to supply the biogas plants and dispose of their digestate in 2011. The comparison of carbon fluxes inside and outside of this biogas fingerprint areas is an easily applicable instrument to assess the influence of biogas production on the region's SOC input.

Areas affected by biogas production showed a high carbon input to soil, but this was very reliant on the application of digestate. It could be beneficial for governments to develop 'good farm practices' for agricultural systems operating biogas plants. Furthermore, an adequate farm management planning has to be developed to deal with this different type of fertiliser.

3. Large-scale integrated assessment of soil carbon and organic matter-related nitrogen fluxes in Saxony (Germany)[*]

3.1 Chapter summary (abstract)

Changes in land-use, agricultural management and climate affect the turnover and storage of organic carbon in soils (SOC) as well as the nitrogen mobilisation from soil organic matter (SOM), with potential side effects on nitrogen availability and leaching. When addressing the requests for increased carbon storage in soil as well as for the reduction of nitrogen losses, integrated approaches on regional scales are required that take into account the actual changes in agricultural management and climate. This study investigated the arable land (7345 km^2) of Saxony (Germany) with regard to the following: (1) the trends of SOC storage and organic matter-related nitrogen fluxes, including their sub regional and annual dynamics, (2) changes in the carbon input to arable soils and the turnover of organic matter, and (3) the contribution of different drivers (climate, crop production and fertilisation, tillage system) to the simulated SOM changes for the period 1998–2014 on a 500 m grid. The model CANDY carbon balance (CCB) was specifically adapted for large-scale simulations of SOM turnover to link spatial data on soils and climate with regional statistics on agricultural management. This new 'regional mode' of CCB has been validated using data from 391 plots across different European locations. The initial SOC levels for Saxony assumed steady state conditions at the beginning of the simulation period and have been validated using data from 667 monitoring sites. The results showed an increase in the SOC stocks of the arable soils of Saxony of 785 x 10^3 t C (1.24‰ annually) during the simulation period. At the same time, the model simulated an average increase in organic nitrogen stored in SOM of approximately 7.5 kg N ha^{-1} a^{-1}, with considerable differences between individual years and subregions. Both the increase in carbon inputs to soil (+8%) and the reduction of carbon turnover rates (-10%) had positive effects on SOC storage. While the increased use of conservation tillage was the most important driver for the overall increase in SOM storage in Saxony, climate variability and crop production and fertilisation had the largest effect on its annual dynamics.

3.2 Introduction

Agriculture in Central Europe is currently faced with new challenges and opportunities. New markets for agricultural raw materials (e.g., bioenergy) created a strong incentive to intensify agricultural production (Fischer et al., 2010; Lotze-Campen et al., 2010). At the same time, the

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demands on agriculture to further minimise the negative effects of land use on the environment (e.g., nitrate leaching and loss of soil carbon) are increasing. Changing climate conditions exert additional pressure and require an adaption of agricultural management (Olesen et al., 2011; Olesen & Bindi, 2002; Reidsma et al., 2010).

Against the backdrop of changes in agricultural management but also with regard to climate change, impacts to the soil organic matter (SOM) balance, carbon to nitrogen (C:N) ratios and nitrogen leaching can be expected (Bindi & Olesen, 2011; Smith et al., 2005). Processes of enrichment and depletion of carbon and nitrogen in SOM significantly influence the preservation of soil fertility and the release of nutrients from the organic pool. They also influence the soil functions related to carbon storage. To address these problems, integrated approaches are necessary that consider organic nitrogen pools as well as organic carbon pools with individual C:N ratios (N. Gruber & Galloway, 2008).

To avoid a trade-off between further intensification and the growing requirements for resource efficient and sustainable production, it is necessary to improve the understanding on current trends in soil organic carbon (SOC) and nitrogen storage and to evaluate the impacts of agricultural use on larger scales. However, the large-scale spatially distributed quantification of carbon and nitrogen dynamics in soil is especially challenging. Data availability is typically limited with respect to agricultural management and SOM monitoring data, and the results must be evaluated under consideration of the respective conditions of the landscape and its management.

The aim of this study was to 1) quantify the recent changes in SOC storage and organic matter-related nitrogen fluxes in the arable land of Saxony (Germany) and to highlight their subregional and annual dynamics; 2) analyse changes in the carbon input to arable soils and the turnover rates of organic matter; and 3) quantify the impact of different drivers (climate, crop production and fertilisation, tillage system) on the observed changes in SOM. The modelling approach was implemented on a 500 m grid using the CCB model (CANDY carbon balance; Franko et al., 2011), specifically adjusted for large-scale problems of SOM turnover.

3.3 Materials and Methods

3.3.1 Study area

The federal state of Saxony in East Germany is dominated by agricultural land use (52%). Arable land covers approximately 7,345 km^2 and is intensively used due to its fertile loess soils. Data on soils, climate, land-use and agricultural management have been provided by the 'State Agency for the Environment, Nature Conservation and Geology of Saxony' (LfULG) and GALF bR ('Gesellschaft für Angewandte Landschaftsforschung'). The underlying database has already been used successfully for the quantification of diffuse matter transport in the river catchment areas of Saxony using the model STOFFBILANZ (Gebel et al., 2010, 2013, 2016; Halbfaß et al., 2009). The STOFFBILANZ database has been transferred into a format suitable for the CCB model used in this study (see section 3.3.3).

The modelling approach was based on a grid with a cell size of 500 m. Each grid cell was considered homogenous in terms of topography, soil, land use and climate. For this study, only arable land was considered, resulting in 29,380 grid cells for the whole area. The parameterisation of climatic conditions was based on data from the regional climate information system ReKIS (www.rekis.org). For the period 1998 to 2014, monthly data on a 1 km^2 raster were taken from the ReKIS climate database and interpolated according to the spatial (500 m) and temporal (annual) resolution requirements of this study.

Climatic conditions in Saxony are temperate but vary substantially between the lowlands (8 °C to 10 °C; 500 to 800 mm precipitation) and low mountain ranges (6 °C to 8 °C; 900 mm to 1200 mm). The average contents of clay, silt and stones in the topsoil were derived from the soil map series of Saxony (LfULG, 2012). Arable land is dominated by silty soils, especially loamy silt (44%) and sandy silt (25%). Raster cells containing peat soils have not been considered for modelling.

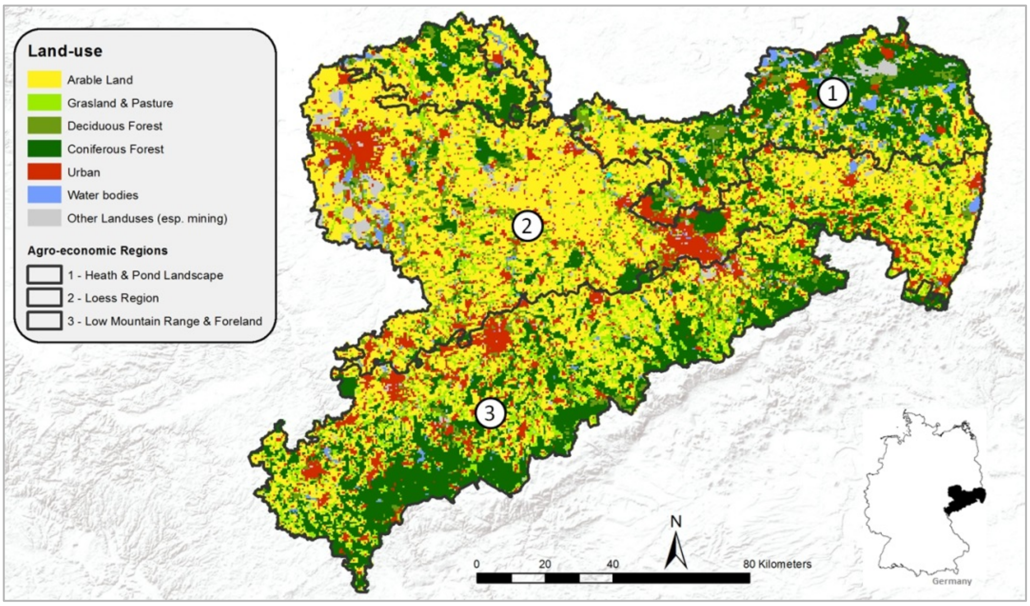

Figure 11: Land-use and agro-economic subregions of the study region Saxony

The study area is subdivided into three ‘agro-economic regions’ according to landscape characteristics and agricultural structure (LfL, 1999): (1) Saxon heath and pond landscape, (2) Saxon loess region, and (3) Saxon low mountain range and foreland (Figure 5). Table 7 summarises the important properties of these three agricultural regions.

Table 7: Land-use and physiogeographic characterisation of the agro-economic regions of Saxony. Average values for the specified periods.

	Heath & Pond Landscape	**Loess Region**	**Low Mountain Range & Foreland**
Arable land [%]	31.9	52.5	28.4
Grassland & pasture [%]	8.1	9.8	16.7
Temperature[1] [°C]	9.6	9.3	7.8
Precipitation[1] [mm]	736	770	961
Clay content[2] [%]	4.4	9.5	13.8
Silt content[2] [%]	22.8	65.3	58.2
Stone content[2] [%]	10.4	7.4	16.2
Conservation tillage 2000/2012 [%]	13.3 / 26.5	14.5 / 34.3	14.9 / 52.1
Catch crops[3] [%]	4.5	4.0	4.6

[1] Period 1990-2014, [2] of agricultural land (topsoil), [3] Period 2000-2012

3.3.2 Agricultural parameters

Each grid cell with arable land-use holds information on crop harvest areas and yields for 20 different crops (Table 8) as well as information on catch crops, tillage systems and fertiliser applications. The land management data were available for five time slices: 2000, 2005, 2010, 2011 and 2012. Data related to crop cultivation and tillage systems were based on regional statistics at the municipality level and InVeKoS data (Integriertes Verwaltungs- und Kontroll-system).

Table 8: Average crop shares and crop yields in Saxony for the period 2000-2012

	Crop Share [%]	**Yield** [t ha^{-1}]
Winter Wheat	24.5	6.9
Winter Barley	13.5	6.5
Winter Rye & Triticale	10.8	5.8
Spring Cereals	8.5	4.8
Winter Rape	15.4	3.8
Maize for Silage	8.7	45.2
Field Grass	2.7	37.2
Clover Grass	2.6	39.1
Other[1]	13.2	

1 fallow, sugar beet, grain maize, vegetables, legumes, sunflowers, potatoes

In the period under review, cereals were the dominant crops (58%) in Saxony followed by winter rape (15%) and maize for silage (9%). The cultivation of catch crops became more important in the investigated period (2000: 3.0%, 2012: 6.6%). Furthermore, the share of conservation tillage increased strongly (2000: 14.4%, 2012: 37.1%). Based on expert knowledge of the state agency LfULG, it was assumed that by-products (esp. straw, beet leaves) of relevant crops were removed from 20% of the arable land.

The quantities of fertilisers applied are based on an analysis of the fertilisation advisory system BEFU (Förster, 2013) for Saxon farmers. It covers the application of organic and mineral nitrogen as well as the N input from atmospheric deposition. For organic fertilisation, slurry and manure were considered in the simulation. Information on other organic fertilisers (e.g., biogas digestate, compost) was not available.

3.3.3 Modelling approach

CCB Model

In this study, the CCB model (Franko et al., 2011) was used to simulate the soil-related carbon and nitrogen dynamics of arable land in Saxony. CCB is based on the model CANDY (Franko et al., 1995) and was developed to answer practice oriented research questions. Due to simplified process modelling, it has fewer requirements regarding data input. It describes the turnover of decomposable carbon in annual time steps for average site conditions depending on crop yields, input rates of fresh organic matter and the initial organic carbon content of the soil. The modelling of turnover is based on first-order kinetics using the Biological Active Time (BAT) as time variable according to the concept in CANDY (Franko & Oelschlägel, 1995). BAT is estimated from site conditions (soil physical parameters of the topsoil, tillage system, annual precipitation and air temperature).

Within CCB, the carbon input to SOM is aggregated to a ‘soil carbon reproduction flux’ (C_{rep}). It includes all carbon from fresh organic matter (FOM), which is transformed to SOC and considers the quality of the different sources of FOM regarding the formation of new SOC. C_{rep} either originates from the non-harvested biomass of the cultivated crops (crop residues and crop by-products) or from organic amendments. The turnover of organic nitrogen in CCB is controlled by the dynamics and the C:N ratios of the FOM and SOM pools. Outputs of CCB include the annual dynamics of SOC concentration, SOC mineralisation and SOC reproduction from FOM as well as soil organic nitrogen dynamics, with particular attention to nitrogen mineralisation from FOM and SOM and immobilisation in SOM. A simplified overview of the pools and fluxes of the CCB model provided in the supplementary material (appendix section 6.2, Figure A1).

Model adjustments for large-scale assessments

Several model adjustments have been necessary to use CCB for large-scale studies such as this. In contrast to previous model applications on plot scale, the simulation objects are not homogeneous in space and time (such as agricultural fields) but represent a gridded integration over several management units. In this new ‘regional mode’, the model is driven by the area average and the proportional coverage of the individual management activities (cropping, tillage etc.) within one spatial modelling unit (e.g. farm, pixel, or municipality). In particular, the ability to use crop share statistics instead of crop rotations can be essential for large-scale modelling approaches. However, the adjustments to run the model with aggregated data also included the handling of crop by-products, application rates of fertilisers and spatial shares of conservation tillage. The adapted procedure of modelling conservation tillage is based on a soil texture-dependent reduction of BAT and has been published by Franko and Spiegel (2016).

Applying CCB to larger scales made it necessary to optimise its data management and computational efficiency. This included the possibility of providing discontinuous management data in the form of time slices (e.g., 2000, 2005, 2010) as well as a framework of parallel computing of one CCB database. All new developments of CCB, which enable the simulation at meso to large scales, have been summarised in a special module ('regional-mode') to enable easy changing between different modelling tasks.

In addition to the technical implementation, it was evaluated whether the modified handling of management data causes systematic errors in the modelled output. Here, it must be considered that the aggregation of management data includes a temporal and a spatial aspect: the temporal aggregation of the crop rotations of one site into crop harvest area relations as well as the spatial aggregation of pools and fluxes of neighbouring sites. The CCB validation database (Franko et al., 2011) was used for this analysis, which covered 391 treatments from long-term field experiments at 40 different locations and 4794 measurements of SOC. The original management data included in this database cover yearly information on cultivated crops and yields, handling of by-products, fertiliser applications and irrigation. To analyse the effects of data aggregation, the management variety of all 391 treatments was spatially aggregated to 40 locations homogeneous in soils and climate conditions. The results of the treatment-specific simulations were compared to the simulations using aggregated management data.

Initialisation of soil carbon levels of Saxony

For the quantitative assessment of SOC dynamics and related nitrogen fluxes, it was necessary to initialise SOC concentrations for the complete study region. In CCB, long-term stabilised SOC (C_{lts}) must be distinguished from decomposable SOC (C_{dec}). Large-scale monitoring data regarding SOC concentration in agricultural soils in Saxony were not available. It was therefore assumed that the fraction of C_{lts} is typical for individual site conditions. To assess C_{lts}, the SOC parameterisation of the STOFFBILANZ model for Saxony was used, which is based on soil type and elevation. The amount of initial C_{dec} was calculated individually for every grid cell. The calculation assumed that the agricultural management and climate of the years 1998-2004 was also applicable for the time period before 1998 and that the initial SOC was in a steady state, which corresponds to this agricultural management and climate. Thus, the initial C_{dec} was determined using the C_{rep} fluxes and BAT values of this time period.

The initialisation of SOC levels was evaluated using data from the long-term SOC monitoring network operated by the state agency LfULG. In total SOC measurement data of 667 permanent monitoring plots throughout Saxony have been considered for this analysis, all located on arable land and have been sampled at least three times. To have a common basis for the evaluation, both (i) the grid-based initialisation of the CCB model and (ii) the SOC measurements of permanent plots were aggregated based on soil type and agro-economic region.

Model application and sensitivity assessment of different drivers

The soil-related carbon and nitrogen dynamics of the arable land in Saxony were simulated for each of the 29,380 grid cells (500 m x 500 m) using the agricultural parameters and initialisation of SOC concentration as stated in the previous sections. The simulation was run in yearly time steps, covering the period 1998–2014. Data on agricultural management were used in time slices: the parameterisation of the management stayed constant during the simulation until the data of a new time step was available.

A scenario approach was used to assess how the most important drivers - climate, crop cultivation and fertilisation, tillage systems – and their development over time individually contributed to the yearly dynamics and overall changes in SOC during the simulation period. Three different model runs were carried out, where each time only one of the three drivers kept the parameterisation of the original (reference) scenario, while the other two drivers got a temporally constant parameterisation for each grid cell based on their average value in the initialisation period (1998-2004) (Table 9).

The results from the individual scenarios allow for a ranking concerning the relative importance of the temporal development of each analysed driver. As a quantitative measure, the correlation coefficient was calculated between the results of the reference scenario (original dynamics of all drivers) and the individual test scenarios where only one driver was kept in its original dynamic. Furthermore, the net change in SOM storage between 1998 and 2014 was quantified.

Table 9: Sensitivity assessment of the contribution of different drivers to system dynamics (Reference = dataset 1998-2014)

		Analysed driver		
		Climate	Crop cultivation & fertilisation	Tillage system
Dataset used	Climate	Reference	Avg. 98-04	Avg. 98-04
	Crop cultivation & fertilisation	Avg. 98-04	Reference	Avg. 98-04
	Tillage system	Avg. 98-04	Avg. 98-04	Reference

3.4 Results

3.4.1 Validation of the CCB module for large-scale simulation

The new ‘regional-mode’ of CCB was successfully validated by comparing 391 treatment-specific simulations (using plot-specific management data) with 40 upscaled simulations (‘regional-mode’) using management data aggregated to the level of experimental location (see supplementary material in the appendix section 6.2, Figure A2). The standard simulation of the 391 experimental treatments resulted in very good statistical quality criteria, using 4794 SOC measurements for validation. The root-mean-square error (RSME) was 1.2 g kg^{-1}, the mean absolute error (MAE) was 0.9 g kg^{-1} and the coefficient of determination (r^2) was 0.94. With a percent bias (PBIAS) of 0.3% and a mean error (ME) of 0.03 g kg^{-1}, systematic errors were negligibly small.

The simulation on the scale of experimental locations (‘regional-mode’) slightly worsened the absolute quality criteria RMSE (1.7 g kg^{-1}), MAE (1.2 g kg^{-1}) and r^2 (0.9) but still gave acceptable results. As a result of input data aggregation, the heterogeneity in the simulated SOC dynamics between the different experimental plots of a location was lost. Nevertheless, PBIAS (0.2%) and ME (0.02 g kg^{-1}) slightly improved, and the general trend in the timeline of carbon storage of a location was adequately represented.

3.4.2 Initialisation of SOC concentration for the arable land of Saxony

The average initial SOC concentration of the arable land of Saxony was 15.09 g kg^{-1}, which is in a reasonable range as reported in other studies (Rank et al., 1999). RMSE of the model initialisation compared to the respective monitoring data of the 667 permanent plots was 3.3 g kg^{-1} when aggregating the data based on soil type and geographic location (Figure 12). The monitoring data showed a high variability in measured values, but correlated satisfactorily with the steady state initialisation (r^2=0.55). There was a tendency to underestimate SOC concentrations in light (sandy) soils while overestimating SOC concentrations in heavier (loamy) soils. Because no management data for the permanent plots were available, the reasons for this pattern could not be analysed. However, the linear regression equation was very close to the ideal 1:1 line, having a slope of 0.93. Because the SOC initialisation was representative of an average management of larger regions, its overall variability was lower than in the individual permanent plots.

