Assessing the Quality of Organic Amendments in Terms of Their Carbon-, Nitrogen & Phosphorus-Dynamics on Arable Soil

Dissertation
zur Erlangung des
Doktorgrades der Naturwissenschaften (Dr. rer. nat.)

der

Naturwissenschaftlichen Fakultät III

Agrar- und Ernährungswissenschaften, Geowissenschaften und Informatik

der Martin-Luther-Universität Halle-Wittenberg

vorgelegt von

Herrn Gasser, Stefan Anton Albert

Date of Defense: 29.04.2024

Referee 1: Prof. Dr. Martin Volk

Referee 2: Associated Prof. Dr. Katharina Meurer

Abstract

Human activity and, increasingly, the impacts of climate change set soils and their functions under great pressure. On the one hand, high yields are to be achieved on agricultural land, but on the other hand, soils fulfill a multitude of ecosystem services, which should not be regarded as a contradiction to maximizing yields, but rather must be brought into accordance with them. This can be achieved by using matter and nutrients from the same or a linked system in order to close material cycles. On arable soils, organic substrates such as manure, digestates, compost and also the crop residues are reintegrated into the soil cycle. These substrates consist of a variety of different components, which leads to a diverse behavior of these substrates and their components on soils and brings with it a wide variety of fertilization properties. However, these dynamics and the behavior of the interlinked soil cycles are often unclear. This thesis contributes to a better understanding of the carbon (C), nitrogen (N), and phosphorus (P) cycles on arable soils and develops methods to evaluate organic (org.) amendments and to model their dynamics on arable soils. For the quality assessment of org. amendments, the mineralization dynamics of incubation experiments, in which the CO_2 release is measured over time, are investigated using mechanistic C landscape models. From this, a quality parameter can be derived, which provides information about the contribution of an organic amendment to the build-up of humus. Besides the derivation of a quality parameter, the obtained turnover parameters can be used to determine the dynamics of C, N, and P on arable soils. Thus, various org. amendments from laboratory experiments can be parameterized to be subsequently transferred to the field scale. Here, not only the external input of organic material plays a role, but also the residues produced in the field, which are returned to the nutrient cycle. In addition to the quality of these residues, the quantity also has an influence and must be taken into account accordingly. The present work provides methods for this and shows approaches to parameterizing org. residues. Further, the P cycle is introduced into the CCB model structure and established as new

CNP-model. The P-module is closely coupled with the C cycle, but further mineral P matter fluxes have also been integrated into the model concept. Thus, another macronutrient for plants and its dynamics on arable soils can be studied, and a more comprehensive picture of the dynamics of org. substrates on arable soils can be generated. Here, the C cycle plays a crucial role in the dynamics of plant-available P in soils. The soil cycles of the elements C, N, and P are directly interconnected and mutually dependent. Individual cycles cannot be adequately considered separately; to analyze the behavior of individual elements, their interactions must also be considered. These interactions can be captured to a certain extent using model approaches. The methods and approaches developed here can be used, on the one hand, to evaluate org. substrates with respect to their humus-building quality, but also further to parameterize the CNP-model in order to successfully simulate C, N, and P dynamics in arable soils. Based on these results, different stakeholders can derive and develop management options to improve soil fertility and secure yields under the influence of climate change. Furthermore, the results can help to predict the long-term effects of organic fertilizers in order to create predictable developments towards more sustainable and productive agricultural systems.