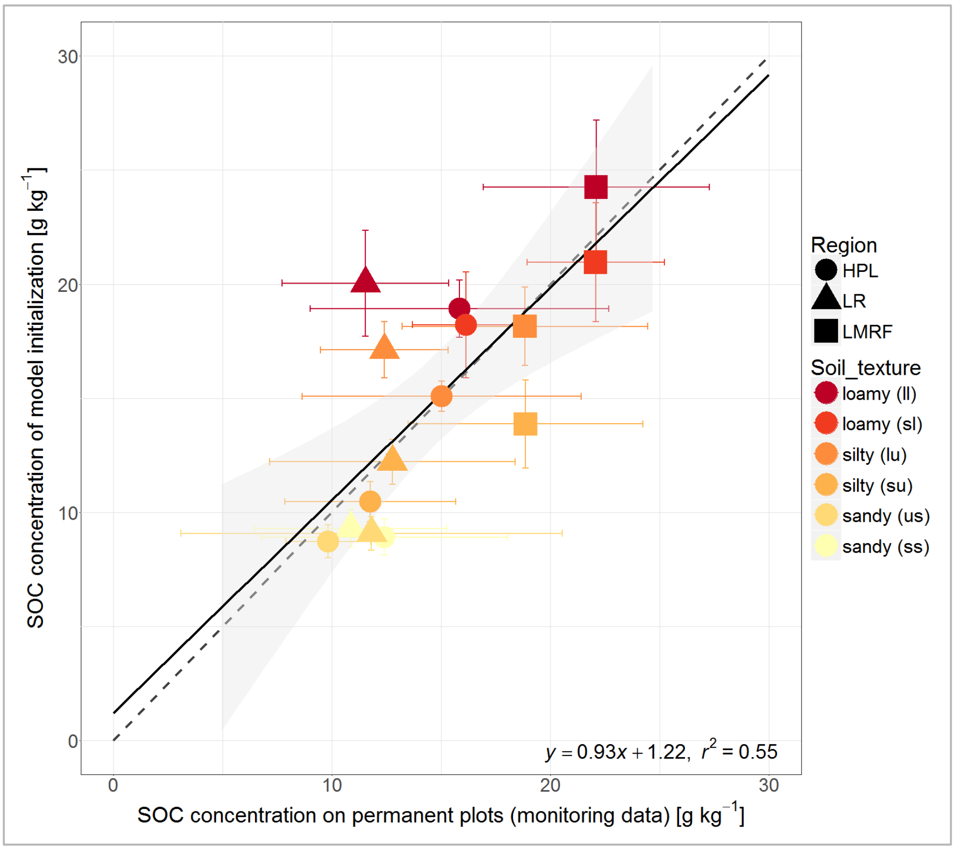

Figure 12: Comparison of the SOC concentration (topsoil, 0 - 30 cm) from the monitoring of permanent plots and the calculated initial values assuming 'steady-state' conditions for the year 1998. The measured data of the permanent plots and the initialised model values of the CCB grid cells were aggregated based on soil type and agro-economic region (HPL = Saxon heath and pond landscape, LR = Saxon loess region, LMRF = Saxon low mountain range and foreland). Soil texture classes (Ad-Hoc-Arbeitsgruppe Boden, 2005): sandy soils (ss = sandy sand, us = silty sand), silty soils (su = sandy silt, lu = loamy silt), loamy soils (sl = sandy loam, ll = loamy loam).

3.4.3 Trends in regional SOC stocks

During the simulation period, the average SOC storage in the topsoil of Saxon arable land increased from 15.1 g kg^{-1} (1998) to 15.4 g kg^{-1} (2014) and so by approximately 2%. The total increase in carbon storage of 0.3 g kg^{-1} in topsoil (30 cm) corresponds to approximately 785.3 x 10^3 t C. Compared to initial SOC levels, the average yearly increase was 1.24‰. In 2.9% of the total simulation area, the gains in SOC were higher than the currently discussed target of 4‰ (Minasny et al., 2017). Nevertheless, the individual trend values exhibit considerable heterogeneity and on 14.9% of the arable land SOC stocks decreased.

When looking at individual regions in Saxony, there have been considerable differences in the average SOC concentration as well as in the trends of carbon storage (Figure 13). In 2014, the arable land of the low mountain ranges had the highest average SOC value (19.7 g kg^{-1}), followed by the loess areas (15.3 g kg^{-1}) and the heath and pond landscape (10.0 g kg^{-1}). With respect to trends of carbon storage, a similar pattern was observed: the low mountain ranges (76.3 kg C ha^{-1} a^{-1}) and the loess areas (69.8 kg C ha^{-1} a^{-1}) stored more than twice as much additional carbon in SOC during the simulation period than the heath and pond landscapes

(23.6 kg C ha^{-1} a^{-1}). Relative to the initial carbon content in 1998, the total gains were 2.1%, 1.8% and 1.3%, respectively.

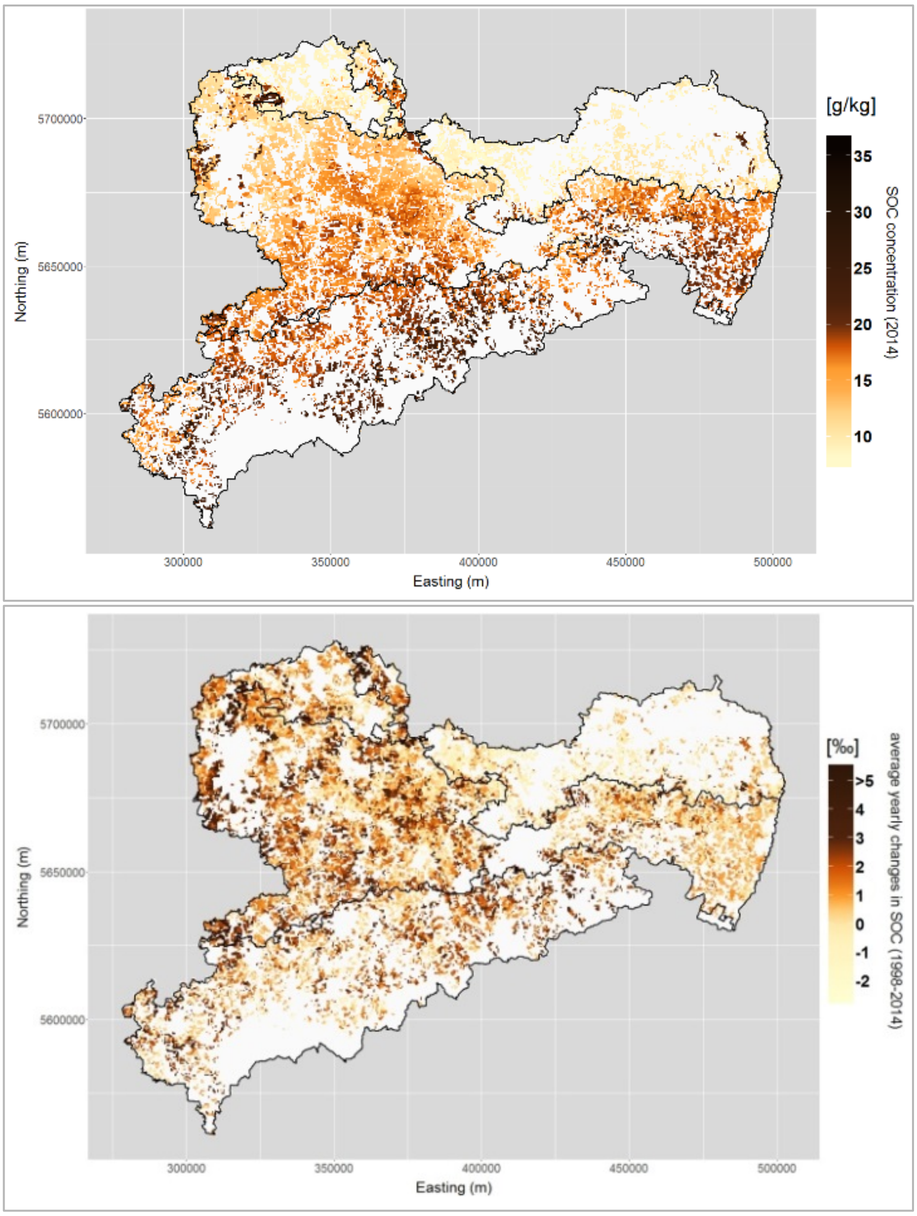

Figure 13: SOC concentration 2014 [g kg-1] (top) and average yearly changes in SOC [‰] for the period 1998–2014 (bottom).

3.4.4 Input and turnover of soil-related carbon

The simulated changes in SOC storage are driven by changes in turnover conditions and carbon input to soil. Within CCB, carbon from FOM that is transformed into SOC is represented by the carbon reproduction flux C_{rep}. Turnover conditions for all carbon pools are aggregated within the model variable BAT. Both model variables changed significantly between the two periods 1998-2004 and 2010-2014. Although showing a high variability between individual sub-regions (Figure 14), the average temporal development of both variables indicated positive effects on SOC storage. For all of Saxony, BAT decreased from 24.4 days (1998-2004) to

22.0 days (2010-2014) and so by approximately 10%. At the same time, the average C_{rep} flux increased from 1220 kg ha^{-1} a^{-1} to 1314 kg ha^{-1} a^{-1} (+8%).

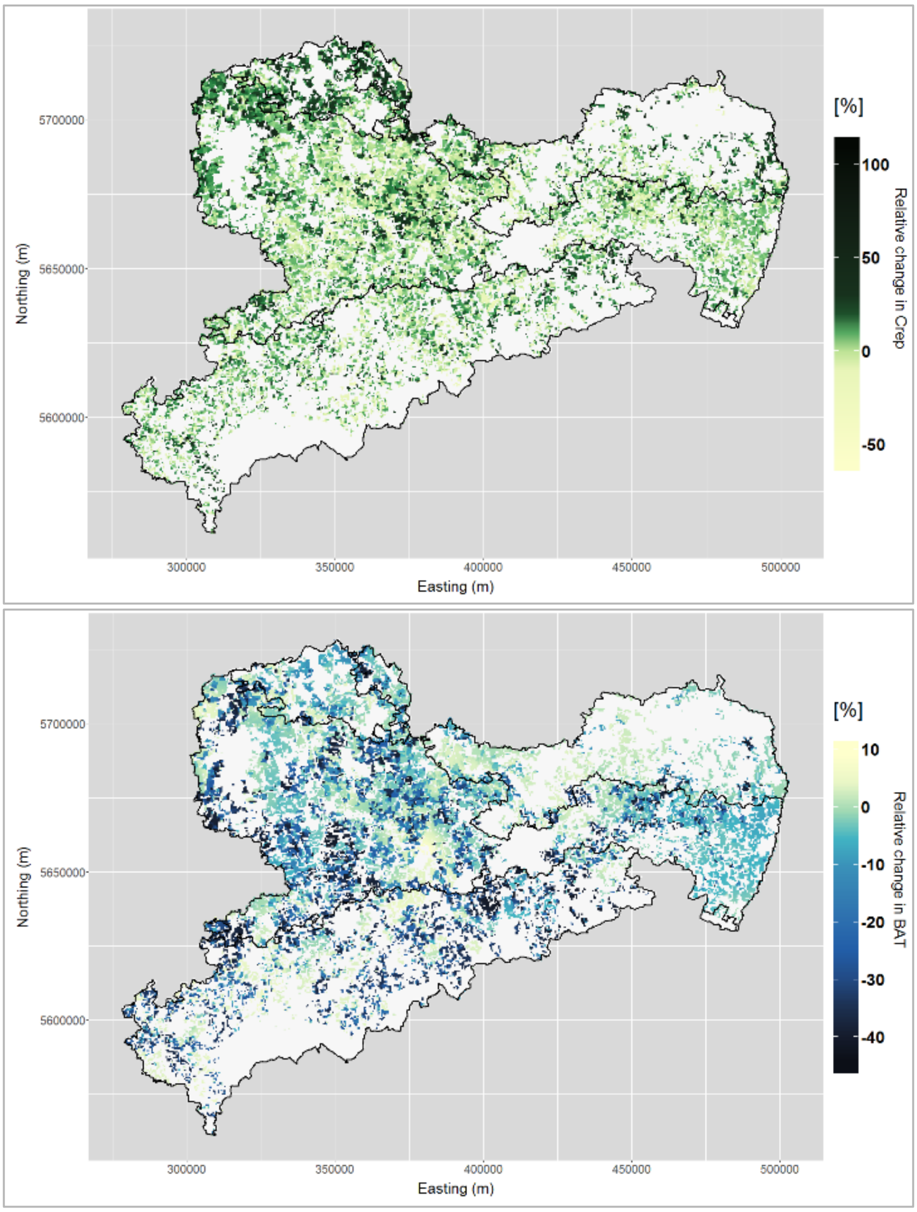

Figure 14: Relative changes in carbon input to SOC (top; expressed as C_{rep}) and SOC turnover conditions (bottom; expressed as BAT) comparing the average values of the two periods 1998-2004 and 2010-2014. Darker colours represent a positive effect on SOC storage.

Climatic variability had considerable impact on the annual turnover of organic carbon but also to some extent on the C_{rep} flux into soil (see supplementary material in the appendix section 6.2, Figure A3) due to, e.g., yield variation. Carbon turnover generally benefited from higher temperatures. The effect of precipitation was more heterogeneous. Light (sandy) soils showed higher turnover rates with increasing precipitation, while for heavier (loamy) soils, too much precipitation had inhibitory effects on the turnover of organic matter. Additionally, changes in tillage systems strongly reduced the average turnover of organic carbon (see also section 3.4.6).

The main sources of FOM changed considerably during the simulation period. In particular, FOM input from winter rape, maize, winter wheat and sugar beet increased, while the contribution of all cereals other than winter wheat declined. These developments were primarily caused by changes in the cultivated area of the individual crops and less by changes in yield. Furthermore, the C_{rep} flux originating from organic amendments increased by 20.2%.

3.4.5 Organic matter-related nitrogen fluxes

The model predicted a total increase of organic nitrogen stored in SOM of approximately 93.2 x 10^3 t N during the simulation period, corresponding to an average gain of 7.5 kg N ha^{-1} a^{-1}. When looking at the average annual N cycle in Saxony, 141.7 kg N ha^{-1} a^{-1} was mobilised from SOM due to SOM mineralisation, while annual reproduction of SOM (humification of FOM to SOM) stored 149.1 kg N ha^{-1} a^{-1} at the same time. The immobilisation of nitrogen due to SOM reproduction increased from 145.5 kg ha^{-1} a^{-1} (1998-2004) to 154.5 kg ha^{-1} a^{-1} (2010-2014). Depending on the C:N ratio of the original carbon source, this N flux into SOM originates in various proportions from the carbon source itself or from the mineral N pool of the soil. On average, 65.2 kg (44%) of this N flux into SOM originated from FOM, while 83.9 kg N ha^{-1} a^{-1} (56%) was immobilised from the N_{min} pool during the turnover of FOM to SOM. Crop residues and by-products from winter wheat, winter rape and winter barley contributed the most to the immobilisation of N_{min} during the turnover of FOM to SOM (Table 10). The total flux of organic nitrogen from FOM to SOM increased from 61.8 kg ha^{-1} a^{-1} (1998-2004) to 69.4 kg ha^{-1} a^{-1} (2010-2014) (+12%).

Table 10: Amount of mineral nitrogen immobilised during the turnover of FOM (crop residues and by-products) to SOM (in addition to the N content of the original carbon source) due to the low carbon to nitrogen ratio of SOM compared to most types of FOM.

	1998 [10^3 t N]	**2014** [10^3 t N]
Winter Wheat	20.1	18.8
Winter Barley	10.9	9.4
Winter Rye & Triticale	8.3	5.8
Winter Rape	6.1	9.8
Spring Cereals	4.4	5.3
Maize for Silage	2.3	3.5
Field Grass	1.7	2.0
Grain Maize	1.3	3.7
Sugar Beet	0.7	1.0
Other crops[1]	3.2	0.6

[1] Fallow, vegetables, legumes, sunflowers, potatoes, clover grass, catch crops, mustard, pea, soy-bean

The annual dynamics of turnover conditions and FOM input (section 3.4.4) had large effects on the annual balance of organic nitrogen and related nitrogen fluxes (Figure 15). These dynamics are an important factor for nitrogen leaching and crop fertilisation. A high turnover of SOM in 2003 led to a strong mobilisation of nitrogen, especially in the loess region. On the other hand, large amounts of nitrogen have been stored in SOM in the years 2005, 2010 and 2013. Due to differences in cultivated crops, the agro-economic regions of Saxony differed substantially in regard to their regional nitrogen balance. The net immobilisation was 2.6 kg N ha^{-1} a^{-1} for the heath and pond landscapes, 8.3 kg N ha^{-1} a^{-1} for the loess region and 9.1 kg N ha^{-1} a^{-1} for the low mountain ranges.

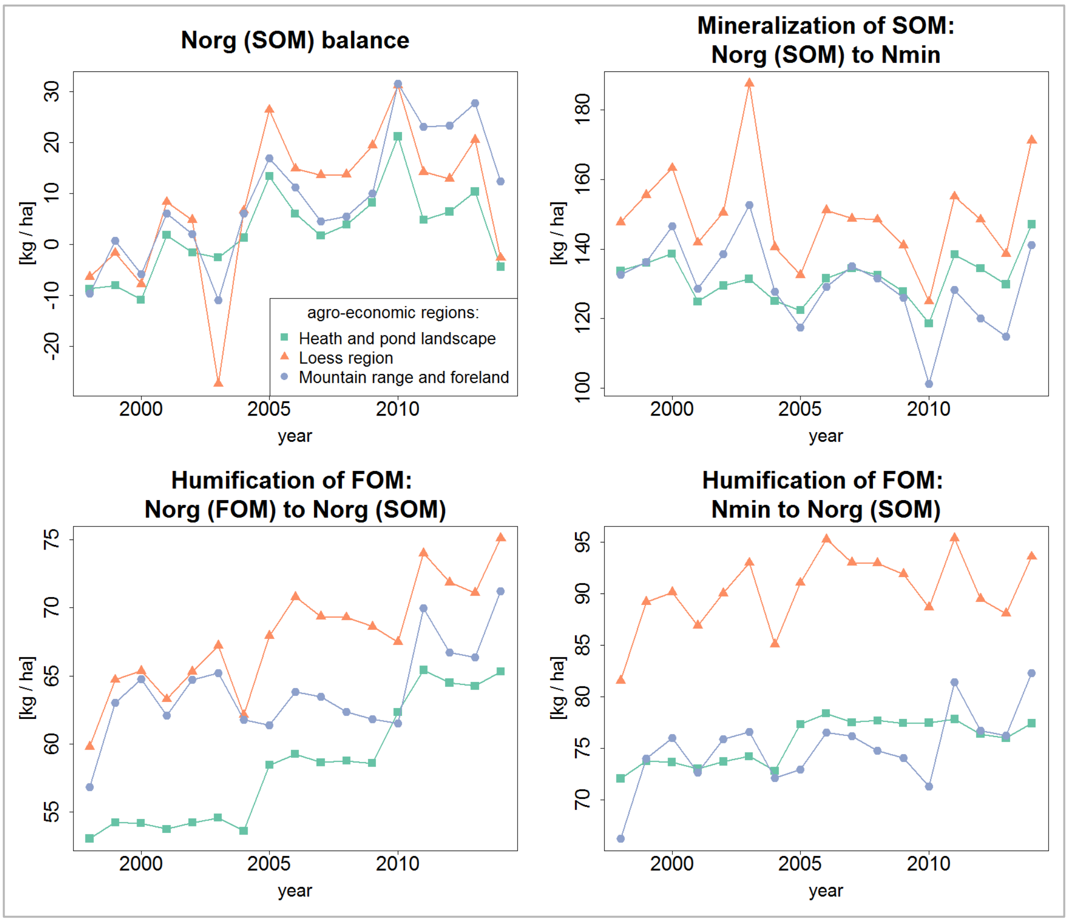

Figure 15: Annual dynamics in the balance of organic nitrogen stored in SOM as well as in the nitrogen fluxes into (humification) and out of the SOM pool (mineralisation).

3.4.6 Contribution of different drivers to changes in SOM

The three main drivers (climate, crop cultivation and fertilisation, tillage system) and their changes during the simulation period all had a positive effect on the SOC storage (Figure 16). However, the simulated scenarios demonstrated an unequal contribution of the individual drivers to the net increases in SOC concentration. Compared to the initial SOC concentration, the driver scenarios led to net increases of 0.02 g kg^{-1} (climate), 0.16 g kg^{-1} (crop cultivation and fertilisation) and 0.25 g kg^{-1} (tillage system) for the simulation period 1998-2014. The combination of all drivers (reference simulation) increased SOC storage by 0.3 g kg^{-1}, which is only 78% of the sum of individual effects. The outcomes of the driver analysis, especially the effects of conservation tillage, differed considerably between the individual agro-economic regions. Within the Saxon heath and pond landscape, the trends in conservation tillage and climate led to decreasing SOC levels.

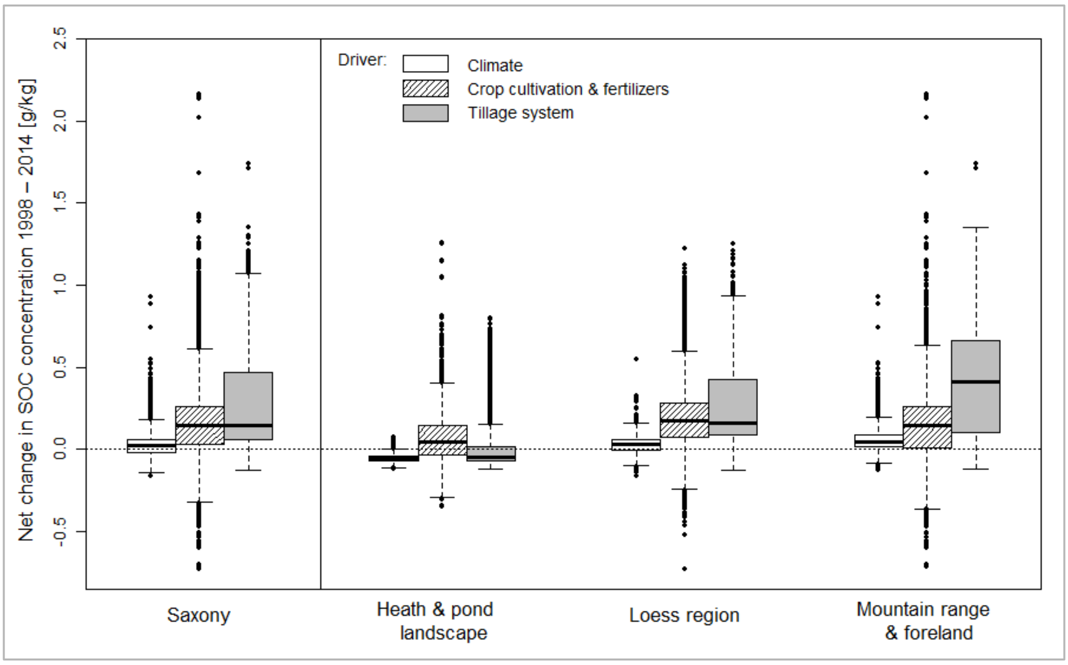

Figure 16: Analysing the effects of the three main drivers on the net changes in SOC concentration within the simulation period (1998–2014). The changes in SOC concentration between 1998 and 2014 were calculated for every grid cell.

The sensitivity of the drivers was different when considering the Pearson’s correlations between reference simulation and individual driver scenarios and thus considering more the annual dynamics in SOM storage. The SOC dynamics of the ‘crop cultivation and fertilisation’ scenario were more similar to those of the reference simulation ($r^2 = 0.78$) than those of the model runs focusing on tillage system ($r^2 = 0.70$) or climate ($r^2 = 0.58$). The annual dynamics in the balance of organic nitrogen stored in SOM revealed a different picture. Here, the dynamics have been considerably stronger than the net changes over the whole simulation period. Climate was identified as a main driver in Saxony ($r^2 = 0.65$), followed by crop production and fertilisation ($r^2 = 0.62$) and tillage system ($r^2 = 0.52$). Nevertheless, for every agro-economic region, there was a different key driver behind the annual dynamics in the balance of organic nitrogen (see supplementary material in the appendix section 6.2, Figure A4).

3.5 Discussion

3.5.1 Large-scale simulation of SOM dynamics using CCB

While selected CCB-based indicators have already been used for large-scale analysis of carbon input and turnover conditions in soil (Franko et al., 2015; Witing et al., 2018), this is the first application of CCB for the large-scale simulation of SOM turnover and storage. The CCB model was extended by a 'regional mode', which has the benefit of using aggregated data on agricultural management that are typically available at lager scales. The application of this methodology was successfully demonstrated for Saxony by quantifying changes in SOC concentration and organic matter-related nitrogen storage on a 500 m grid (29,380 cells).

Although the specific model adaptations have been successfully validated, it must be noted that a simulation using regionally aggregated data can only represent the average area-wide balance of that region and averages the management diversity of individual sites within it. With respect to the dataset used for validation, it must be considered that the analysed experimental sites of one location often have extreme types of fertilisation. It can be expected that the different management strategies aggregated within census data are more homogenous.

A proper initialisation of SOC pools is a challenging task in SOC modelling (Dimassi et al., 2018; Foereid et al., 2012), especially when the simulated spatial units represent a set of diversely managed agricultural fields. This problem was approached by assuming steady state conditions in SOC storage for the starting period of the simulation. While the validation of this approach was satisfactory, further improvements could be achieved by including the management data of the permanent plots used for validation within the generation of the initial values. Unfortunately, these data were not available for this study. Nevertheless, the approach of steady state initialisation has the benefit of highlighting the effects of external drivers on SOM levels during the simulation period.

3.5.2 Dynamics of SOC and related organic nitrogen stocks in Saxony

For the vast majority of the arable land of Saxony, an increase in SOC concentration during the study period was observed. Although the currently discussed target of 4‰ (Minasny et al., 2017) is only achieved in selected locations (2.9%), the observed average yearly increase of 1.2‰ is considerable. The results are in accordance with other studies that observed that SOC stocks in central European regions started to rise from the beginning of the 21st century (Kaczynski et al., 2017). Both the overall decrease in turnover conditions and the overall increase in carbon input to soil led to this positive development in SOC storage.

Considering the 4‰ target and the observed trends in Saxony it is important to emphasise their dependency on the continuous presence of casual drivers. If the driver behind positive trends in SOM storage is lost, the stored amounts of C and N will be released again. This is especially critical if gains in SOM storage are based on changes in agricultural management that are not repeatable. The results indicated that a large part of the increase in SOC storage is due to the increased use of conservation tillage. Despite this, the prevalence of conservation tillage in Saxony might be variable and dependent on the existence of subsidy programs (SMUL, 2008, 2014, 2017). Upcoming subsidy programs should consider not only future carbon storage potentials but also the maintenance of current carbon stocks.

With respect to organic matter-related nitrogen, variations between individual years have been more dominant than the overall trends in storage. Nevertheless, a significant amount of N has been immobilised in SOM. The model results contribute to an integral and spatially distributed understanding of the N and C cycles of arable land. Processes of enrichment and depletion of N in humus significantly influence the preservation of soil fertility but also affect nitrate leaching.

3.5.3 Effects of drivers, changes in carbon input and turnover conditions

The use of conservation tillage has been shown to be the most important contributor to the overall gains in topsoil SOC concentration. A considerable decrease in overall turnover conditions of organic matter in Saxony was observed, which is largely related to the increase in conservation tillage and the original reason for gains in SOC storage at constant carbon input to soil. The positive effect of conservation tillage on soil carbon storage is widely studied (Alvarez, 2005; Lal & Kimble, 1997; Luo et al., 2010), although there is discussion about the soil depth that has to be considered (Baker et al., 2007).

The indicator C_{rep} aggregates the effect of different carbon sources on SOC storage by considering the quality of the different sources of FOM for the formation of SOC (Franko et al., 2011; Kolbe, 2010). The study revealed considerable gains in C_{rep} fluxes during the simulation period, which were mainly caused by changes in the composition of cultivated crops and in the application of organic amendments and less by changes in the actual yield of individual crops. An important driver for this is the inclusion of biogas production in the agricultural systems of Saxony (Witing et al., 2018).

The effects of climate on the net balance of SOM in the whole simulation period have been minor but became important for its annual dynamics, especially with respect to organic matter-related nitrogen. To give scientifically substantiated recommendations on how to further improve agricultural management in Saxony with respect to SOM storage, it would be important to include long-term climate scenarios in future studies as they effect turnover conditions but also crop yields and therefore the carbon inputs to soil (Davidson & Janssens, 2006; Robertson et al., 2017; Sanderman, Creamer, et al., 2017).

3.5.4 Conclusion

With the quantification of selected parameters of the soil-related carbon and nitrogen balance on large scales, the CCB model system takes an important step towards an integrated, spatially distributed view on the carbon and nitrogen cycle of arable land. The application of this methodology was successfully demonstrated for Saxony, where we could consider a diverse set of input data thus overcoming a typical limitation for the large-scale simulation of SOM dynamics. Spatial data on soils and climate have been combined with statistical information on agricultural management on various levels. The presented approach has the benefit of reflecting real changes in agriculture and climate. However, due to the resolution of some statistical data sources, the results should not be used for the detailed analysis of individual spots (grid cells).

With respect to the study region of Saxony, considerable amounts of C and N have been stored in SOM of arable soils during the period 1998-2014. However, there have also been significant regional differences, including decreasing SOC levels in 14.9% of the area. The low mountain ranges and the loess areas stored more than twice as much additional carbon in SOC than the heath and pond landscapes. While the increased use of conservation tillage was the most important driver for the overall increase in SOM storage, climate variability had strong effects on its annual dynamics. Nevertheless, changes in the composition of cultivated crops and in the application rate of organic amendments also had considerable impacts. It is important to emphasise that if the driver behind the positive trend in SOM storage is lost the stored amounts of C and N will be released again. Future subsidy programs should consider not only future carbon storage potentials but also the maintenance of current SOM stores. Otherwise, SOM stores could pose a risk for climate change mitigation and cause nitrate leaching.

4. Modelling soil organic carbon dynamics of arable land across scales: A simplified assessment of alternative management practices on the level of administrative units*

4.1 Chapter summary (abstract)

Regional assessments of soil organic carbon (SOC) trends and the carbon sequestration potential of alternative management practices (AMP) are highly relevant for developing climate change mitigation strategies for the agricultural sector. Such studies could benefit from simplified SOC modelling approaches on the scale of administrative units as this often corresponds to the level of policy-making and data availability. However, there is a risk of systematic errors in such scaling operations. To overcome this problem, we performed a scaling experiment where we simulated the SOC dynamics of the arable soils of the State of Saxony (Germany) across a series of scales using the CANDY Carbon Balance (CCB) model. Specifically, we developed model set-ups on four different administrative levels (NUTS1, NUTS2, NUTS3, and LAU) and evaluated the simulation results of the upscaled models against a 500 m grid-based reference model. Furthermore, we quantified the carbon sequestration potential of selected AMP scenarios (addressing field grass, cover crops, and conservation tillage) across all scales. The upscaled model set-ups adequately simulated the SOC trends of Saxon arable land compared to the grid-based reference simulation (scaling error: 0.8–3.8%), while providing significant benefits for model application, data availability and runtime. The carbon sequestration potential of the AMP scenarios (1.33 Mt C until 2050) was slightly overestimated (+0.07–0.09 Mt C) by the upscaled model set-ups. Regardless of the scale of model set-up, we showed that the use of aggregated statistical input data could lead to a systematic underestimation of SOC trends. LAU and NUTS3 levels were shown to be a suitable compromise for effectively quantifying SOC dynamics and allowed for an acceptable spatial prioritisation of AMPs. Such simplified, scale-adapted assessments are valuable for cross-regional comparisons and for communication to and among decision-makers, and might provide a quantitative basis for discussions on the effectiveness of AMPs in various stakeholder processes.

4.2 Introduction

Soil organic carbon (SOC) is an important contributor to global carbon cycles, and increasing the carbon storage in soils could contribute to climate change mitigation (Lefèvre et al., 2017).

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The importance of this positive impact is underlined by the '4 per 1000' initiative that has been launched at the COP 21 (Lal, 2016; Minasny et al., 2017). This initiative aims to demonstrate that agricultural soils can play a crucial role in food security and climate change, which stimulates current discussions about the feasibility of CO_2 certificates for carbon sequestration in soils (Amundson & Biardeau, 2018; Wiesmeier, Mayer, Paul, et al., 2020). Political, socio-economic and environmental drivers affect the carbon storage of agricultural soils by changing carbon turnover conditions (e.g. climate change, choice of tillage system) or the amount of carbon influx to soil (e.g. cultivated crops, organic amendments from livestock or biogas plants) (Franko & Witing, 2020). The scale of origin and impact of these drivers can be very different. Developing scale adequate strategies for managing and fostering SOC storage thus requires assessing the impact of different drivers and measures across various scales as well. This is also important for reaching a targeted communication, as a scale adapted view would ease discussion between different groups of stakeholders (Primmer & Furman, 2012).

Consistent approaches are thus needed that could be used for assessing the effects of specific drivers and measures on SOC over different scales and thus be able to locally adapt and prioritise specific targets or measures. Ideally such an approach should be easily applicable and allow for quantitative assessments, at least on most of the scales that are relevant for policy and environmental management. Hierarchical administrative units could be an important basis for scaling levels (Zen et al., 2019). Although administrative units typically do not have a relation to environmental processes like carbon sequestration, they are essential in terms of external drivers and data (Raudsepp-Hearne & Peterson, 2016). They have own sets of policies, are relevant in a variety of planning processes and are often used for cross-regional comparison and communication. Furthermore, most of the relevant statistical datasets are maintained and provided on the level of administrative units.

A prominent example for such administrative units are the European 'Nomenclature of Territorial Units for Statistics' (NUTS) and 'Local Administrative Units' (LAU). The current classification of Europe lists four levels of administrative units: NUTS1 (92 regions), NUTS2 (244 regions), NUTS3 (1,215 regions) and LAU (99,387 regions) (European Commission, 2016). Several studies that developed spatially distributed estimations of SOC stocks on regional to large scales at least partly made use of input datasets that were aggregated on those administrative levels (Aguilera et al., 2018; Borrelli et al., 2016; Kaczynski et al., 2017; Lugato et al., 2014). Lugato et al. (2014), for example, estimated the SOC stocks of agricultural soils across Europe using NUTS3 and NUTS2 level statistics on agricultural land-use and management in the agro-ecosystem SOC model CENTURY. Kaczynski et al. (2017) modelled the regional SOC trends of a 1,800 km^2 case study area using the Rothamsted C model (RothC) and LAU level information on agricultural management. Farina et al. (2017) used statistical datasets (e.g. on crop yields) for a spatially distributed modelling of SOC stock changes and CO_2 emissions in Southern Italy using the RothC10N model and RothCIS tool. Also outside of Europe the use of statistical input data on administrative levels is often without an alternative for SOC modelling. Begum et al. (2018), for example, estimated regional carbon sequestration potentials of rice cropland on the level of 64 districts of Bangladesh using the model DayCent because most of the information available were at the district level.

For many of the existing large-scale simulations of SOC stocks and trends, the scalability of the quantitative approaches is sparsely tested. Due to a lack of data, different datasets with varying spatial resolution are often combined in a high-resolution model set-up. This raises two important questions: (1) does the use of aggregated input data (such as agricultural parameters on NUTS level) lead to systematic errors in the modelled SOC dynamic? (2) is it reasonable (for certain research questions) to model SOC dynamics directly on the level of administrative units and thus make use of the various benefits such an upscaled approach is promising to provide? To the best of our knowledge, this paper is the first study that explicitly addresses those questions and presents a scaling experiment for the assessment of alternative management practices on arable land, which could provide important impulses for regional SOC management.

We simulated the current stocks and trends in SOC for the arable soils of the State of Saxony (NUTS 1 region in Eastern Germany) using five different model set-ups. In the first four set-ups the spatial resolution of the models and all input data were scaled to the four administrative levels of Europe (LAU, NUTS3, NUTS2, NUTS1). The fifth set-up was a 500 m grid-based reference model of the arable land of Saxony (Witing et al., 2019) that was used to evaluate the simulation quality of the upscaled model set-ups. Furthermore, we selected two alternative management practices (AMP) for our scaling experiment that are in line with Saxony's policy efforts and assessed their effects on all of the mentioned scales. Specifically, the AMPs addressed policies that aim to increase the share of grass mixtures in the fodder system, and prevent soil erosion by increasing the use of winter cover crops and conservation tillage (Sächsisches Staatsministerium für Energie, Klimaschutz, Umwelt und Landwirtschaft, 2015). On all of the five scales considered in this study the same model approach as well as type and source of input data has been used, but all set-ups had their own spatial resolution of input data. We expect that such simplified and scale adapted assessments of different drivers, measures and pathways could be valuable for political, economic and environmental considerations as well as eases applicability and communication.

4.3 Materials and Methods

4.3.1 Study area

The Federal State of Saxony is a NUTS1 region in Eastern Germany (Figure 17), which is dominated by agricultural land-use (52%). The arable areas (7,330 km^2) are managed rather intensively due to the fertile soils (esp. loamy silt and sandy silt) and accordingly high yield potential. However, three 'agro-economic regions' can be distinguished, which are characterised by quite different agricultural activities, landscape characteristics and soils (LfL, 1999): (1) the heath landscape in the north/north-east, (2) the loess region in the centre, and (3) the low mountain range in the south/south-west of Saxony. A detailed characterisation of these regions is given in in the supplementary materials (appendix section 6.1, Table A1). The climate is temperate, but the lowlands (8-10 °C; 500-800 mm) are considerably drier and milder than the low mountain range (6-8 °C; 900-1200 mm). The most important crops cultivated in Saxony are different types of cereals (esp. winter wheat, winter barley, winter rye, triticale) as well as winter oilseed rape and silage maize.

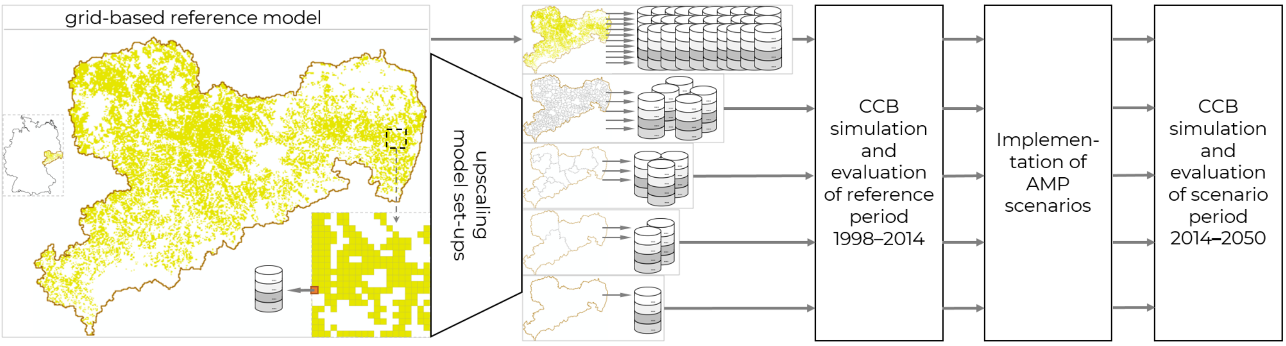


Figure 17: Workflow for assessing the SOC dynamics of arable land of Saxony and the carbon sequestration potential of alternative management practices (AMP) across a series of scales. Upscaled model set-ups on four different administrative levels of Europe (NUTS1, NUTS2, NUTS3, and LAU) were evaluated against the simulation results of a 500 m grid-based reference model.

4.3.2 Modelling Approach

CCB model

The CCB model (CANDY Carbon Balance; (Franko et al., 2011)) is a simplified version of the CANDY model (Carbon And Nitrogen-DYnamics; (Franko, 1996; Franko et al., 1995)) and requires less input data because it was developed for practice oriented research questions. It has been validated over various site conditions and cropping systems in Europe and applied in several case studies, especially in Germany and Austria (Diel & Franko, 2020; Farina et al., 2021; Franko et al., 2011, 2022; Franko & Merbach, 2017; Franko & Ruehlmann, 2018; Franko & Schulz, 2021; Franko & Spiegel, 2016; Gasser et al., 2022, 2023; Spiegel et al., 2018; Witing et al., 2019). CCB was selected for this study as it is capable to simulate in a specific regional mode (Witing et al., 2019), where the model can be driven by proportional coverages and area averages of different management activities (cropping, tillage, fertilisation, etc.) in any kind of spatial modelling unit (e.g. field, farm, pixel, municipality). The ability to use common input data like crop share statistics is essential for being able to model directly on the level of administrative units.

CCB simulates carbon dynamics in annual time steps considering three different pools of soil organic matter (SOM) (active, stabilised, long-term stabilised) as well as a set of pools for fresh organic matter (FOM). FOM pools are differentiated by the origin of the organic substances, specifically organic amendments (e.g. slurry), crop by-products (e.g. straw) and crop residues (e.g. roots). The simulation of carbon turnover is controlled by land management and site conditions. To quantify turnover conditions CCB uses the 'Biological Active Time (BAT)' approach (Franko & Oelschlägel, 1995), which provides an absolute measure that considers soil physical parameters, climate (precipitation, temperature) and information on tillage systems. In CCB the decomposition of FOM results in a 'soil carbon reproduction flux' (C_{rep}), which recreates SOM. The calculation of C_{rep} considers the properties of the FOM and allows to calculate an integrated value across all different FOM sources. A detailed description of CCB's pools and fluxes is given by Franko et al. (2011) and in supplementary materials (appendix section 6.2, Figure A1).

The indicators BAT and C_{rep} can be used to describe and compare the state and development of SOC across different sites or regions (Franko & Ruehlmann, 2022). Their usage in CCB allows for and simplifies the scalability of model-setups. The spatially upscaled model set-ups in our study should have a similar amount of C_{rep} and BAT as the reference model.

Reference model set-up

Basis for our scaling experiment was a grid-based CCB model set-up for the arable soils of Saxony that uses the best information available to local public authorities of agriculture and water sectors, including inter alia field discrete cultivation data (Witing et al., 2019). The grid-based reference model was developed by Witing et al. (2019) and introduced a 'regional-mode' of the CCB model, which allows to handle various spatially and temporally aggregated input datasets related to agricultural management and climate. The results of this reference model are used to evaluate the performance of a second set of CCB models that have been set-up with aggregated input data (as described below). The reference model was set-up on a 500 m grid and included 29,319 modelling units (Figure 17), where each unit had a specific parameterisation of soil, climate and agricultural management. Soil properties were derived from the soil map series of Saxony (LfULG, 2012), climate data originates from the regional climate information system ReKIS (www.rekis.org) and cultivation data (crops, yields, tillage systems, fertiliser, etc.) were based on field scale IACS data (Integrated Administration and Control System) and regional statistics at the municipality level. Data on agricultural management was available for five time periods (2000, 2005, 2010, 2011 and 2012) and stayed constant between two periods. The simulation period covered 17 years between 1998 and 2014. More details on the set-up of the reference model are given by Witing et al. (2019). The initialisation of SOC-levels was updated according to the approach of Drexler et al. (2020), which provides typical organic matter contents for the agricultural soils of Germany based on land-use, soil texture, C:N ratio and annual precipitation (more details are provided in the supplementary materials: appendix section 6.3, Explanation A1).