Zusammenfassung

Durch menschliches Handeln und verstärkt durch den Klimawandel stehen Böden in ihren Funktionen unter großem Druck. Auf der einen Seite sollen auf landwirtschaftlichen Flächen hohe Erträge erzielt werden, doch darüber hinaus erfüllen Böden eine Vielzahl von Ökosystemleistungen, welche nicht als Widerspruch zur Ertragsmaximierung betrachtet werden sollten, sondern vielmehr damit in Einklang gebracht werden müssen. Hierzu können Kreislaufwirtschaften dienen, bei welchen Stoffe und Nährstoffe aus dem gleichen oder einem verketteten System verwendet werden, um Stoffkreisläufe zu schließen. Auf Agrarflächen kommen unter anderem organische Substrate wie Stallmiste, Gärreste und Komposte zum Einsatz, aber auch die auf dem Feld anfallenden Residuen werden wieder in den Bodenkreislauf integriert. Diese Substrate bestehen aus einer Vielzahl unterschiedlicher Bestandteile, was zu einem diversen Verhalten dieser Substrate und deren Bestandteile auf Böden führt und verschiedenste Düngeeigenschaften mit sich bringt. Doch diese Dynamiken und das Verhalten der verketteten Bodenkreisläufe sind oft unklar. Diese Thesis trägt dazu bei, ein besseres Verständnis für die C, N und P Kreisläufe auf Ackerflächen zu gewinnen und erarbeitet Methoden, um org. Reststoffe zu bewerten und deren Dynamiken auf Ackerflächen zu modellieren. Für die Qualitätsbewertung von org. Reststoffen werden die Mineralisationsdynamiken von Inkubationsversuchen, bei welchen die CO_2 Freisetzung über die Zeit gemessen wird, mithilfe mechanistischer C-Landschaftsmodelle untersucht. Hieraus kann ein Qualitätsparameter abgeleitet werden, welcher Auskunft über den Beitrag eines org. Reststoffes zum Aufbau von Humus gibt. Neben der Ableitung eines Qualitätsparameters können die gewonnenen Mineralisationsparameter dazu benutzt werden, die Dynamiken von C, N und P auf Ackerflächen zu bestimmen. Somit können verschiedenste org. Reststoffe aus Laborversuchen parametrisiert werden, um anschließend auf die Feldskala übertragen zu werden. Hierbei spielt nicht nur der externe Input von org. Material eine Rolle, sondern auch die auf dem Feld anfallenden Residuen, welche

wieder in den Nährstoffkreislauf zurückgeführt werden. Neben der Qualität dieser Residuen hat auch die anfallende Menge einen Einfluss und muss demensprechend berücksichtigt werden. Die vorliegende Arbeit liefert hierfür Methoden und zeigt Ansätze auf, wie sich org. Reststoffe parametrisieren lassen. Weiterführend wird der P-Kreislauf in die Modellstruktur und Modellrechnungen eingeführt, das CCB Model wird um ein P-Modul erweitert und als CNP-Modell etabliert. Das P-Modul ist eng an den C-Kreislauf gekoppelt, wobei auch mineralische Stoffflüsse integriert wurden. Somit kann ein weiterer Makronährstoff für Pflanzen und dessen Dynamiken auf Ackerflächen untersucht, sowie ein vollständigeres Bild von den Dynamiken org. Substrate auf Ackerflächen erzeugt werden. Hierbei spielt der C-Kreislauf eine entscheidende Rolle für die Dynamiken von pflanzenverfügbarem P in Böden. Die Bodenkreisläufe der Elemente C, N und P sind unmittelbar miteinander verbunden und bedingen sich wechselseitig. Einzelne Kreisläufe können nur unzureichend alleinstehend betrachtet werden; um das Verhalten einzelner Elemente zu analysieren, müssen auch ihre Wechselwirkungen mit in Betracht gezogen werden. Diese Wechselwirkungen können bis zu einem gewissen Grad mit Modellansätzen erfasst werden. Die hier entwickelten Methoden und Ansätze können zum einen dazu dienen, org. Substrate hinsichtlich ihrer Humusaufbauqualität zu bewerten, aber auch weiterführend, um das CNP-Modell zu parametrisieren um damit erfolgreich die C-, N- und P-Dynamiken auf Ackerböden zu simulieren. Hiermit können der aktuelle Zustand der Böden und deren Stoffflüsse bestimmt werden. Hieraus können wiederum unterschiedliche Akteure Handlungsoptionen ableiten und Managementoptionen entwickeln, die dazu beitragen, die Bodenfruchtbarkeit zu verbessern und Erträge unter dem Einfluss des Klimawandels zu sichern. Weiterführend können die Resultate dazu beitragen, die Langzeitwirkung von organischen Düngern vorherzusagen, um so planbare Entwicklungen hin zu nachhaltigeren und produktiven Agrarsystemen zu schaffen.