4.3.3 Upscaling of model set-ups, agricultural parameters, climate and soils

The case study region Saxony is a NUTS1 unit and its further administrative division includes 3 NUTS2 units, 13 NUTS3 units and 414 LAU units (European Commission, 2016). A large set of environmental and agricultural statistics relevant for SOC modelling is available especially on the level of NUTS regions, either provided by Eurostat (Eurostat, 2023b, 2023a) or in the statistical reports of the individual administrative units (for Saxony e.g. Statistisches Landesamt Sachsen (2023)). However, within our study we did not directly use those statistics, but aggregated the more detailed input data of our grid-based reference model to the level of administrative units. We thus mimicked the procedure of creating agricultural census data, which typically aggregates the information of smaller reporting units. In doing so, we excluded potential quality issues of different publicly available datasets and focused our analysis on the effects that may arise when upscaling model set-ups.

Spatial reference for the data aggregation procedure were the NUTS and LAU boundaries of the year 2016 (Eurostat, 2023c) (©EuroGeographics for the administrative boundaries). Based on a spatial overlay, each of the 29,319 grid-based modelling units of the reference model has been assigned to a specific administrative unit. This has been done for all four administrative levels. Subsequently, for each input dataset of the reference model an aggregation operation was conducted. Agricultural parameters were aggregated using the area-weighted mean of the grid-based datasets within one administrative unit, specifically considering: harvest areas and yields of 20 crop types, cultivation of cover crops, management of crop by-products, tillage systems, and fertiliser applications. As the 'regional mode' of CCB is capable of processing area shares of crops and management operations (Witing et al., 2019), the results of the input data aggregation could be directly used in the upscaled model set-ups. With respect to climate data the area-weighted mean was calculated from the 500m grid for annual mean temperature and annual precipitation. In contrast to agricultural management and climate, soil texture is rather constant and is barely changed by management and other external drivers besides erosion. Furthermore, soil texture and related soil physical properties are important drivers of SOC storage (Wiesmeier et al., 2019). Thus, we kept all of the existing soil types and did only aggregate the shares of different soil types within one administrative unit. In the CCB model set-ups, each soil type of an administrative unit was thus considered as an own modelling unit, but can be seen as a property of that administrative unit without spatial reference. Accordingly, all soil types within one administrative region got the same input-data on agricultural management and climate. For the initialisation of SOC-levels the same approach that is used in the reference model was applied (Drexler et al., 2020). Table A2 (supplementary materials: appendix section 6.1) provides a descriptive summary of the aggregation procedure for all relevant datasets.

4.3.4 Alternative management practices

We simulated two alternative management practices (AMP) on all five scales considered in this study (500m-grid, LAU, NUTS3, NUTS2, NUTS1). Both AMP are in line with current policy efforts in Saxony, which aim at increasing the share of grass mixtures in the fodder system, and prevent soil erosion by increasing the use of cover crops and conservation tillage (Sächsisches Staatsministerium für Energie, Klimaschutz, Umwelt und Landwirtschaft, 2015, 2022). The alternative management practices have been selected to analyse the sensitivity and suitability of the upscaled model set-ups regarding two different types of processes – input und turnover of soil related carbon. The scenario assumptions of both AMPs are summarised in Table 11.

To address changes in carbon input we considered an increase of field grass cultivation, based on a reduction of silage maize and winter fodder barley as well as an increased use of winter cover crops on areas that are cultivated by summer crops (silage maize, sugar beet, summer barley). In order to enable comparability of the AMP-1 scenario across all model set-ups, we applied relative changes to the mix of cultivated crops of each modelling unit of each model set-up. Specifically, the areas cultivated with silage maize and winter fodder barley have been reduced by 35% within each modelling unit (e.g. 100 ha to 65 ha), which led to absolute changes on the level of Saxony show in Table 11. Accordingly, the absolute share of field grass cultivation increased by 8.3% in the first AMP scenario. Furthermore, the absolute share of areas under cover crop cultivation in Saxony was increased by 10%, which ensured winter soil coverage of nearly all areas under summer crop cultivation within the AMP-1 scenario.

As a second alternative management practice (AMP-2) an increase in conservation tillage has been parameterised, which changes the turnover conditions of fresh and soil organic matter. Specifically, 30% of the areas with conventional soil management were converted into minimum tillage within each modelling unit, which led to a total increase in conservation tillage of 18.9% for Saxony (Table 11). The simplified scenario assumptions are meant to represent a 'moderate' degree of AMP implementation with the main objective of testing the scaling experiment of this study.

Table 11: Parameterisation of the alternative management practice (AMP) scenarios summarised on the level of Saxony (NUTS1).

	crop shares & soil management	2014	2015-2050
AMP-1	silage maize	11.4%	7.4% (-4%)*
	winter barley	12.2%	7.9% (-4.3%)*
	field grass	3.1%	11.4% (+8.3%)
	winter cover crops	6.6%	16.6% (+10%)
AMP-2	conservation tillage	37.1%	56.0% (+18.9%)**

*cultivated areas have been reduced by 35% (compared to the status of 2014) and transferred to field grass; **30% of the areas with conventional soil management were converted into conservation tillage

For implementing the AMP scenarios into the models, we adapted the management parameterisation of the year 2014 within all five model set-ups and simulated this setting for 37 years (2014-2050). The final year of the scenario runs has been set to 2050 as this is the target year for reaching net-zero emissions as adopted by the IPCC (Intergovernmental Panel on Climate Change, 2018) and the European Green Deal (The European Green Deal COM/2019/640 Final, 2019). To have a clear baseline the original 2014 parameterisation has been applied to this simulation period as well. This 'business-as-usual' (BAU) scenario served as a basis for comparing the effects of the two alternative management practices. All other parameterisations including climate have been kept and repeated during the scenario runs.

4.3.5 Model application, post-processing and evaluation

In total 15 different models have been set-up, considering the aforementioned five scales (500m-grid, LAU, NUTS3, NUTS2, NUTS1) as well as three scenarios (BAU, AMP-1, AMP-2) for each scale. All model set-ups have been pre- and post-processed using the R Statistical Software (R Core Team, 2022) and the simulations were carried out using the CCB version 20.16.2.26. The results of the grid-based reference models were aggregated to the level of administrative units and compared to the results of the upscaled model-setups. Due to the concept and structure of CCB, all soil types of an administrative unit were modelled individually in the upscaled model-setups and the related carbon stocks have been aggregated in the post processing. Both AMP scenarios have been related to the BAU scenario to extract the AMP driven effects from the overall trends in SOC of the period 2014-2050. All analyses were done for the case study of Saxony as a whole as well as for all spatial units of the upscaled model set-ups. To identify the drivers behind potential scaling errors, a series of correlation analysis was conducted considering CCB internal indicators (C_{rep}, BAT), soil properties as well as different datasets that have been aggregated within the upscaling process (e.g. climate parameters, tillage systems). Specifically, spatial dispersion parameters (regional standard deviation) of the mentioned predictors have been used. The analysis of the CCB databases as well the visualisation of the results were done in R using the packages ggplot2 (Wickham, 2016), ggthemes (Arnold, 2021), PerformanceAnalytics (Peterson & Carl, 2020), PupillometryR (Forbes, 2020), raster (Hijmans, 2022), reshape2 (Wickham, 2007), RODBC (Ripley & Lapsley, 2021), scales (Wickham & Seidel, 2020) and viridis (Garnier et al., 2021).

4.4 Results

4.4.1 Comparing model complexities and overall trends in SOC dynamics

The case region of Saxony (NUTS1 region) represents the main spatial reference unit of this study. Table 12 provides an overview of the five model set-ups for Saxony and the SOC dynamics simulated with different input data sets for the reference period (1998-2014). The differences in model complexity have been substantial between the five set-ups as demonstrated by the number of modelling units that ranged between 49 and 29,319. Only for the grid-based approach the number of modelling units equals the number of spatial units, as in this set-up a spatially explicit soil type, agricultural management and climate data set was assigned to each grid cell. The upscaled set-ups considered the distribution of soil types in each spatial unit (without their exact location; see section 4.3.3) and an averaged climate and agricultural management condition. Obviously, the number of soil types per administrative region increases with larger administrative levels. While each LAU included on average 4.8 different soil types, it was already 18.1 for each NUTS3 unit and up to 49 for the NUTS1 level of Saxony. The difference in model complexity can also be described in database sizes and computation time of the respective model set-ups, which ranged between 7-467 megabyte and a few seconds up to several hours respectively on a standard personal computer. The initialisation of soil carbon levels was similar for all levels of aggregation and only minor deviations to the grid-based model set-up have been observed (Table 12).

Table 12: Overview of model complexities and general trends in SOC dynamics of the Saxon arable land (NUTS1 region) simulated for the reference period (1998-2014). A grid-based reference set-up is compared with four upscaled model set-ups simulating SOC dynamics at the level of administrative units.

Simulation level	**Number of spatial units**	**Number of modelling units**	**SOC initialisation [Mt]**	**Soil carbon sequestration within the simulation period 1998-2014**		
				[Mt C]	[kg C ha^{-1} y^{-1}]	[‰ y^{-1}]*
GRID	29,319	29,319	41.40	2.65	212.56	3.76
LAU	414	1,980	41.40	2.63	210.92	3.73
NUTS3	13	253	41.40	2.56	205.81	3.64
NUTS2	3	100	41.41	2.55	204.48	3.62
NUTS1	1	49	41.40	2.56	205.75	3.64

* based on SOC stocks of 1998

Despite the differences in model complexity, the simulated SOC trends of the case study region as a whole have been very similar across all model set-ups. All models predicted a carbon sequestration in the Saxon arable soils of about 2.6 Mt C (+/- 0.05 Mt C) for the reference period (1998-2014). This equals to an overall annual increase in carbon storage of 205-213 kg C ha^{-1} y^{-1} or 3.6-3.8‰ when related to the SOC stocks of the model initialisation. However, we could observe that all model set-ups using aggregated input data showed an underestimation of the simulated SOC trends when compared to the grid-based reference simulation. While the LAU-level simulation still was close to the reference (-0.8%), the stronger upscaled simulations showed more significant deviations of up to -3.8% for the NUTS2 set-up.

4.4.2 Spatial analysis and scale transitions

To investigate if the upscaling of the model set-ups to and across administrative levels leads to systematic errors in the simulated SOC dynamics we compared the individual sub-regions of each aggregation level with the reference simulation. Figure 18 shows maps of the average annual change in SOC stocks simulated with the five different model set-ups. In this section we show the simulated SOC trends in per mille (‰) per year and thus relate the results to the initial SOC stocks of 1998, which allows for easy relation to the targets of the '4 per mille' initiative (Lal, 2016; Minasny et al., 2017).

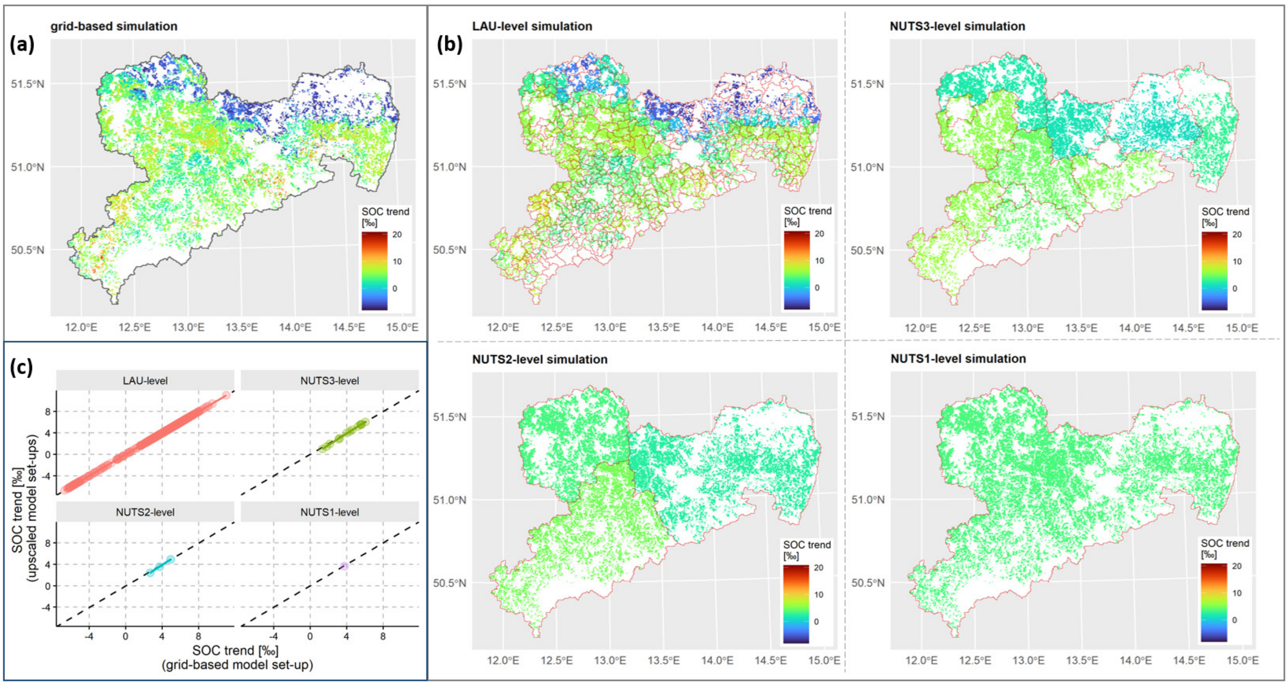
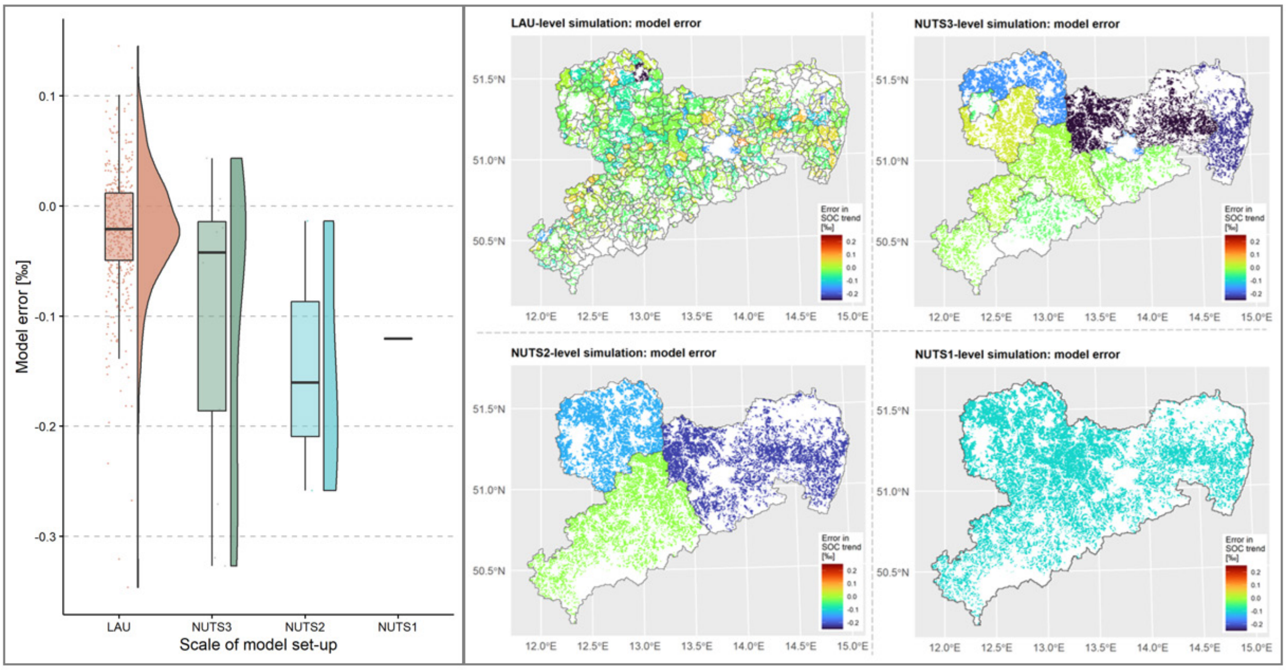


Figure 18: SOC trends [‰ per year; based on SOC stocks of 1998] of the case study area Saxony (NUTS1 region in Germany) simulated with five different levels of data aggregation for the period 1998-2014. **(a)** Results of the grid-based reference simulation (29,319 grid-cells). White areas represent non-arable land. **(b)** Results of the simulations using upscaled model set-ups on the level of administrative units (NUTS1, NUTS2, NUTS3, LAU). **(c)** Scatter plots comparing results of the upscaled and the (grid-based) reference model set-up on the level of the individual administrative units (NUTS1: n=1, NUTS2: n=3, NUTS3: n=13, LAU: n=414). ©EuroGeographics for the administrative boundaries.

Obviously, the upscaled simulations can only assess the overall trends for the simulated spatial units and not their inner heterogeneity. Thus, the total range of simulated SOC trends is considerably smaller, especially when simulated above the scale of LAU. However, when analysing the regional trends on the level of individual administrative units, all the aggregated model set-ups could reproduce the results of the grid-based reference simulation in a reasonable range (scatter plots in Figure 18c). The scatter plots also show that there are no clear outliers where the upscaling did not work for specific administrative units. The root-mean-square error (RMSE) for this trend comparison ranges between 0.06‰ for the LAU regions and 0.18‰ for the NUTS2 regions. Accordingly, the mean absolute error (MAE) varies between 0.04‰ (LAU regions) and 0.14‰ (NUTS2 regions), while having a mean overall trend of 3.7-3.8‰ per year in the upscaled model set-ups. A correlation analysis between the aggregated and grid-based simulation of SOC trends shows an adjusted r^2 of 0.999 for all four administrative levels considered. However, the slopes of the linear regression models are decreasing with increasing size of the administrative units: 1.001 (LAU), 0.929 (NUTS3), 0.902

(NUTS2), indicating a systematic underestimation of SOC trends in the highly upscaled set-ups.

Figure 19a shows the distribution of the observed model error when comparing the upscaled model set-ups with the grid-based reference simulation for each administrative unit. For the individual LAU regions, the model error ranges between +0.15‰ and -0.35‰, which equals +10.1 and -17.3 kg C ha^{-1} y^{-1}. However, this needs to be related to a mean trend in SOC stocks of 212 kg C ha^{-1} y^{-1} across all regions in Saxony. With increasing size of the simulated regions, the range in observed model errors decreases, but at the same time shifts toward a more distinct underestimation of SOC trends. For the NUTS2 model set-up the average annual trend in SOC stocks of all three spatial units was underestimated, while for the NUTS3 set-up 11 out of 13 regions showed an underestimation of SOC trends (Figure 19). The NUTS1 set-up (with only one spatial unit simulated) showed slightly better results than the NUTS2 set-up.



(a) **(b)**

Figure 19: (a) Distribution of the model errors observed when comparing the SOC trends of the upscaled model set-ups with the grid-based reference simulation on the same administrative levels. **(b)** Maps of the observed errors in the trend of SOC stocks for upscaled model set-ups. White areas represent non-arable land. ©EuroGeographics for the administrative boundaries.

While for the LAU set-up the simulation errors of the individual regions are rather evenly distributed within Saxony, a clear spatial pattern can be observed for the NUTS2 and NUTS3 set-ups (Figure 19b). Here, an underestimation of SOC trends can be observed especially in the northern and western regions of the case study area. These regions are characterised by a variety of different soil types (sandy soils and loamy silt soils) and cultivation systems.

4.4.3 Analysing the drivers behind errors in upscaled SOC simulations

Scaling of SOC simulations goes along with aggregating the input and turnover conditions of soil-related carbon, which both have a strong influence on the simulated dynamics in SOC stocks. Within CCB, the carbon flux from FOM to SOC (C_{rep}) and the turnover variable BAT, that aggregates the environmental conditions, are the two most important indicators for describing the state and development of SOC. Our results show that C_{rep} and BAT were scaled satisfactory to and across administrative levels.

For all model set-ups the average annual sum of the carbon reproduction flux C_{rep} of Saxony was 0.93 Mt C y^{-1} within the simulation period 1998-2014. The upscaled model set-ups showed a slight overestimation of the total C_{rep} flux with a range of +0.06% - +0.11%, which equals about 1.3 kg C ha^{-1} y^{-1}. A somewhat higher range of deviations was observed when considering the individual administrative regions (NUTS2 regions: -0.09% - +0.05%; NUTS3 regions: -0.17% - +0.34%; LAU regions: -1.3% - +0.92%) or the annual development of C_{rep} (e.g. NUTS1: -0.91% - +0.93%). However, the analysis did not show a systematic over- or underestimation of the C_{rep} flux for the upscaled model set-ups.

Regarding the carbon turnover conditions of Saxony, a minor underestimation in the total BAT was observed for the aggregated model set-ups with a range between -0.07% for the LAU set-up and -0.93% for the NUTS1 set-up. The tendency for underestimation of BAT was confirmed when analysing the individual regions on LAU and NUTS levels (NUTS2 regions: -0.46% - +0.09%; NUTS3 regions: -0.92% - +0.14%; LAU regions: -1.65% - +1.19%). The SOC turnover indicator BAT also showed higher annual deviations, with e.g. up to -3.02% - +1.48% for the NUTS1 set-up.

To analyse if the model upscaling and thus loss of variation in the drivers leads to systematic errors in simulated SOC dynamics we carried out a series of correlation analyses, starting with the main indicators C_{rep} and BAT, but also considering the original factors that drive carbon turnover conditions (climate parameters, tillage system, soil properties). Specifically, spatial dispersion parameters of the mentioned predictors have been correlated to the observed absolute errors in the simulated trends of SOC. Accordingly, Figure 20 shows a set of correlation matrices for the LAU level (414 spatial units) and the NUTS3 level (13 spatial units) simulations. Due to the low number of data-points this analysis was not available for the NUTS2 (3 units) and NUTS1 (1 unit) set-up.

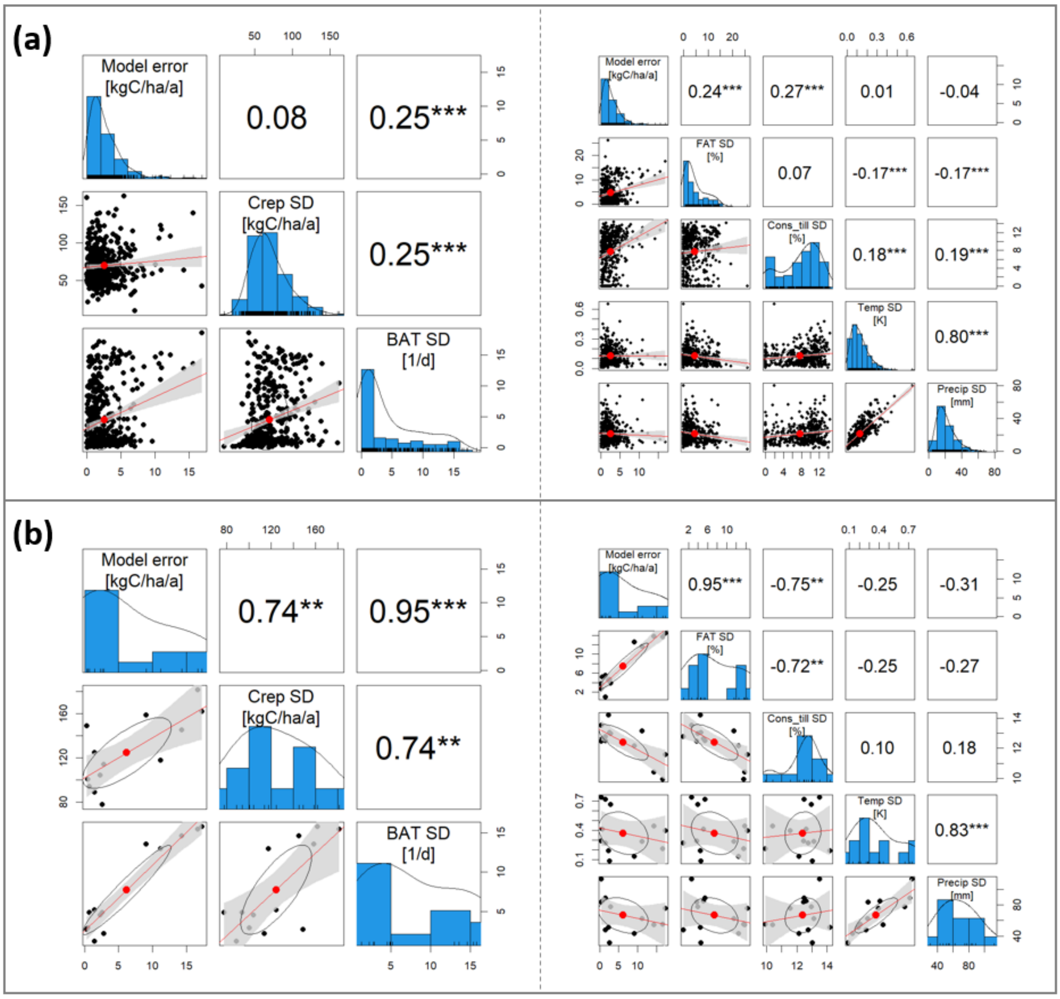
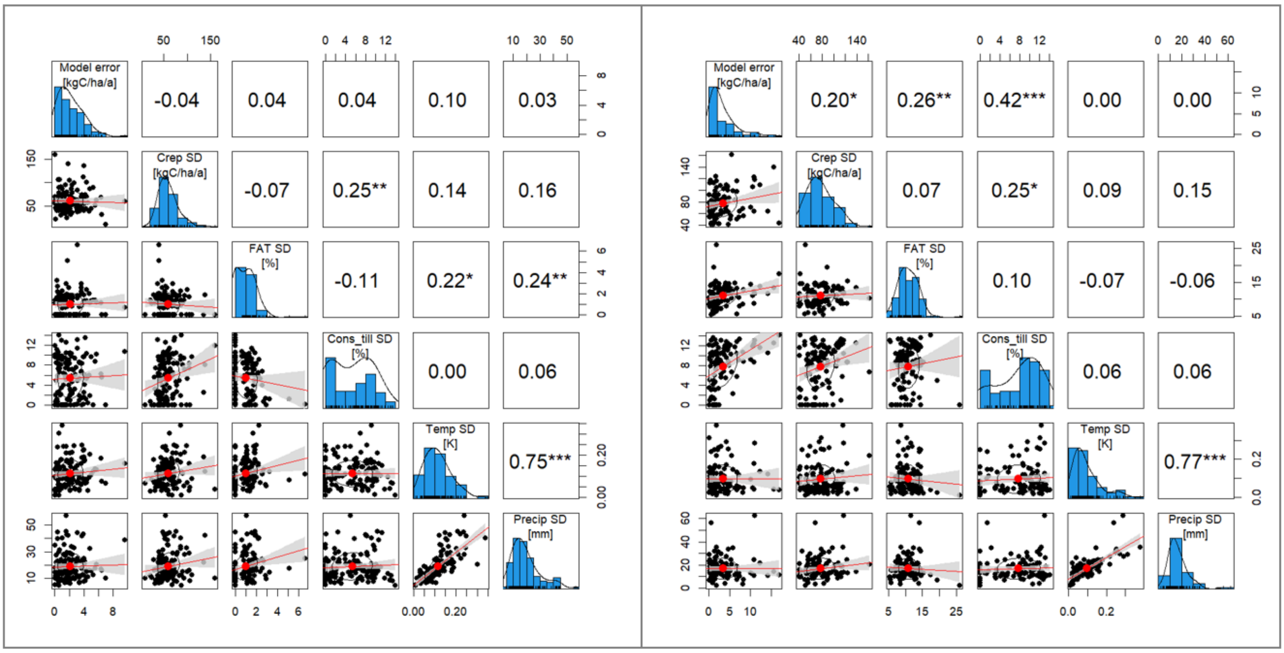


Figure 20: Correlation matrices between the absolute errors of the upscaled model set-ups (comparing SOC trends of the upscaled model set-ups with the grid-based reference simulation on the level of individual administrative units) and the spatial dispersion (standard deviation) of a set of predictor variables describing the input and turnover conditions of soil-related carbon. **(a)** Correlation matrices for the LAU-level model set-up; **(b)** Correlation matrices for the NUTS3-level model set-up. The predictors of the matrices are the soil carbon reproduction flux (C_{rep}), the carbon turnover indicator BAT, the soil fine particle content (FAT), conservation tillage shares (Cons_till), annual mean temperature (Temp) and annual precipitation (Precip). For each predictor its regional dispersion (standard deviation - SD) within an administrative unit has been calculated from the reference dataset and used for the correlation matrix. The distribution of each variable is shown on the diagonal. Below this diagonal the bivariate scatter plots with a fitted line are displayed. Above the diagonal the value of the correlation is shown as well as its significance level (stars), where the p-values <0.001, <0.01 are associated to the symbols *** and ** respectively.

For the LAU level simulation (Figure 20a) the matrices show a rather low correlation between the predictor variables and the observed model error. Nevertheless, a high spatial dispersion of a region's turnover conditions (BAT) and specifically its soil fine particle content (FAT) as well as conservation tillage shares (Cons_till) significantly favours higher model errors in simulated SOC trends (p-values < 0.001). For the NUTS3 simulation (Figure 20b) this picture becomes more pronounced and strong correlations between the dispersion of C_{rep}, BAT, FAT and conservation tillage and the model error were found. However, the results are affected by cross-correlations, e.g. between BAT and C_{rep}, as variations in soil properties often go along with variations in yields. The climate related predictors (regional dispersion in temperature and precipitation) had no statistically significant correlation to the observed errors of the aggregated models.



(a) (b)

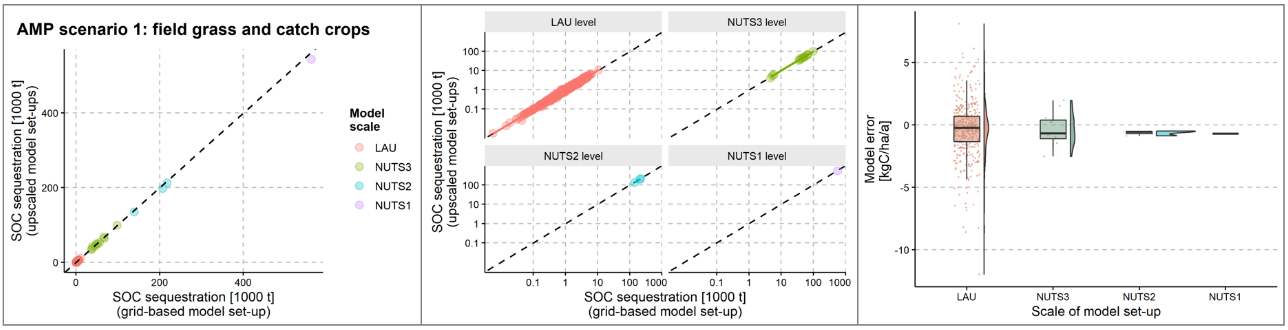
Figure 21: Correlation matrices between the absolute errors of the LAU-level model set-up and the spatial dispersion (standard deviation) of a set of predictor variables. **(a)** Correlation matrix for a subset of LAU regions that show a low variability in carbon turnover conditions (BAT); **(b)** Correlation matrix for a subset of LAU regions that show a high variability in carbon turnover conditions (BAT). The predictors of the matrices are the soil carbon reproduction flux (C_{rep}), the soil fine particle content (FAT), conservation tillage shares (Cons_till), annual mean temperature (Temp) and annual precipitation (Precip). For each predictor its regional dispersion (standard deviation - SD) within an administrative unit has been calculated from the reference dataset and used for the correlation matrices. The distribution of each variable is shown on the diagonal. Below this diagonal, the bivariate scatter plots with a fitted line are displayed. Above the diagonal, the value of the correlation is shown as well as its significance level (stars), where the p-values of < 0.001, <0.01 are associated with the symbols *** and **, respectively.

An individual correlation matrix for LAU regions with high and with low variability in BAT (Figure 21) can be used to further investigate the role of regional carbon turnover conditions on the observed model error. The analysis shows that for administrative units with low standard deviation in regional carbon turnover conditions (Figure 21a) the observed model errors were lower and that there was no significant correlation of the model error with any of the predictors. For administrative units with high variability in turnover conditions (Figure 21b) the observed model error can be partially explained by the regional variability in C_{rep}, FAT and conservation tillage. The range in the spatial dispersion of C_{rep} and conservation tillage shares is nearly the same in both matrices, but the variability in soil fine particle content increased. As shown in Figure A5 (supplementary materials: appendix section 6.2) the relevance of regional deviations in soil fine particle content (FAT) is higher for regions with high spatial dispersion of C_{rep}. For regions with both, high spatial dispersion of C_{rep} and BAT, C_{rep}

is the most significant predictor for the observed error of the LAU-level model set-up (Figure A6 in the supplementary materials: appendix section 6.2).

4.4.4 Assessing alternative management practices across scales

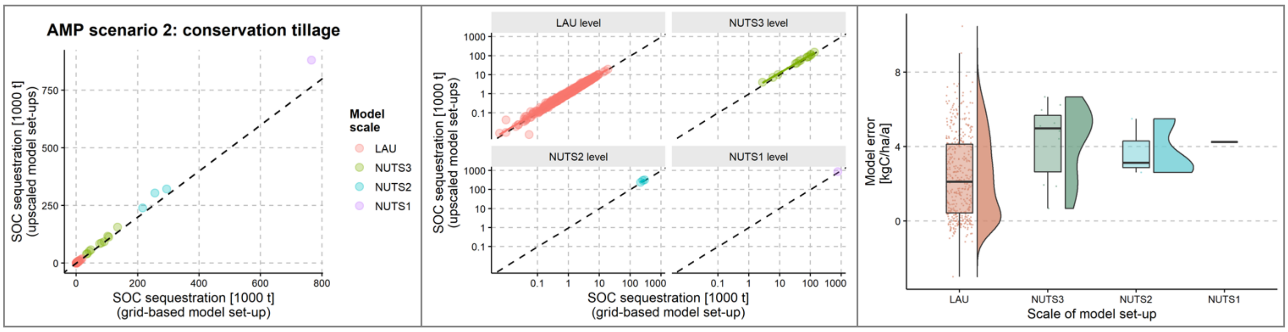
Two scenarios have been used to assess the ability of the upscaled model set-ups for quantifying the carbon sequestration potential of alternative management practices (AMP). Both AMP scenarios have been related to a ‘business-as-usual’ scenario to extract the AMP driven effects from the overall trends in SOC stocks. Our results show that the upscaled model set-ups could reproduce the results of the grid-based reference model for both scenarios in a reasonable range, although some limitations do apply.



(a) **(b)** **(c)**

Figure 22: Carbon sequestration potential of the first alternative management practice (AMP-1; increasing soil carbon influx based on increased cultivation of field grass and cover crops) simulated with five different model set-ups. **(a)** The results of the grid-based reference simulation are compared to the four upscaled model set-ups. **(b)** Same content as (a), but using a logarithmic scale for better visualisation of carbon sequestration in smaller LAU regions. **(c)** Model errors in the assessment of AMP-1 for individual administrative units.

The first AMP, addressing an increase in soil carbon input based on changes in the cultivation of fodder crops and cover crops, resulted in a carbon sequestration of 0.56 Mt C within the grid-based reference simulation (2014-2050), which equals 20.7 kg C ha^{-1} y^{-1}. The upscaled model set-ups underestimated these results to a small extend ranging between -0.13 kg C ha^{-1} y^{-1} (LAU set-up) and -0.71 kg C ha^{-1} y^{-1} (NUTS1 set-up), which equals -0.6% to -3.4% of the of the overall AMP effect respectively. Figure 22a and Figure 22b show that on the level of the individual administrative regions the simulated carbon sequestration potentials of the first AMP scenario are scattered along the 1:1 line for all model set-ups. For the individual LAU regions, the deviation of the model error was highest and included some relevant outliers (Figure 22c).



(a) **(b)** **(c)**

Figure 23: Carbon sequestration potential of the second alternative management practice (AMP-2; reducing carbon turnover conditions by increasing the use of conservation tillage) simulated with five different model set-ups. **(a)** The results of the grid-based reference simulation are compared to the four upscaled model set-ups. **(b)** Same content as (a), but using a logarithmic scale for better visualisation of carbon sequestration in smaller LAU regions. **(c)** Model errors in the assessment of AMP-2 for individual administrative units.

The second AMP scenario addressed a different driver of SOC dynamics and reduced carbon turnover conditions by increasing the use of conservation tillage within Saxony. For the reference simulation this scenario resulted in a SOC sequestration of 0.77 Mt C for the period 2014-2050, which equals to 28.2 kg C ha^{-1} y^{-1}. The upscaled model set-ups significantly overestimated these results within a range of +2.7 and +4.2 kg C ha^{-1} y^{-1}, which equals +9.5% to +15.0% of the of the overall AMP effect respectively. The absolute model error on the level of Saxony was highest for the NUTS1 set-up, which simulated a total SOC sequestration of the second AMP scenario of 0.88 Mt C. Figure 23c is comparing the simulated effects of the conservation tillage scenario on the level of the individual administrative regions, showing that the deviation of the model error was highest in LAU-level model set-up. Furthermore, the scatterplots of Figure 23a show that the results of the upscaled simulations are clearly above the 1:1 line and systematically increase for administrative units with high C sequestration potential.

The spatial distribution of the carbon sequestration potential simulated with both AMP scenarios is mapped in Figure A7 (supplementary materials: appendix section 6.2). Accordingly, the highest total carbon sequestration can be reached in the loess regions of central Saxony. The NUTS3 and LAU level model-setups allowed for an acceptable spatial prioritisation AMPs, which was not the case for the set-ups on the scales above.

4.5 Discussion

An effective management of the SOC stocks of arable land requires an understanding of the scalability of the drivers affecting the SOC dynamics. Furthermore, it is necessary to find appropriate reference scales that simplify applicability, scalability and communication of SOC assessments. Ideally a consistent approach could be used for assessing the effects of specific drivers and measures on SOC over different scales and thus enable a local adaptation and prioritisation of targets or measures. In this paper we discuss administrative units as a promising spatial basis for scaling levels, and demonstrate the potential and limitations of such an approach. We also discuss whether the use of aggregated statistical data sources may lead to an underestimation in regional SOC trends regardless of the actual process model in use and the scale of its set-up. For each point of discussion, we conclude with recommendations for how to better incorporate scale related aspects in the assessment and management of SOC.

4.5.1 Administrative units as an adequate compromise for scaling SOC assessments, communication and policy-making

Like many other ecosystem services, soil carbon sequestration tends to be heterogeneously distributed over space. Due to partly existing mismatches on the scale of production, management and benefits the dynamics of carbon sequestration need to be evaluated and assessed across different scales (Raudsepp-Hearne & Peterson, 2016). Ecosystem services are frequently analysed and mapped in the highest possible resolution and later aggregated to a desired spatial unit, which is often the management level in policy-making (Zen et al., 2019). Despite the averaging effect, which results in a loss of information, this approach seems to be adequate for soil carbon related assessments (Grêt-Regamey et al., 2014; Raudsepp-Hearne & Peterson, 2016), which is not always the case for other ecosystem services (e.g. tourism, maple syrup and timber production (Grêt-Regamey et al., 2014; Raudsepp-Hearne & Peterson, 2016)). However, the availability of some key datasets (e.g. agricultural parameters) of regional SOC assessments is often limited to larger scales - specifically low-resolution statistics on the level of organisational boundaries or administrative units, which also equals to the level of policy making.

The results of our study showed that the simulation of SOC dynamics on the scale of administrative units can be feasible and leads to significant benefits for model set-up, application and runtime. The degree of model simplification was substantial, while the simulation error introduced by upscaling the model set-ups was in an acceptable range in our case study set-up. The LAU-level set-up reduced the number of modelling units by a factor of 15 (6.8% of the units of the grid-based reference setup), while the NUTS1-level set-up even resulted in a reduction by a factor of 600 (0.17% of the grid-based reference setup). At the same time the model scaling error on the level of Saxony was -0.8% and -3.2% for the LAU and NUTS1-level set-ups respectively and thus in a reasonable range having in mind the uncertainties that come along with large-scale assessments. Obviously, the decision if such a simplified assessment is acceptable depends on the scale of interest and higher errors have been observed for individual units on smaller administrative levels.

Upscaling the modelling framework to administrative units led to a simplified application of CCB, easy scenario implementation and allowed for scalability across administrative levels. By using two contrasting scenarios we showed that the approach could be used for a scale adequate quantification of the anticipated effects of alternative management practices (AMPs) on carbon sequestration. Here, the simulation of AMPs addressing changes in soil carbon input (e.g. cultivated crops, residues management, organic fertiliser) has shown to be more robust on larger scales than AMPs, which influence carbon turnover conditions (e.g. tillage systems). In the latter case, we observed an overestimation of the carbon sequestration potential in the upscaled model set-ups of up to 15%. As administrative regions are also often the level of policy making, communication and cross-regional comparisons, the approach shown in this study could promote discussions on the effectiveness of AMPs on a quantitative basis, which could be helpful in various stakeholder processes.