List of Publications

The following publications are part of this cumulative thesis:

Chapter II: Gasser, S. A. A., Diel, J., Nielsen, K., Mewes, P., Engels, C., & Franko, U. (2021). A model ensemble approach to determine the humus building efficiency of organic amendments in incubation experiments. *Soil Use and Management.* doi:10.1111/sum.12699 (published)

Chapter III: Gasser, S. A. A., Nielsen, K., & Franko, U. (2022). Transfer of carbon incubation parameters to model the SOC and SO dynamics of a field trial with energy crops applying digestates as organic fertilizers. *Soil Use and Management.* doi:10.1111/sum.12810 (published)

Chapter IV: Gasser, S. A. A., Nielsen, K., Eichler-Löbermann, B., Armbruster, M., Merbach, I., & Franko, U. (2023). Simulating the soil phosphorus dynamics of four long-term field experiments with a novel phosphorus model. *Soil Use and Management.* doi:10.1111/sum.12881 (published)

Author Contributions Summary

Gasser et al. (2021), Chapter II: AG designed and conducted the research, developed the model averaging and wrote the manuscript. KN, CE, PM, conducted the experiments and provided the data, UF and JD assisted with the model implementation, UF assisted with the development of the research idea and revised the manuscript.

Gasser et al. (2022), Chapter III: AG developed the research idea, designed and conducted the research and wrote the manuscript. KN conducted the experiments, provided the data and contributed formulating the corresponding sections. UF contributed formulating the corresponding sections and revised the manuscript.

Gasser et al. (2023), Chapter IV: AG developed the research idea, designed and conducted the research and wrote the manuscript. KE-L, MA, and IM conducted the experiments, provided the data and helped formulating the corresponding sections. UF contributed to the model development and implementation and revised the manuscript.

Danksagung

Auf dem Weg zur Fertigstellung dieser Arbeit ist einiges an Zeit ins Land gegangen und viel Kaffee die Kehle hinuntergeflossen. Während dieses Prozesses hatte ich das Glück, von einer Vielzahl von Menschen unterstützt und begleitet zu werden, ohne welche ich nicht an diesen Punkt gekommen wäre. Ihnen allen gebührt mein Dank, doch einige lobende Erwähnungen möchte ich dennoch aussprechen.

Die Arbeit ist im Rahmen des vom FNR geförderten Verbundprojekts HUMOR: „Bewertung der Humus und Nährstoffwirkung von organischen Reststoffen“ entstanden (FKZ: 22410718). In diesem Zusammenhang möchte ich den Projektpartner*innen für den wissenschaftlichen Austausch und die Kooperation danken. Besonders Kerstin Nielsen für die gute wissenschaftliche Zusammenarbeit und dem zur Verfügung stellen von Daten. Des Weiteren gebührt mein Dank Ines Merbach, ebenfalls für die wissenschaftliche Zusammenarbeit, sowie bei der Unterstützung bei der Probennahme auf dem Dauerfeldversuch in Bad Lauchstädt.

Weiterhin möchte ich den Mitarbeitenden des UFZ und des Departments BOSYS für die gemeinsame Zeit in Halle danken. Hierbei besonders Julius Diel für die Zusammenarbeit, das Ausdiskutieren von Ideen und die gemeinsame Zeit im Büro, auch wenn ich nicht allzu oft dort war. Darüber hinaus möchte ich Martin Volk für die große Bereitschaft danken, mir trotz begrenzter Zeit, immer mit Rat und Tat zur Seite zu stehen.

Meinen aufrichtigen Dank möchte ich Uwe Franko aussprechen, der mich zum einen an die mechanistische Modellierung herangeführt und mir geholfen hat, meine Kompetenzen in diesem Bereich auszubauen. Zum anderen auch dafür, meine Arbeit auch während des wohlverdienten Ruhestands als Mentor, Kollege und Freund unterstützt zu haben.