The scaling experiment presented in this study represents an idealised framework of the overall concept. By upscaling the input data of our reference model to the level of administrative units we ensured that the scaling effects we observed were not caused by different types and qualities of data sources. However, we showed that this type of scaling is reasonable as well as that CCB is a capable tool for this kind of analysis. We expect that other soil carbon models may be suitable for such scaling operations as well, given that these models accept input data in the form of proportional coverages and area averages of different management activities. One examples for such models that could be used to confirm our results is the C-N-P model (Carbon-Nitrogen-Phosphorus; a further development of CCB) (Franko, 2023; Franko et al., 2023). Furthermore, it is essential to consider that at least the distribution of soil types in a region should be included in an upscaled model set-up. An exclusion of soil types, e.g. by using the dominant soil of an administrative unit, will strongly affect the overall scaling error. For very heterogeneous regions, especially in terms of soils and yield potential, the upscaling of input data could lead to systematic errors (see also the following section 4.5.2). However, this effect was rather minor for the case study of Saxony despite its diversity in agricultural systems, landscape characteristics and soils. Regarding the administrative levels of Europe, the LAU regions showed to be the most suitable compromise between model simplification and observed model error. However, also the model set-ups on the larger NUTS3, NUTS2 and NUTS1 levels provided scale-adequate results and have the benefit of better data availability and relevance for communication and policies.

4.5.2 Data driven underestimation of SOC trends in regional assessments

Our results indicate that regional heterogeneity in the carbon input and turnover conditions of a study area may drive systematic errors in regional SOC assessments. Specifically, we observed a slight, but systematic underestimation of SOC trends within our upscaled model set-ups. While in our study this error was introduced by the upscaled modelling approach, it might be relevant for all regional assessments of SOC that make use of regional statistics in their input data. Due to the widespread limitations in data availability the use of statistical datasets on administrative levels is quite common in regional to large scale estimations of SOC stocks (Aguilera et al., 2018; Begum et al., 2018; Borrelli et al., 2016; Farina et al., 2017;

Kaczynski et al., 2017; Lugato et al., 2014). We showed that with increasing heterogeneity in turnover conditions (e.g. driven by different soil types or tillage systems) the use of aggregated input data (especially on agricultural management) leads to an increasing model error.

This effect can be best discussed at the example of a fictional region that has two different soil types: (1) sandy soils with high carbon turnover conditions and low yield potential and (2) silty soils with lower SOC turnover conditions and high yield potential. Obviously, both soil regions have different amounts of biomass available to be returned into soil, which may lead to vastly different steady state levels of SOC. The agricultural parameters (e.g. yield) reported in statistical datasets of this fictional region will only provide an average value across both soil types, which might then be applied as a uniform value to both soil types within a model set-up. Accordingly, an overestimation of the carbon influx to the sandy soils and an underestimation of carbon influx to the silty soils can be expected. However, as the residence time of carbon in sandy soils is shorter than in silty soils, the virtual transfer of carbon from silty soils to sandy soils leads to an underestimation of a region's SOC sequestration. This effect is purely input data driven and regardless of the model in use or the scale of model set-up.

With a series of correlation analyses we showed the relevance of this effect and it became clear that regional heterogeneity in soil properties and tillage systems are the most relevant variables that drive the scaling error in our framework. For regions that have high turnover conditions for soil related carbon also the regional heterogeneity in soil carbon input levels becomes relevant, which is not the case for regions with low heterogeneity in turnover conditions. The overall effect on our case study results was rather low, however we recommend that regional SOC assessments should consider this effect in their uncertainty analysis (Diel & Franko, 2020).

4.5.3 Supporting SOC sequestration in the case study region Saxony

The SOC stocks of the Saxon arable land show a positive trend within the reference period due to positive developments in agricultural management practices like the increased use of conservation tillage (Lülfs-Baden et al., 2020; Witing et al., 2019). Within our study we quantified a total carbon sequestration in the arable soils of 2.6 Mt C for the period 1998-2014, which equals a trend of 3.7‰ per year based on the SOC stocks of 1998. This is considerably higher than the results reported by Witing et al. (2019). Updates in the initialisation of CCBs SOC pools according to the approach of Drexler et al. (2020) are the main reason for the differences observed and underline the widespread challenges of model initialisation in regional SOC assessments (Dimassi et al., 2018; Foereid et al., 2012).

Our results also show that an increased use of conservation tillage as well as increased cultivation of field grass and cover -crops could substantially support future SOC sequestration in Saxony. We quantified that moderate changes in management (absolute increase of 8.3% in field grass and 10% in conservation tillage) could potentially store additional 1.33 Mt C (48.9 kg C ha^{-1} y^{-1}) in the Saxon arable soils until 2050. This is lower than the results of similar scenarios that have been reported for the arable land of Great Britain (Jordon et al., 2022), but still in a reasonable range. Future studies should investigate other potential management actions as well as effective and reasonable degrees of implementation, which were not in the focus of this study. Promising management activities in the local context are for example related to the management of crop by-products and residues, self-planted fallow greening, or an adapted management of field margins (Sächsisches Staatsministerium für Energie, Klimaschutz, Umwelt und Landwirtschaft, 2015, 2022). Also the biogas sector became an important factor for the SOC dynamics in Saxony (Witing et al., 2018) and together with implication induced by upcoming changes in climate (Franko et al., 2015, 2019) and dietary habits a re-evaluation of the carbon fluxes of the agricultural system may be required (Tiefenbacher et al., 2021).

The use of conservation tillage showed higher carbon sequestration potential in Saxony than the increased cultivation of field grass and cover crops. However, CCB does only simulate the carbon dynamics of the topsoil (30cm) and potential negative impacts of reduced tillage on the SOC levels of deeper soil layers could not be investigated (Baker et al., 2007; Haddaway et al., 2017). Furthermore, management decisions need to consider that SOC accumulation rates decrease over time and are always accompanied by major changes in nitrogen cycles and stocks (Lugato et al., 2018; Witing et al., 2019).

4.5.4 Conclusions

Regional and quantitative assessments of SOC stocks and trends as well as of the carbon sequestration potential of alternative management practices (AMP) are highly relevant for developing climate change mitigation strategies of the agricultural sector. However, such assessments are still rarely done due to limitations in the availability of input data and the complexity of the model set-ups. This study showed that a simplified, upscaled assessment of AMPs on the level of administrative units can be feasible for several applications. By using the 'regional mode' of the CCB model we could apply a consistent approach for quantifying SOC dynamics over different scales, which enables a local adaption and prioritisation of targets or measures. In general, and not only for upscaled model set-ups, modelers need to be aware that the use of statistical input data (esp. on agricultural management) may lead to a systematic underestimation of SOC trends, regardless of the model in use. However, simplified and scale adapted assessments of SOC dynamics using commonly available data could be valuable for cross-regional comparisons, communication and policy making and could provide a quantitative basis for discussion on the effectiveness of AMPs in various stakeholder processes. Regarding the administrative levels of Europe, the LAU and NUTS3 regions showed to be the most suitable compromise between model simplification, data availability and observed model error and allowed for an acceptable spatial prioritisation of AMPs.

5. Synthesis

5.1 Key findings and contributions of the thesis

Agriculture is the primary land use in Germany and the European Union and is facing numerous challenges and conflicts (Boix-Fayos & de Vente, 2023; Fellmann et al., 2018; Kirschke et al., 2021; Pe'er et al., 2020). The increasing demand for high-quality food and materials must be met sustainably and in an environmentally friendly manner, while also adapting to a changing climate and mitigating emissions and pollution (Kay, 2018; Tilman et al., 2002). Productive and resilient agriculture relies on soils, whose fertility, stability and functioning are closely linked to their organic matter content (Vogel et al., 2019; Wiesmeier et al., 2019). An appropriate management of SOM is therefore part of many of the already ongoing adaptation and mitigation strategies. However, SOM stocks exhibit significant spatial heterogeneity both within and across agricultural landscapes (Aksoy et al., 2016; de Brogniez et al., 2015; Lugato et al., 2014; Rial et al., 2017) due to a variety of drivers at different scales that affect the SOM cycle or related environmental boundaries. Therefore, managing SOM presents a significant challenge, requiring appropriate approaches to assess the impact of drivers or measures on SOM across a set of relevant scales and system boundaries. The overarching objective of this thesis was to improve the understanding of SOM in agricultural landscapes from a spatial and systems perspective, thereby facilitating the development of integrated SOM management strategies. In order to address important research gaps in this context, the preceding chapters of this dissertation presented a regional perspective on SOM dynamics and their management, and analysed various carbon fluxes in agricultural systems. The following provides a concise overview of the key findings presented in chapters 2, 3, and 4 and relates them to the research questions set out in chapter 1.

The first research question of this dissertation dealt with the land requirements of biogas production systems in Saxony and the potential impact of the growth of the biogas sector on regional agricultural carbon fluxes to soils. **Chapter 2** introduces a new conceptual approach called 'biogas fingerprint area' (BFA), which aggregates the effects of location and management of a biogas plant into valuable indicators for the analysis and differentiation of bioenergy production systems on regional scales. Specifically, the land requirements for the production of biogas feedstock and disposal of digestate are determined and characterised, together with the associated direct soil carbon fluxes. The comparison of carbon fluxes inside and outside of a BFA proved to be an easily applicable instrument to assess the influence of a biogas plant on regional SOC cycles. It is therefore proposed to be used as an indicator to characterise the sustainability of a biogas plant. The results demonstrated that areas impacted by biogas production can have a greater return flow of agricultural carbon compared to the surrounding agricultural land, as well as compared to the carbon fluxes prior to the installation of a biogas plant. Within Saxony, the application of digestate could fully compensate for the ‘loss’ of livestock-related carbon from the traditional matter cycling. Due to the use of plant material in the feedstock mix for biogas production, additional carbon remains in the agricultural carbon cycle and is returned to the soil via biogas digestate, instead of being exported as food. Though, when excluding digestate, the carbon flux from agricultural cultivation (crop residues and crop by-products) is lower in areas affected by biogas production than in the surrounding areas. This is primarily because the BFAs in Saxony have a higher area share of maize and a lower area share of cereals, which are typically rich in crop by-products such as straw.

The BFA approach also contributes to a better understanding of the relationship between power supply and area requirements of different renewable energy sources (Evans et al., 2009; Lechon et al., 2011; Popp et al., 2014; Scheidel & Sorman, 2012; H. Wüstemann et al., 2017). It became evident that the area requirements of a biogas plant are highly dependent on its location (effecting crop yields, livestock mix), installed capacity and substrate mix. Larger biogas plants typically require less area per kW of installed electrical capacity due to lower indirect feedstock requirements, especially animal excrements. The study found that, on average, biogas production in Saxony influenced an area of 2.0±0.4 ha kW_{el}^{-1}. However, only 0.4±0.1 ha kW_{el}^{-1} of that were related to the cultivation of energy crops on arable land. Biogas production also has an impact on carbon fluxes in arable land used for fodder crop cultivation, primarily through changes in organic amendments. In Saxony, this is the largest area affected by biogas production systems, with an average of 1.2±0.3 ha per kW of installed electrical capacity.

In summary, Chapter 2 presented a novel approach for examining the impact of bioenergy production on regional soil carbon cycling through an ex-post analysis of biogas production in the agricultural landscapes of Saxony. The concept of a biogas ‘fingerprint’ was successfully demonstrated, providing novel insights into agricultural carbon and matter fluxes, as well as the regional area requirements of biogas production. It was shown that biogas plants in Saxony can be operated sustainably with regard to SOC recycling, but this is highly dependent on the application of digestate and accompanied by considerable land requirements.

The second research study of this thesis expanded and generalised the approach of Chapter 2, which had focused on the soil carbon input fluxes of conceptual spatial units (‘biogas fingerprint areas’). In contrast, **Chapter 3** employed a grid-based approach for an integrated simulation of the entire soil carbon cycle and related fluxes of organic nitrogen, while investigating a series of significant drivers. Accordingly, the second research study introduced a series of model adjustments that have been implemented to utilise the SOM model CCB for regional studies. In this new ‘regional mode’, CCB can be operated using the proportional coverage of a variety of management activities within a flexible type of spatial modelling unit, such as farm, pixel, or municipality. In particular, the new ability to employ crop share statistics instead of crop rotations is a crucial prerequisite for large-scale modelling approaches. The validation of the innovative model developments was successful using data from long-term field experiments conducted at various sites across Europe. Accordingly, this new CCB module has the potential to be applied to numerous case studies to gain an integrated, spatially distributed view on the regional carbon and nitrogen cycles of arable land.

The methodology was successfully applied to 7,345 km^2 of arable land in Saxony, where a diverse set of input data could be considered, overcoming typical limitations for the large-scale SOM simulations. The results showed that considerable amounts of carbon (0.79 Mt C) and nitrogen (0.09 Mt N) have been stored in the SOM of the arable soils of Saxony during the period 1998-2014. However, significant regional differences were observed. Both the increase in carbon inputs to the soils (+8%) and the reduction of carbon turnover rates (-10%) had a positive effect on SOC storage. The most significant driver for the overall increase in SOM storage was the increased use of conservation tillage, while climate variability had a strong impact on its annual dynamics. It is crucial to note that if the factor driving the positive trend in SOM storage is lost, the stored amounts of carbon and nitrogen will be released. Therefore, future subsidy programs should not only consider the potential for future carbon sequestration but also the maintenance of current SOM stocks.

In summary, the newly developed 'regional mode' of the CCB model demonstrated its capability to simulate regional trends in SOM stocks using aggregated agricultural management data and gridded modelling units. The study revealed that between 1998 and 2014 regional SOM stocks increased across most of Saxony's arable land, but with distinct regional differences and largely driven by the increased use of conservation tillage. The simulated average annual increase in SOC of 1.2‰ is significant, but falls short of the '4 per 1000' target set by the COP21. Along with the increase in SOC, a significant amount of nitrogen was immobilised. Still, the year-to-year variations were more dominant than the overall trends in nitrogen storage.

The third research study built upon the model developments of Chapter 3, with the objective of operationalising SOM modelling for policy support by enhancing the applicability and comparability of SOM assessments. It was questioned whether SOM dynamics and carbon sequestration scenarios can be directly simulated for spatial units and scales that are relevant to policy and environmental management, such as administrative units, even though such units are typically not directly related to environmental processes. **Chapter 4** demonstrated that simplified, upscaled assessments of alternative management scenarios at the level of administrative units are feasible for several applications. The degree of model simplification was substantial (reduction in modelling units by a factor of 15 - 600 compared to a grid-based set-up), while the simulation error introduced by upscaling the model set-ups was within an acceptable range. The innovative scaling experiment demonstrated that a consistent approach can be applied to quantify SOC dynamics on a 500 m grid up to the NUTS1 level. This enables the assessment of alternative management strategies at a large scale and in a quantitative manner, while allowing for the local adaptation or prioritisation of these measures using the same modelling approach. Furthermore, it is highly relevant as it allows researchers and stakeholders to operate at scales that align with the level of policy-making, data availability, cross-regional comparisons and communication. The study results indicate that that the use of statistical input data, in particular agricultural management data, may result in a systematic underestimation of SOC trends. This is a general picture driven by soil heterogeneity and is independent of the model in use or the scale of its set-up. For the Saxon arable land, the average scaling error was quantified to be in the range of 0.8–3.8% when using the new 'regional mode' of the CCB model, which is a reasonable range having in mind the uncertainties that come along with large-scale assessments.

The study showed that that making moderate changes in agricultural management, such as increasing field grass, cover crops, and conservation tillage by 8.3-10%, could potentially store additional 1.33 Mt C in the Saxon arable soils by 2050. The upscaled model set-ups overestimated the total carbon sequestration potential of the scenarios by up to 0.09 Mt C. Simulation of management scenarios that address changes in soil carbon input (e.g. field grass, catch crops) has proven to be more robust on larger scales than scenarios that influence carbon turnover conditions (e.g. reduced tillage). In the latter case, the study observed an overestimation of the carbon sequestration potential in the upscaled model set-ups of up to 15%. The LAU and NUTS3 regions of Europe are the most appropriate compromise between model simplification, data availability and observed model error, while allowing for an acceptable spatial prioritisation of targets and measures.

In summary, the results for the case study of Saxony demonstrated that simulating SOC dynamics on the scale of administrative units provided feasible results with an acceptable scaling error, while being advantageous for model set-up and application. Field grass, cover crops, and conservation tillage have shown great potential for carbon sequestration in Saxon arable soils. When utilising statistical input data for SOC modelling, in particular agricultural management data, moderate but systematic deviations in simulated SOC trends can be expected due to simplifications in simulated soil and crop yield heterogeneity.

Overall, the three studies significantly improve the spatial and systems perspective on the SOM dynamics in agricultural landscapes by providing novel tools and approaches, case study specific assessments at regional scales, and recommendations for specific measures. As such, the results of this work provide valuable support for future SOM management strategies. It is relevant to highlight that the key findings of this dissertation do not only represent a research-based increase in knowledge. By focusing on a specific case study and providing quantitative assessments, the results are also highly relevant and informative to a variety of stakeholders in the agricultural, governmental and planning sectors. The findings provide a quantitative basis for discussing current developments in the agricultural sector and the effectiveness of potential adaptation measures, as well as the feasibility of CO_2 certificates for carbon sequestration in agricultural soils. Additionally, the results allow for a better understanding of the status-quo, contributing to improved GhG inventories and cross-regional comparisons. A wide range of land-users are provided with a spatially differentiated information base, increasing their awareness of the relevance of SOM and contributing to planning processes at the farm level up to policy-making, such as the development of new incentive systems.

5.2 General discussion

In addition to the key findings described above, the following chapters discuss the contributions of the thesis within the wider context of the recent challenges in SOM management, as outlined in Chapter 1.

5.2.1 Emphasising the requirement for a co-management of carbon and nitrogen pools

Increasing SOM stocks is an important component of many strategies aimed at improving the sustainability of agricultural land use, mitigating and adapting to climate change, or promoting other soil-based ecosystem functions and services (Keesstra et al., 2016). However, carbon sequestration studies and strategies often concentrate on soil carbon, its stability and turnover times (Baveye et al., 2020). Soil nitrogen, on the other hand, is often only partially considered, for example as an additional contributor to GhG emissions (N_2O) or as a driver of SOM turnover (Guenet et al., 2021; Han et al., 2016). Little attention is often paid to the potentially significant changes in soil nutrient stocks that are associated with soil carbon sequestration, despite the fact that SOM binds up to 95% of soil nitrogen (Bingham & Cotrufo, 2016).

The thesis results indicate that agricultural soils in Saxony have stored significant amounts of nitrogen, averaging 7.5 kg N ha^{-1} a^{-1} between 1998 and 2014. Yet, the findings also reveal the magnitude of the annual cycling of soil nitrogen: On average, 142 kg N ha^{-1} is mobilised each year due to SOM mineralisation, while at the same time, about 149 kg N ha^{-1} is immobilised through SOM reproduction. It is obvious that nutrient availability for crop production is closely linked to the annual SOM turnover and will be affected by any management strategy that alters SOM stocks and thus (im)mobilises both C and N. Furthermore, this interdependence with SOM cycling also applies to all other nutrient-related goals and challenges, such as nitrogen leaching into water bodies and gaseous losses, but also soil life activity (Baveye et al., 2020). Although some relationships are understood well, they are not always reflected in legislation and management.

Field crop fertilisation is heavily regulated in Germany, for example through the fertiliser ordinance (Düngeverordnung - DüV, 2017), aiming to achieve fertilisation levels that correspond to the expected plant uptake. Unfortunately, in such calculations, in-field SOM stocks are barely considered, although trends in SOM could be accompanied a significant (im)mobilisation of nitrogen. The challenge of regulating organic nitrogen pools is further demonstrated by the topic of organic amendments: the nutrient content of organic fertilisers is only partially accounted for in fertilisation calculations (keyword: mineral fertiliser equivalent; Albert et al., 2007; Herold et al., 2010; Wiesler et al., 2016; Wissenschaftlicher Beirat für Düngungsfragen, 2015), due to the delayed plant availability of the nutrients and application losses. To enhance the joint management of carbon and nitrogen in agriculture, it is essential to regularly and comprehensively monitor SOM stocks and trends. Though, measuring the organic carbon content of soils is challenging (Smith et al., 2020). In contrast, soil mineral nitrogen levels are relatively inexpensive to measure and are commonly assessed each spring to as part of calculating fertilisation demands. Incorporating SOC monitoring at this stage could be a significant advancement. While German agricultural policy has recognised the need to improve the monitoring of soil nitrate (Bundesministerium für Ernährung und Landwirtschaft (BMEL), 2019), the same cannot be said for SOC, at least not as an integrated part of agricultural practice. Nevertheless, Germany’s first agricultural soil inventory (‘Bodenzustandserhebung’; Jacobs et al., 2018) provided an important first baseline of the SOC stocks in agricultural soils on an 8 x 8 km grid. Improving SOC monitoring is also a requirement for accessing new market opportunities, such as ‘carbon farming’, which allows farmers to benefit from carbon sequestration by selling CO_2 certificates as emission offsets on the carbon market (Mattila et al., 2022; Paul et al., 2023; Sharma et al., 2021). However, also in this context the interrelations with soil nutrients must be considered, as carbon sequestration is accompanied by an increase in soil nitrogen stocks. Little research has been done on the potential risks associated with the accumulation of large quantities of nitrogen in soil, which will be released again if the implemented agricultural measures are not continuously maintained.

Improved collaboration among different stakeholder communities and sectors involved in agricultural matter fluxes or interested in their side effects could lead to better management of carbon and nitrogen in soils. Naturally, each community has its own focus and specific challenges, but a joint effort is necessary for reaching integrated strategies. This thesis demonstrates possibilities to establish an analytical baseline that could facilitate future collaboration across sectors, including agriculture, water management, bioeconomy and other markets related to carbon- and nutrient-based products. This will ultimately benefit ecosystems.

5.2.2 Increasing capacity to assess regional SOM stocks and fluxes

Regional environmental assessments are important tools for considering potential environmental impacts in decision-making processes and should be proactively integrated into planning and policy-making (Benson, 2003; Olagunju & Gunn, 2016). However, although the need for including SOM-related indicators in decision-making processes has been recognised, there are several obstacles that must be overcome (Lorenz & Lal, 2016). The main challenges can be broadly attributed to the lack of data and tools designed for regional-scale assessments. This results in a rather limited number of regional applications compared to other environmental factors, such as water. Accordingly, there is a need for increased capacity to assess SOM stocks and fluxes at a regional level to improve the knowledge base for effective climate change mitigation strategies in the agricultural sector and for achieving sustainable development goals.

To increase capacity, the first step is to improve existing databases of SOC stocks, which requires the establishment of routine, harmonised, and comparable approaches for systematic SOC data collection (Lorenz & Lal, 2016). Large-scale sampling campaigns such as the German soil condition survey (Jacobs et al., 2018) are an important step towards improving future regional environmental assessments. Though, it has been argued that there is a lack of efficient standard approaches for monitoring SOC stocks in both the field/laboratory (Olson et al., 2014) and at the farm/landscape scale (Stockmann et al., 2013). Difficulties can also arise when extrapolating SOC data from a limited number of sampling sites to a larger area (de Gruijter et al., 2016), which is crucial for the initialisation of regional scale SOC models. In this thesis, two different approaches were used to overcome these problems. Firstly, site-condition-typical stocks for the long-term stabilised carbon pool were combined with steady-state assumptions for the decomposable SOC pools (chapter 3). In the second approach (chapter 4), the SOC initialisation was updated using recent data from Drexler et al. (2020), who provide a SOC classification scheme for German agricultural soils based on measurements from nearly 3,000 sites of the German agricultural soil inventory (Jacobs et al., 2018). It is desirable that such large-scale sampling campaigns are continued on a regular basis to provide a time series of data that would facilitate model initialisation and validation of simulated trends in regional SOM stocks.

A further step in increasing the capacity for regional SOM assessments is to continue the development of tools that are appropriate for the scale under study. These tools should, for example, be designed to handle the type of input data that is typically available at regional scales. While the availability of spatially explicit crop cultivation data is improving with remote-sensing-based products (Asam et al., 2022; Blickensdörfer et al., 2022; Preidl et al., 2020a, 2020b), information on other agricultural parameters, such as crop yields, handling of crop residues, tillage and irrigation systems, and fertilisation practices, is likely to remain scarce at larger scales. The newly developed regional mode for the CCB model allows for the use of available statistical information on these agricultural parameters as model input data. This is a significant advancement towards increasing the availability of tools for regional scale assessments. The results of this dissertation demonstrate that this approach can be applied to different spatial units, ranging from grid cells to large administrative regions, and will facilitate the application of regional SOM assessments. However, there is no one-size-fits-all approach for assessing SOM stocks and fluxes at larger scales. The complex feedback loops justify the use of several types of assessment. loops. The regional analysis of FOM fluxes to soils, as performed for the biogas system in chapter 2 of this thesis, can also provide valuable information for decision-makers. Overall, there are significantly fewer regional applications addressing SOM compared to other environmental objectives that are commonly assessed at a large scale, such as water quantity and quality. This is despite the fact that there is a clear link between the water retention capacity of a landscape and its SOM stocks.

5.2.3 Agricultural management options, potentials and recommendations for Saxony

Agriculture has a great potential to increase SOM stocks in arable soils by influencing carbon inputs and turnover through farm management decisions (Singh et al., 2018). This thesis contributes to a better understanding of the carbon sequestration potential of various agricultural practices for the case study Saxony, including conservation tillage, organic amendments, cover crops and field grass cultivation.

In particular, the results of the dissertation suggest that conservation tillage has been the primary factor contributing to the recent gains in SOC stocks of arable soils in Saxony (chapter 3). Furthermore, conservation tillage demonstrates a high potential for continued soil carbon sequestration until 2050 (chapter 4). These findings align with the positive effects of conservation tillage that have been studied and promoted for decades (Krauss et al., 2022), such as its ability to sequester carbon for many years (Ogle et al., 2019). Several funding programmes were established in Saxony at an early stage, including the agri-environmental programme ‘Umweltgerechte Landwirtschaft’, which began in 1993 (Sächsische Landesanstalt für Landwirtschaft, 2007), and the funding directive ‘Agrarumweltmaßnahmen und ökologische Waldmehrung –AuW/2007’, which started in 2007 (Hüttinger et al., 2014). Accordingly, conservation tillage has been widely adopted in Saxony, with two-thirds of farmers permanently applying it or using it for specific crops (Lülfs-Baden et al., 2020). Despite ongoing debates about its effects on deep soil layers (Krauss et al., 2022; Luo et al., 2010; Meurer et al., 2018), it is relevant to continue these practices to prevent the release of already stored carbon and nutrients. However, it is crucial to acknowledge the existing knowledge gaps and work towards filling them. Furthermore, conservation tillage provides additional co-benefits that are highly relevant for Saxony. The increased water infiltration and retention result in reduced erosion and nutrient losses. These benefits are likely to become increasingly important to protect Saxony’s fertile loess soils under changing climate conditions and to meet the Water Framework Directive targets. Existing trade-offs, such as those related to pest management, should be mitigated and create a need for unconventional pest control practices (Alletto et al., 2010; Jasrotia et al., 2023).

Changes in cultivated crops and their rotations were significant during the period considered in this dissertation, partly due to the inclusion of bioenergy production in the agricultural system. As a result, the composition of FOM sources in Saxony shifted, with maize, rapeseed and winter wheat increasing their contribution while other cereals such as barley and rye decreased (chapter 2). Overall, the thesis results indicate that the changes in cultivation patterns have led to a moderate increase in the total crop-based carbon flux into soil, which also contributed to the recent trends in SOC (chapter 3). The results also highlight the potential of field grasses to replace maize and barley as fodder crops, and cover crops by 2050. The current Saxon funding directive ‚Agrarumwelt- und Klimamaßnahmen - FRL AUK/2023‘ also acknowledges this fact by supporting the cultivation of legume-grass mixtures (Sächsisches Staatsministerium für Energie, Klimaschutz, Umwelt und Landwirtschaft, 2022). Crop rotation diversity often yields in distinctly higher SOM stocks (Tiefenbacher et al., 2021), but its potential for policy regulation is limited due to its susceptibility to market demands. Accordingly, efforts should also be made to develop and implement new crop varieties, including deep-rooting and perennial (grain) crops such as intermediate wheatgrass (Thinopyrum intermedium) (Crews & Cattani, 2018; Thorup-Kristensen et al., 2020), and to increase in-field diversity, for example through intercropping (Meena et al., 2020; Q. Wang et al., 2010). Structural elements, ranging from hedges and grassed waterways to agroforestry systems, could complement these efforts, providing a wide range of ecosystem functions in otherwise featureless agricultural landscapes (Follain et al., 2007; Simelton et al., 2021).

Organic amendments are a significant carbon source in agricultural systems, but also have an indirect effect on carbon sequestration by stimulating net primary production (Jacobs et al., 2020). The availability and use of organic fertiliser were found to be highly dynamic over the period studied in this dissertation, due to changes in livestock numbers and the rise of the biogas sector (chapter 2). The application of biogas digestate could offset the loss of livestock excrements and the increased cultivation of maize for silage in Saxony. While numerous studies emphasise the potential of organic amendments for carbon sequestration, it is important to note that merely relocating carbon sources does not necessarily result in an increase in global net carbon storage (Schlesinger & Amundson, 2019; Wiesmeier, Mayer, Burmeister, et al., 2020). Overall, the potential of organic amendments for Saxony remains uncertain and depends on the full life cycle of potential carbon sources, but also on other factors such as future dietary habits that affect livestock numbers and the availability of excreta.

One overarching concept that may be highly relevant for achieving carbon sequestration targets is carbon farming (Mattila et al., 2022; Paul et al., 2023; Sharma et al., 2021). At the European level, discussions are taking place on how to implement incentives for carbon farming, including the awarding of emission certificates for carbon sequestration and certifying products based on carbon farming (European Commission, 2020). This could enable farmers to generate economic benefits from increased SOC stocks. However, there are several limitations that raise discussions about the feasibility of this concept. One of the main challenges is the permanence of carbon sequestration, which cannot be guaranteed and therefore affects the long-term accountability of the carbon certificates (Paul et al., 2023; F. Wüstemann et al., 2024). Furthermore, potential leakage effect and difficulties in ensuring the additionality of the stored carbon, as well as a lack of long-term monitoring data, pose additional challenges (Thamo & Pannell, 2016; F. Wüstemann et al., 2024). Nevertheless, the potential contributions of carbon farming to climate change mitigation could be significant and it is important to conduct further studies before deciding on a strategy. One possible approach could be to focus on short-term removals of atmospheric carbon to prevent exceeding climatic tipping points (McDonald et al., 2023; Meyer-Ohlendorf et al., 2023; Paul et al., 2023).

In addition to the potential of specific measures and concepts for SOM enrichment, it is important to consider a systems and landscape perspective on land-use and management in Saxony. There has been a significant increase in the use of life cycle assessments to evaluate agricultural and food systems in peer-reviewed articles (Notarnicola et al., 2017). This emphasises the need for new conceptual frameworks to assess agricultural production (van der Werf et al., 2020). Such frameworks should have a broad and interdisciplinary perspective to include different kinds of environmental issues on a landscape perspective, as well as indirect effects beyond specific regions (Fehrenbach et al., 2022). In chapter 2 of this dissertation, a first step towards a systems perspective on the bioenergy production in Saxony has been made. However, food production systems and their associated supply chains have an intrinsic variability and complexity (Notarnicola et al., 2017). The methods developed in this thesis contribute to a tailoring of assessment methods and dedicated modelling approaches.

5.2.4 Limitations of this thesis and future research needs

This doctoral thesis analysed the dynamics of soil organic carbon and nitrogen in Saxony from a regional perspective and developed novel spatially-explicit approaches to do so. The studies carried out were accompanied by a number of methodological challenges related to the definition of system boundaries, data availability, process knowledge and model capabilities, as well as the complexity of drivers occurring at the regional scale. The following paragraphs discuss important assumptions and limitations associated with these challenges.

The definition of system boundaries is a necessary element in impact assessments, particularly when focusing on a specific case study (Tillman et al., 1994). This involves establishing the thematic and spatio-temporal framework for the assessment to be conducted. When studying a region that represents an administrative unit, such as Saxony, the geographical boundaries of the study are politically determined and address specific levels of decision-making. This reflects the potential effects of governance on agricultural management. However, the definition of the spatial framework is not driven by process understanding, which has led to specific thematic assumptions being made. For the analysis of the biogas production system in Saxony, only biogas plants that did not require additional substrate input from outside the study region were considered. Additionally, indirect land-use changes, such as those caused by fodder imports from outside the study region, could not be considered. However, Thrän et al. (2020) found no evidence to suggest that the expansion of the biogas system in Germany has resulted in indirect land use changes. The relatively small potential effect size of these factors is supported by statistics on the share of domestic fodder production in Germany, which remained at around 90% between 2000 and 2011 (Deutscher Bundestag, 2012). Similar limitations regarding the spatio-temporal framework apply to the scaling experiment of Chapter 4, which was designed to support decision-making on policy-based geographical units (NUTS) using commonly available data.

Data availability is a major limitation in many model-based environmental assessments. Within this thesis, this was particularly true for SOM monitoring data as well as certain agricultural management parameters. The limited availability of observation time series has an impact on the initialisation of regional SOC levels, as well as on the opportunities for model validation and, as a result, the reliability of model predictions (Dimassi et al., 2018; Foereid et al., 2012; Le Noë et al., 2023). Therefore, the validation of the newly developed regional mode for the CCB model was constrained to data from long-term field experiments of the CCB validation database (Franko et al., 2011). With regard to the agricultural parameters, several simplifications and estimates were necessary, although the information used represented the most accurate data available to the regional authorities. These data limitations include statistical information on crop yields and fertilisation schemes (Förster, 2013), as well as assumptions regarding the removal of by-products such as straw. All of these simplifications contribute to increased projection uncertainty and restrict the analysis of single pixels in the simulations based on the 500m grid. As data on such agricultural parameters are likely to remain scarce, further research is required to determine the optimal methodology for parameterising an agricultural system at a regional scale for carbon sequestration assessments.

The scale of model use is also an important factor in model selection, as SOM models can have different scales of the model hypotheses, which impose different types of limitations (Campbell & Paustian, 2015; Manzoni & Porporato, 2009). CCB was designed to function with limited input data, while considering all relevant site conditions that influence SOC stocks (Schwengbeck et al., 2023). This renders it an appropriate tool for regional assessments. Nevertheless, several simplifications in CCB constrain its capabilities. These include the single soil layer design, which focuses on the topsoil (30 cm). Moreover, CCB does not allow for the simulation of crop yields, which could be a potential means of at least partially compensating for the limitations in the spatial resolution of crop share statistics. Finally, the regional mode of CCB does not consider any spatial fluxes of soil carbon, such as those related to soil erosion. It is evident that soil erosion has the potential to redistribute a considerable amount SOC in agricultural landscapes (Chappell et al., 2016; Kirkels et al., 2014; Ritchie et al., 2007). While the majority of SOM models exhibit limitations in their spatial framework, this is typically a strength of eco-hydrological models. Such models, including the Soil and Water Assessment Tool SWAT+ (Bieger et al., 2017), are simulating water, nutrient and sediment fluxes in the landscape as well as crop yields, but still have limitations in their representation of the SOC cycle.

The capabilities of models, though, go hand in hand with the extent of process knowledge, which is often incomplete, for instance with regard to deeper soil layers (Gross & Harrison, 2019). Deep SOC cycles on longer timescales and its responses to changes in management and climate are likely to be different from surface SOC, yet remain poorly studied (Pries et al., 2023). For this reason, the carbon sequestration effectiveness of the alternative management practices studied in this thesis cannot be extrapolated to the entire soil profile. While the effects on the topsoil could be simulated with CCB, the deep soil layers could not be investigated, which is particularly controversial in the case of conservation tillage (Baker et al., 2007; Haddaway et al., 2017). In general, only a limited number of management practices and other drivers could have been studied in this thesis. The majority of these practices align with those commonly studied in the literature, including tillage, fertilisation, residue management and cover crops (Beillouin et al., 2022). Other measures, such as crop rotation, agroforestry, deep-rooted annual crops or perennial grain crops, warrant further investigation and should be the focus of future studies.

The diversity, complexity and interconnectedness of the drivers of SOM dynamics in agricultural landscapes are large, including climate, policy and market, farm- and land management practices, and soil properties (Franko & Witing, 2020). This dissertation has addressed this complexity from different perspectives and by using novel methodological approaches. A clear market perspective, nevertheless, is lacking, both from a historical and a future point of view. While an improved consideration of the market perspective could assist in the assessment of future developments of other interrelated drivers, its historical evolution has strongly influenced the current SOM status in a given land-use system. It is recommended that future studies enhance the market perspective by linking food and land system research, which would involve consideration of the food value chain (Meyer et al., 2023). Furthermore, the market perspective could be integrated by employing agent-based modelling approaches to simulate farmers' decisions and reasonable pathways towards improved SOM management (Marvuglia et al., 2022; Ravaioli et al., 2023).

5.3 Final conclusions

The Earth's carbon cycle is an essential aspect of all ecosystems and is of fundamental importance for sustainable development. This thesis has shown that a sound management of the world's largest terrestrial carbon reservoir, namely soil organic carbon, requires integrated approaches that consider a multitude of drivers operating at diverse scales. Comprehensive approaches to SOM management can yield a multitude of benefits, including the preservation of soil fertility, climate regulation, soil biodiversity support, compound retention for water quality improvements and erosion control. However, the challenges to develop sustainable

SOM management practices for arable land are substantial. This thesis has contributed to the clarification and quantification of significant carbon and matter fluxes in agricultural systems, and provided novel tools and approaches to assess the impact of climate and best management practices on SOM at different scales.

It has been shown that biogas plants in the case study region Saxony can be operated sustainably in terms of SOC recycling, but this is highly dependent on the application of digestate and accompanied by considerable land requirements. The newly developed 'regional mode' of the CCB model demonstrated its ability to simulate regional trends in soil organic carbon stocks and associated nitrogen fluxes using aggregated agricultural management data on gridded modelling units. This is an overarching requirement for operationalising SOM assessments for policy support. The new capabilities of CCB have been applied to simulate SOC dynamics at the scale of administrative units, showing that this approach can provide feasible results with an acceptable scaling error. For the case study region Saxony, it has been revealed that regional SOM stocks increased for large parts of the arable land between 1998 and 2014, but with marked regional differences and largely driven by the increased use of conservation tillage. Along with the increase in SOC, a significant amount of nitrogen was immobilised. Field grass, cover crops, and conservation tillage have shown great potential for future carbon sequestration in Saxon arable soils.

Uncertainties and limitations of regional assessments remain large, yet this thesis has made a valuable contribution to enhancing capacity and providing specific recommendations on how to improve SOM management and assessment for the case study region of Saxony and beyond. In order to further strengthen the evidence base, future studies should incorporate a greater number of measures that can be classified as frontier technologies, incorporate spatial fluxes of SOM in the landscape, include additional drivers such as an improved market perspective, and establish an appropriate long-term monitoring of SOM stocks to improve opportunities for validation of regional assessments.

6. Appendix

6.1 Supplementary material - tables

Table A1: Characterisation of the agro-economic regions of Saxony.

	Heath & Pond Landscape	Loess Region	Low Mountain Range & Foreland
Temperature[1] [°C]	9.6	9.3	7.8
Precipitation[1] [mm]	736	770	961
Clay content[2] [%]	4.4	9.5	13.8
Silt content[2] [%]	22.8	65.3	58.2
Stone content[2] [%]	10.4	7.4	16.2
Arable land [%]	31.9	52.5	28.4
Grassland & pasture [%]	8.1	9.8	16.7
Conservation tillage 2000/2012 [%]	13.3 / 26.5	14.5 / 34.3	14.9 / 52.1
Cover crops[3] [%]	4.5	4.0	4.6

[1] Average annual values of the period 1990-2014,

[2] Average values across all soil types of agricultural land (topsoil),

[3] Average values of the period 2000-2012

Table A2: Descriptive summary of the data aggregation procedure for upscaling a grid-based set-up of the CCB model to the level of administrative units.

Type of dataset	**Scale of model set-up**	
	Grid-based (500m)	**Administrative units**
Soils	One soil type for each grid cell.	The area shares of the soil types within an administrative unit were aggregated and used as a property of the administrative unit. Subsequently, each soil type within one administrative unit was parameterised as an own CCB modelling unit (without spatial reference).
Climate	One time series dataset for temperature and precipitation (annual values) for each grid cell.	One time series dataset for temperature and precipitation (annual values) for each administrative unit, based on the area-weighted mean of the grid-based datasets within one administrative unit.
Crop types	One dataset for the crop types cultivated and their area share (annual values) for each grid cell.	One dataset for the crop types cultivated and their area share (annual values) for each administrative unit, based on the area-weighted mean of the grid-based datasets within one administrative unit.
Crop yields	One dataset on crop yields (annual values; crop type specific) for each grid cell.	One dataset on crop yields (annual values; crop type specific) for each administrative unit, based on the area-weighted mean of the grid-based datasets within one administrative unit.
Management of crop by-products	One dataset on the removal rate of crop-by products (annual values; crop type specific) for each grid cell.	One dataset on the removal rate of crop-by products (annual values; crop type specific) for each administrative unit, based on the area-weighted mean of the grid-based datasets within one administrative unit.
Fertiliser	One dataset on fertiliser application rates (annual values; fertiliser type specific) and the area share of their application for each grid cell.	One dataset on fertiliser application rates (annual values; fertiliser type specific) and the area share of their application for each administrative unit, based on the area-weighted mean of the grid-based datasets within one administrative unit.
Soil management	One dataset on the share of tillage systems (annual values) for each grid cell.	One dataset on the share of tillage systems (annual values) for each administrative unit, based on the area-weighted mean of the grid-based datasets within one administrative unit.
Initial SOC	Grid-specific initial SOC according to the approach of Drexler et al. (2020) and the soil type and climate of the grid cell.	Administrative unit- and soil-specific initial SOC according to the approach of Drexler et al. (2020) and the soil types and climate of the administrative unit.