Des Weiteren möchte ich meinen Eltern für die Unterstützung während der Jahre meines Studiums und der Promotion danken. Sie haben mich stets unterstützt und mir ermöglicht meine Ziele zu verfolgen. Außerdem danke ich meinen lieben Mitbewohner*innen, Johanna, Moritz und Marie fürs Begleiten in guten und schlechten Zeit während der letzten Jahre. Da ich dem Winter in Deutschland nichts abgewinnen kann möchte ich Oli für die tolle Zeit in der winterlichen Schreibwerkstatt und die inspirierenden Gespräche danken. Es war eine willkommene Abwechslung zum tristen Winter. Ich danke außerdem Samira für das Korrekturlesen der Paper auf Englisch und das Verbessern meiner sich wohl immer wiederholenden Grammatik-und Kommafehler. Abschließend gebührt mein herzlichster Dank, Renée für die aufmunternde Unterstützung in der Endphase des Schreibprozesses, ohne welche ich die Arbeit in dieser Form wohl nicht vollendet hätte.

Große Wertschätzung gebührt meinem Opa, der sich zwar in seiner materiellen Form wieder den globalen Kreisläufen angeschlossen hat, aber für mich einen emotional wichtigen Ankerpunkt im Leben darstellt und mich in meinem Sein geprägt hat. Ich widme ihm daher diese Arbeit.

Table of Content

List of Figures

List of tables

List of abbreviations:

A-SOM: active soil organic matter (CCB/CNP-pool)

Al: aluminum

AOM: added organic matter

BAT: biological active time

C: carbon

C-Tool: a model for estimating carbon stock changes in soils

CAN: calcium ammonium nitrate

CCB: CANDY Carbon Balance

CENTURY: a model for estimating carbon stock changes in soils

CO_2: carbon dioxide

Corg: organic carbon

CRL: control treatment

DG: digestates e.g. from biogas plants

d: day

dm: dry matter

E_{HUM}: humus building efficiency

$\overline{E_{HUM}}$: ensemble humus building efficiency

Fe: iron

FOM: fresh organic matter

FYM: farmyard manure

ha: hectare

ICBM: Introductory Carbon Balance Model

LTE: long-term field experiments

LTS-SOM: long-term stabilized soil organic matter (CCB/CNP-pool)

N: nitrogen

NaOH: sodium hydroxide

N_{min}: mineral nitrogen

Nt: total nitrogen

MIN: mineral fertilization

MSE: mean squared error

OM: organic matter

org.: organic

P: phosphorus

P_2O_5: phosphate

P-CAL: phosphorus extracted with calcium acetate lactate method

P-DL: phosphorus extracted with double lactate method

P_{av}: plant available phosphorus

pH: power of hydrogen (in soil solution)

P_{na}: plant non available phosphorus

P_t: total phosphorus

RMSE: root mean squared error

RothC: Rothamsted Carbon Model

S-SOM: stabilized soil organic matter (CCB/CNP Pool)