6.2 Supplementary material - figures

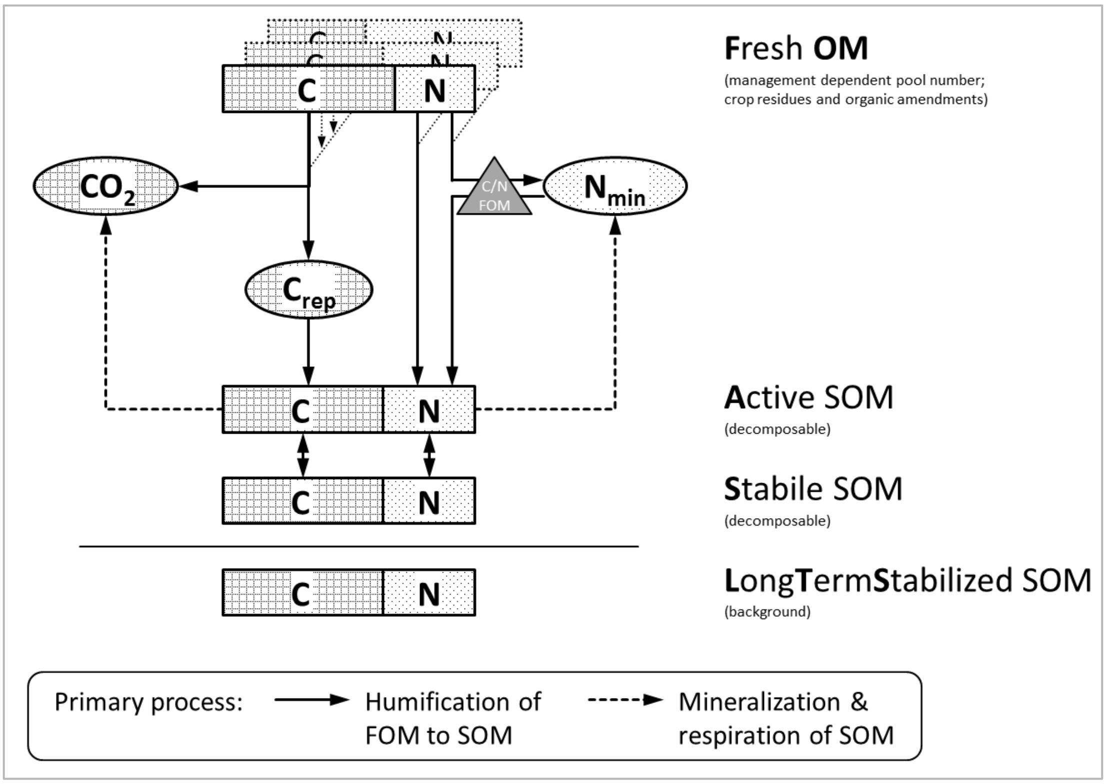


Figure A1: Simplified overview of pools (blocks) and fluxes (arrows) of the CCB model. C_{rep}: carbon reproduction flux from fresh organic matter (FOM) to soil organic matter (SOM). CO_2: release of carbon dioxide. LTS-SOM: long-term stabilised soil organic matter with no turnover during simulation time. Nitrogen fluxes: depending on the C:N ratios of the different FOM and SOM pools additional nitrogen is immobilised from or mobilised into the external pool of mineral nitrogen (N_{min}) during the humification of FOM (modified from (Franko et al., 2011)).

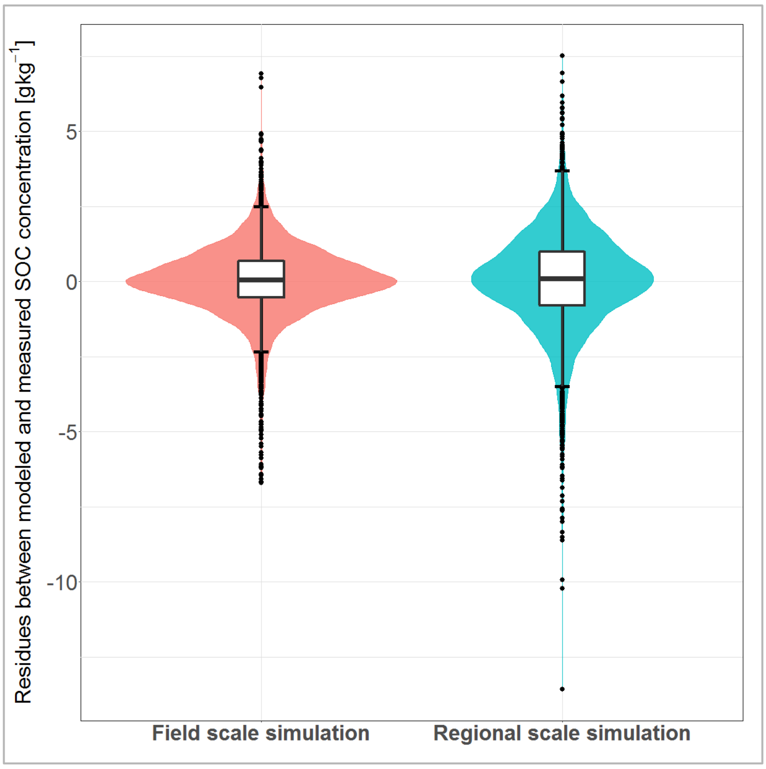


Figure A2: Comparing the residues between simulated (CCB model) and measured SOC concentrations for 4,794 measurements of SOC in 40 different locations in Europe. Left: Simulation of SOC dynamics on the scale of experimental treatments. Right: Simulation of SOC dynamics aggregated to the scale of the experimental location – here, the agricultural management of 391 treatments with different management was aggregated to 40 locations homogeneous in soil and climatic conditions.

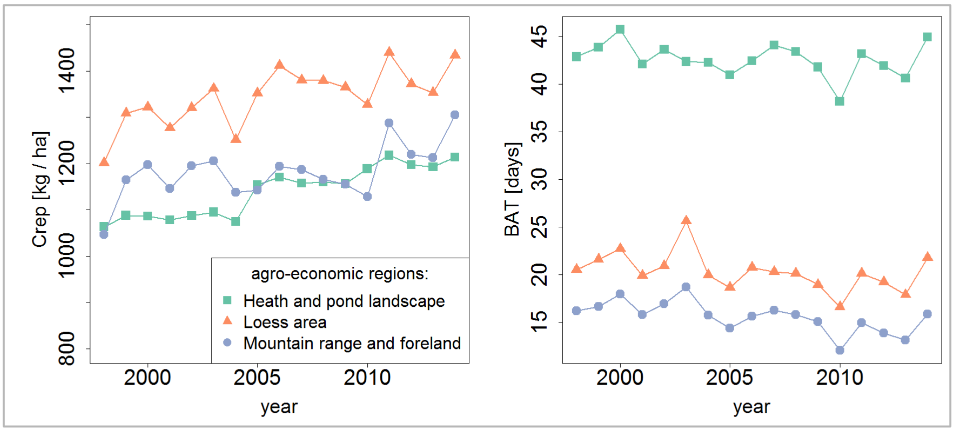


Figure A3: Annual dynamics in carbon input (left; expressed as C_{rep}) and turnover (right; expressed as BAT). C_{rep} aggregates all sources of FOM while considering their quality for the formation of new SOC. BAT aggregates turnover conditions with respect to soil physical parameters, tillage system, annual precipitation and air temperature. During the simulation period, there were several years that had particular effects on regional SOC dynamics. The years 2000, 2007 and 2014 have been outstandingly warm years, while the year 2010 has been a particularly cold one. With regard to precipitation, the year 2003 has to be highlighted as a notably dry year. The years 2002 and 2010 have been the wettest.

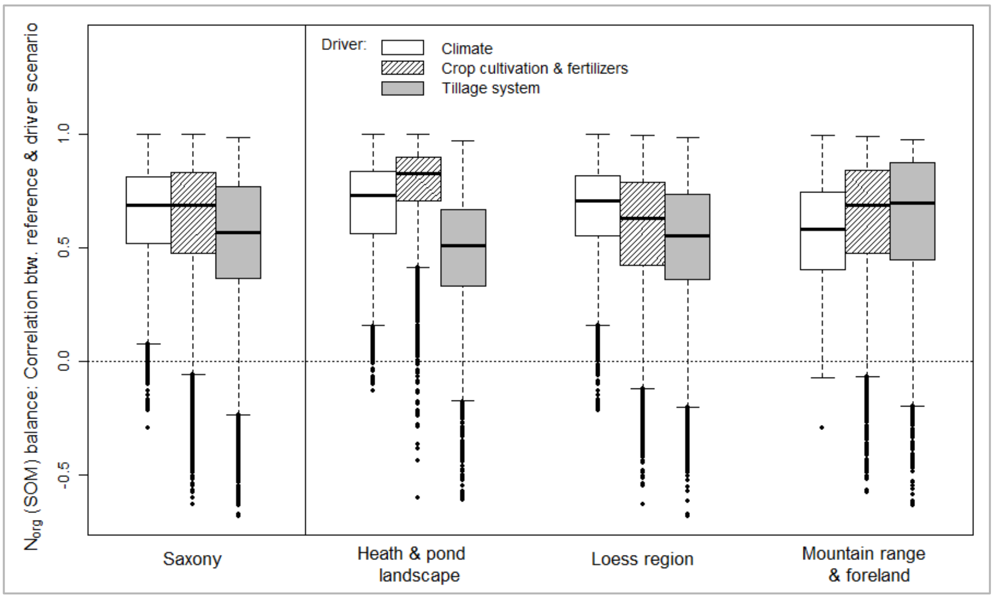
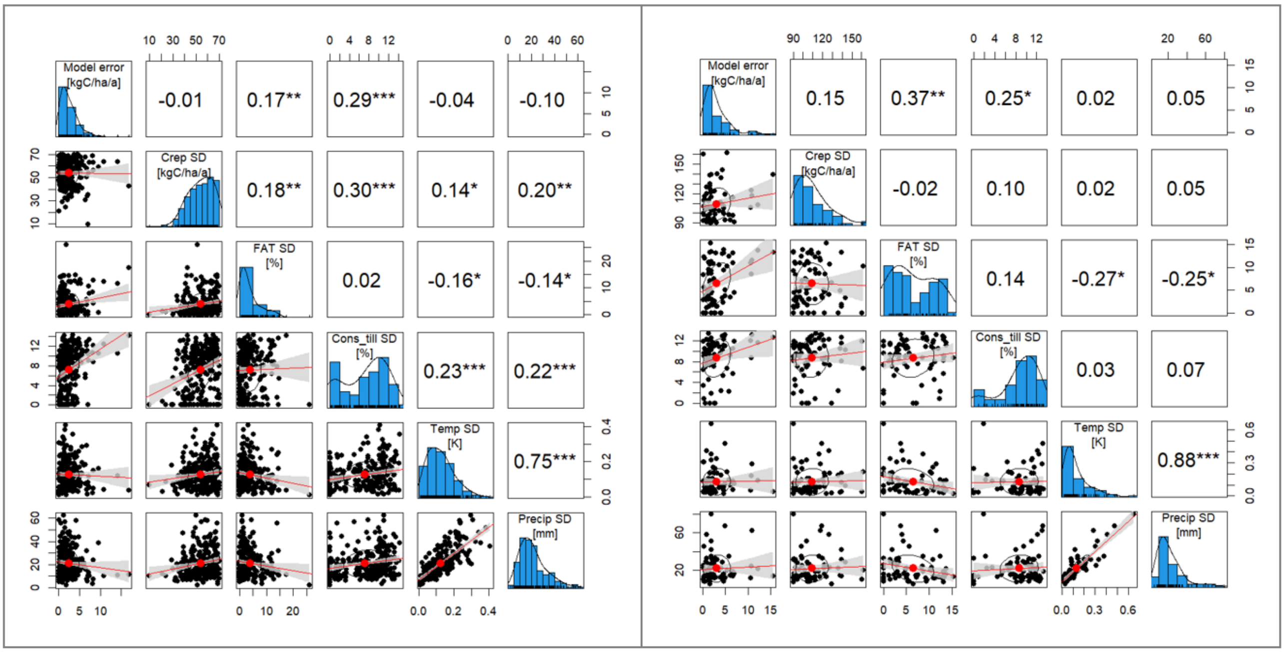


Figure A4: Analysing the effects of the three main drivers on the annual balance of organic nitrogen stored in SOM. Pearson's correlation between the reference simulation and the model runs focusing on individual drivers was calculated for every grid cell.



(a) **(b)**

Figure A5: Correlation matrices between the absolute errors of the LAU-level model set-up and the spatial dispersion (standard deviation) of a set of predictor variables. (a) Correlation matrix for a subset of LAU regions that show a low variability in the carbon influx to SOC (C_{rep}); (b) Correlation matrix for a subset of LAU regions that show a high variability in the carbon influx to SOC (C_{rep}). The predictors of the matrices are the soil carbon reproduction flux (C_{rep}), the soil fine particle content (FAT), conservation tillage shares (Cons_till), annual mean temperature (Temp) and annual precipitation (Precip). For each predictor its regional dispersion (standard deviation - SD) within an administrative unit has been calculated from the reference dataset and used for the correlation matrices. The distribution of each variable is shown on the diagonal. Below this diagonal the bivariate scatter plots with a fitted line are displayed. Above the diagonal the value of the correlation is shown as well as its significance level (stars), where the p-values <0.001, <0.01 are associated to the symbols *** and ** respectively.

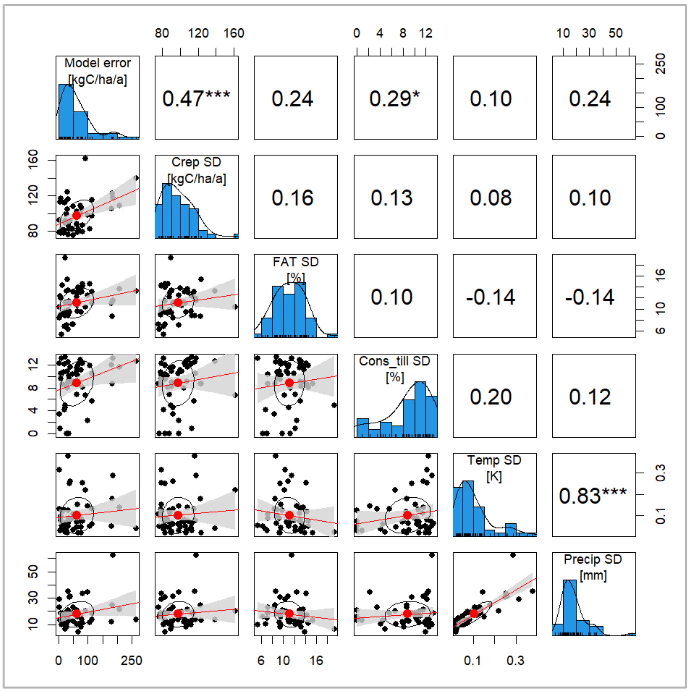
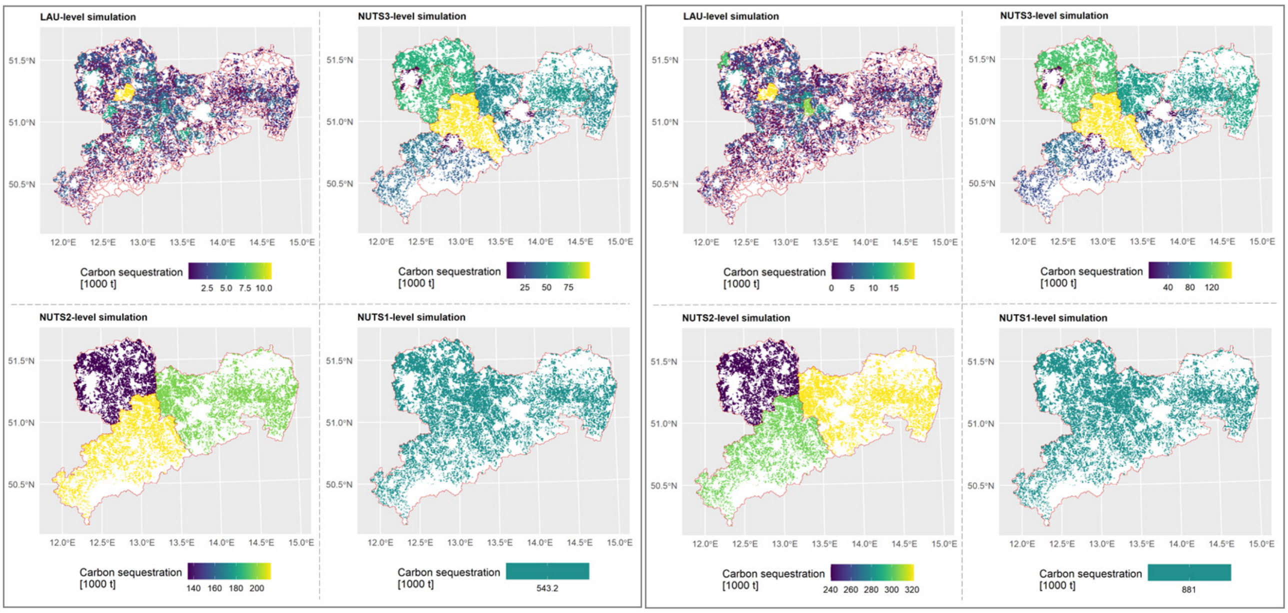


Figure A6: Correlation matrix between the absolute errors of the LAU-level model set-up and the spatial dispersion (standard deviation) of a set of predictor variables. The correlation matrix only considers a subset of LAU regions that show a high variability in carbon turnover conditions (BAT) as well as a high variability in the carbon influx to SOC (C_{rep}). The predictors of the matrix are the soil carbon reproduction flux (C_{rep}), the soil fine particle content (FAT), conservation tillage shares (Cons_till), annual mean temperature (Temp) and annual precipitation (Precip). For each predictor its regional dispersion (standard deviation - SD) within an administrative unit has been calculated from the reference dataset and used for the correlation matrices.



(a) **(b)**

Figure A7: Soil carbon sequestration potential of two alternative management practices simulated with four different levels of data aggregation for the arable soils of the case study Saxony (NUTS1 region in Germany). The simulations were done using upscaled model set-ups on the level of administrative units (NUTS1, NUTS2, NUTS3, LAU). White areas represent non-arable land. (a) Carbon sequestration potential of the first alternative management practice (increasing soil carbon influx based on increased cultivation of field grass and cover crops). (b) Carbon sequestration potential of the second alternative management practice (reducing carbon turnover conditions by increasing the use of conservation tillage). ©EuroGeographics for the administrative boundaries.

6.3 Supplementary material - explanations

Explanation A1: Initialisation of SOC-levels

Initialisation of SOC stocks is a crucial step of SOC modelling and accompanied by high uncertainties. SOC stocks need very long time periods to reach a steady state and changes in land-use, management and climate do always change theoretical steady state levels and associated SOC dynamics. Also, the initial distribution of the total SOC over the different model pools can significantly affect the modelled predictions.

In a recent publication Drexler et al. (2020) provided an extensive analysis of the soil organic carbon contents of the agricultural soils of Germany. The analysis was based on C_{org} measurements on 2,973 sites and resulted in a classification scheme of the site-typical SOC content of the German agricultural soils. Based on information of the land use, soil texture, C:N ratio and annual precipitation of a site it is thus possible to derive site-typical C_{org} values for Germany. We applied this classification scheme to the arable soils of Saxony for setting the initial SOC contents in our CCB model set-ups. Thus, we derived for each soil type in each spatial modelling unit one specific initial SOC, using the C_{org} modal value provided Drexler et al. (2020). The table below shows the distribution of the classes for soil texture and annual precipitation in Saxony based on the classification system of Drexler et al. (2020). The majority of the soils in Saxony are in the soil texture class ‘medium 1’, followed by ‘light’ (sandy) soils. The average initial C_{org} value across all grid-cells simulated in this study was 1.35%.

The distribution of the 29,331 grid-cells of the CCB reference model within the classification system of Drexler et al. (2020) is shown below, considering only soil texture and annual precipitation classes.

	≤700mm	>700mm	≤850mm	>850mm	≤1000mm	>1000mm	≤900mm	Total
light	1,589	4,045						5,634
medium 1			13,573	7,208				20,781
medium 2					2,005	839		2,844
heavy 2							72	72

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8. Lists of figures and tables

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Declaration

Eidesstattliche Erklärung / Declaration under Oath

Ich erkläre an Eides statt, dass ich die Arbeit selbstständig und ohne fremde Hilfe verfasst, keine anderen als die von mir angegebenen Quellen und Hilfsmittel benutzt und die den benutzten Werken wörtlich oder inhaltlich entnommenen Stellen als solche kenntlich gemacht habe.

I declare under penalty of perjury that this thesis is my own work entirely and has been written without any help from other people. I used only the sources mentioned and included all the citations correctly both in word or content.

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2010 - 2011	Research assistant at the UFZ* Department Computational Landscape Ecology
2009	Internship at the UFZ* Department Computational Landscape Ecology
2008 - 2009	Tutor in data processing and geoinformatics at TU Dresden
2007 - 2008	Internship at Horticulture and Food Research Institute of New Zealand Ltd, HortResearch Palmerston North (now Plant & Food Research) at the Department for Sustainable Land Use
2003 - 2011	Student of Geography (Diploma) at the Dresden University of Technology with an academic emphasis on geographical information systems and the minor subjects biology, soil science and meteorology. Participation in the FLOODmaster study program and the supplementary study "Regional Studies of Latin America" (BELA)

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