sd: standard deviation

SLY: slurry

SOC: soil organic carbon

SOM: soil organic matter

SON: soil organic nitrogen

Yasso: a model for estimating carbon stock changes in soils

I. General Introduction

I.1.1 Arable Soils & Organic Amendments

Soils pervade important ecological and economical functions. They are used for agricultural production, serve as a filter in the water cycle, and are the basis of human activities. But today's terrestrial soil systems are under substantial civilizational and ecological pressure (Rillig et al., 2019). Changes in climate will enforce a lot of soil disruptive processes, but since not all regions will be affected with equal intensity, strategies to mitigate climate change effects have to be adapted to site-specific conditions and landforms. Soils supply a huge variety of ecosystem services, which have to be preserved and promoted to mitigate both climate change effects and secure food production (Kopittke et al., 2019). Soil degradation is a major threat to many arable soils, often caused by depleting levels of soil organic carbon (SOC) and the linked loss of soil stability, soil fertility and biodiversity which jeopardizes the sustainability of soil management and food security (Cerecetto et al., 2021). In the past decades, yields have nearly doubled due to mineral fertilizers while SOC levels have decreased. However, organic amendments provide a promising alternative to mineral fertilizers generating similar yields while increasing SOC (Bonanomi et al., 2020). Organic amendments accumulate in production chains and can be reintegrated into the nutrient cycle of soils. This can help to create circular economies and develop production methods that can ensure food security in a more sustainable way, as envisaged by stakeholders such as the EU (Ragossnig et al., 2019). Furthermore, the use of organic amendments leads to the input of plant nutrients, which ensure high yields. Additionally, organic amendments contribute to increasing soil fertility, for instance by improving soil structure, which makes soils less susceptible to drought and increases the water use efficiency (Iizumi et al., 2019). Moreover, organic amendments contribute to increasing microbial and macrobial activity, which in turn promotes the release of nutrients.

There is a large variety of organic residual materials, which are derived from different production chains and can therefore differ greatly in their properties. In agricultural production, additionally to the main products, by-products accrue, which are not the primary goal of cultivation. These by-products are generally parts of the crop which cannot be eaten like straw, leaves, herbage seed pods, etc. Those by-products can be used in a variety of ways, they can be directly incorporated back into the soil to act as organic fertilizer, or they can be used in biogas production to produce methane under anaerobic digestion. In animal husbandry, by-product can be used as feed or bedding in stables, or further as construction material (straw), etc. Some of these applications compete with the use as org. fertilizer, whereas digestates and animal manures in return can be reused as org. fertilizer. Besides manures and digestates, composts are common org. amendments consisting of different mixtures of org. substrates that have undergone aerobic digestion and gained a certain maturity. Furthermore, sewage sludges which arise from industrial or municipal water treatments can be applied as org. amendment to enhance soil fertility (Sayara et al., 2020). A further application of org. amendments is green matter and intercrops which can suppress weeds and reduce the risk of erosion during their growing period and are incorporated into the soil afterwards. Organic amendments can originate from agricultural production, industrial processes or urban wastes, furthermore they can be subject of different treatments like aerobic or anaerobic digestion and even differ in their fraction (solid or liquid) (Urra et al., 2019). Depending on their composition of parent material and former treatments, org. amendments contain different amounts of nutrients and C polymers, which results in a wide variety of potential agronomic uses.

The range of potential org. fertilizers is constantly expanding. This leads to the necessity that this fertilizer pallet must be characterized also regarding their humus and nutrient effects. On the one hand, this includes physical and chemical properties such as the dry matter content or the C-, N-, and P-content. On the other hand, it includes the turnover properties, which are determined by the chemical properties, like the C/N ratio, lignin, cellulose, and hemicellulose content and furthermore by the environmental conditions they are applied to. These elements' interactions with each other and with their environment are highly complex and influenced by a wide variety of biological, chemical, and physical conditions. Nevertheless, these interactions and the prediction of their cycling dynamics are the basis for circular economies and sustainable agricultural practices. There is a need to develop tools to predict the state of those elements and nutrients as well as their behavior under different soil conditions in order to evaluate management practices and generate consulting indicators.

I.1.2 Soil Carbon

Soils are the second largest C sink after the oceans. Thus, soils play a crucial role in the C cycle: Organic matter such as litter is used by microorganisms for their metabolism and C is mineralized to CO_2. While some of the C is used to build up the microbial biomass, the more resilient parts, as well as microbial residues and exudates, build up soil organic matter (SOM), which coalesces with the mineral soil phase (Wiesmeier et al., 2019). The decomposition of fresh organic matter (FOM) and SOC can vary from days to up to > 1000 years (O'Rourke et al., 2015). C sequestration in soils is widely and controversially discussed under the "4 per mille initiative" as a possibility to mitigate climate change, which was introduced at the COP21 by UNFCC. The aim is to sequester 4 ‰ C (0.4 %) every year into soils to compensate the anthropogenic greenhouse gas emissions (Minasny et al., 2017). The approach is mainly criticized for distracting from high CO_2-emitting practices as well as the fact that soils have to be maintained and managed so that they remain a lager sink than a CO_2 source for future generations (Baveye et al., 2018). Furthermore, agricultural land accounts for about 37 % of the terrestrial soils

(Smith et al., 2008), which limits the approach to certain landmasses and does not include peatlands or forests. In addition to C sequestration, increasing SOC stocks promotes further benefits, restores soil functions and can help to set incentives and implement sustainable agricultural practices. High SOC contents can improve the resilience of soils against droughts, improve the soil structure and therefore reduce soil erosion, which is expected to increase in response to climate change and high intensity rain events (Baveye et al., 2020). Besides the improvement of physical soil properties, SOC is essential for micro-and macrobiota, which feed on FOM and SOC and mutually influence the soil structure and water infiltration as well as the nutrient availability. The C-cycle is a driving factor in the cycling of most micro- and macro-nutrients for plants, due to the turnover of FOM and the adsorption of nutrients to SOC.

I.1.3 Soil Nitrogen

Nitrogen (N) is a key constituent of all living organisms and is part of nucleic acids, amino acids and proteins. As N_2, it constitutes 79 % of the atmosphere's gases, nevertheless, N_2 is not available for plants due to its low reactivity. N fixation is the process where N_2 is converted to ammonium (NH_4^+) or ammonia (NH_3) by microorganisms in soils. In leguminous plants, those microorganisms live in symbiosis with the plants, which supply the microorganisms with sugars or nutrients and in return receive accessible N. Nitrification is the process in which NH_4^+ is converted to Nitrite (NO_2^-) and then to Nitrate (NO_3-N). The processes in which N is mineralized to N_2 and reenters the soil air and the atmosphere is called denitrification (Lamb et al., 2014).

For most arable land, mineral N plays a vital role for management practices, where mineral N is applied as fertilizer. In the Haber-Bosch process, N molecules react with hydrogen, using catalysts and high amounts of energy, to form ammonia. The Haber-Bosch processes accounts for most of the world's production of ammonia and thus, mineral fertilizers. Due to the high energy demand, technical ammonia production accounts for 1 % of the worlds energy demand and produces 1.4 % of the world's CO_2 emissions (Capdevila-Cortada, 2019). Thus, a high necessity is given to search for alternatives to mineral N fertilization.

Mineral N constitutes only for a small amount of soil N, around 95 % of soil N is bound to the organic phase. It is therefore closely connected to the C turnover and is, in this form inaccessible for plants. In the course of mineralization, organic N is transformed to NH_4^+ as which it enters the mineral N cycle. FOM with a high C/N ratio can lead to immobilization of N. Bacteria which decompose FOM with high C and low N have to compensate for the low N in FOM, which is required for their growth, from soil N. This can result in depletion of plant-accessible N forms in soils and thus lead to reduced crop production (Walworth, 2013).

Excessive applications of N fertilizers results in N leaching, especially of nitrate, which can be hazardous for aquatic systems and pollute ground water. Furthermore, leaching of N can have economical losses for the farmers (Hess et al., 2020). Thus, management options can be adapted, to minimize N losses. To be able to do so, it is important to know the state of N and to track the N cycle in soils.

I.1.4 Soil Phosphorus

Phosphorus (P) constitutes an essential macronutrient for all living organisms. As such, it is required for growth processes, for energy synthesis and as compartment of the associated adenine triphosphate (ATP). Plants take up P in form of phosphate (P_2O_5), which is water-soluble, although plants can convert lightly bound P into phosphate form. One way this can occur is through the release of root exudates, or the release of acids in the rhizosphere which cause a decrease of the soil pH and desorption of mineral-bound P (Lambers, 2022).

P occurs in soils in various chemical forms, whereby it can be subdivided into inorganic and organic binding forms. The weathering of P-rich primary minerals, such as appatites, strengites and variscites, can extend over long periods of time (Shen et al., 2011). For this reason, mineral P fertilizers are often used on agricultural land to ensure optimal plant nutrition. Most of these fertilizers come from fossil phosphate deposits, although these are limited to a few countries. The largest deposits, accounting for about 80 % of the reserves, are located in Morocco, the USA, China, and South Africa, among others (Vaccari, 2009). These mineral phosphate deposits are estimated to last for another 50-400 years. The estimates vary greatly, which may be attributed to price developments and the associated discovery of new deposits and P-sources caused by technological progress. Additionally, population growth and consumption patterns affect P reserves (Van Kauwenbergh, 2010). Besides the scarcity, fossil P has been found to have high contents of radioactive material, as well as high concentrations of heavy metals, both of which can lead to health hazards (Boer et al., 2019). Fossil P is an essential component of mineral fertilizers used in industrial agriculture, despite the disadvantage that a lot of said P is leaching and translocated. A considerable part of P reaches water bodies through erosion processes and can lead to eutrophication. Alewell et al. (2020) estimate global P-losses from erosion at 4-19 kg ha^{-1} yr^{-1}, with 50 % due to water erosion. In addition, P as a limited resource is diffusely distributed into the oceans and a recovery is almost impossible or financially not worthwhile. Therefore, it is especially important for countries without fossil P reservoirs to establish a functioning recycling economy. Other sources of input into the soil are organic materials, in which P is released by mineralization processes. Here, there is a close link to the C-cycle. Studies show that organic fertilizers have an impact on plant P availability and that organic fertilizers promote microbial activity, which in turn can lead to higher P availability (Khan et al., 2022).

Besides the interaction with the organic soil phase, P availability is influenced amongst others by pH-dependent sorption of P particularly to Al, Fe and Ca ions. In neutral and alkaline soils, P precipitation and adsorption processes with calcium carbonate dominate, in which P is taken from organic sources. This can be of importance since liming is a common practice to regulate the pH value on arable soils. At soil pH of 6-5, the fixation of P to Al dominates, whereas at soil pH values of 4-3, absorption to Fe dominates. It must be noted that pH values below 4 are uncommon in agricultural soils (Barrow, 2016).

The P species and its availability for plants depend on a variety of influencing factors. Further factors worth mentioning in this context are the clay content, which tends to absorb P due to its high surface to volume ratio, microorganisms which take up P for their metabolism, and environmental conditions like temperature or moisture, which influence the turnover of org. substrates. All those organic and inorganic influences lead to a dynamic equilibrium where P is either water-diluted or bound to the soil phase in different degrees of intensity and species. All this summed up makes soil P a highly complex plant nutrient, the understanding and application of which poses challenges for scientists and farmers aming to reduce unwanted P losses and to optimize P availability for crops.

I.2 Research Questions

Mineral fertilizer production consumes vast amounts of energy, and in case of P, is also limited to fossil reservoirs, which are expected to deplete. The use of org. fertilizers is a considerable alternative, which can simultaneously support endeavors to reach CO_2 mitigation goals. The variety of org. substrates is continuously growing, due to increasing biogas production and the occurring digestates, sewage sludges, or similar. Contrary to mineral fertilizers, organic amendments consist of a variety of components and nutrients that depend on the composition of the parent material, and, if applicable, on the processing of those amendments. The nutrients are not always in a plant-accessible form, rater, they are partly organically bound and subsequently released during mineralization. This leads to the issue that the organic substrates vary in their quality regarding their turnover dynamics, and thus in their release of nutrients. On the one hand, this allows a versatile use, e.g., to build-up of SOC and improve soil quality, or the fertilization of nutrients with long term-effects. On the other hand, this behavior is difficult to determine, since the turnover depends not only on the parent material but also on microbial communities and environmental conditions. Consequently, there is a great need to classify and evaluate organic substrates in terms of their humus building efficiency and long-term fertilization effect, so that they can be more specifically adapted to the management strategies. With the aim to provide stakeholders with an advisory tool which can be easily interpreted, the question was investigated:

(1): How can one evaluate the quality of org. substrates under consideration of microbial turnover?

In comparison to laboratory experiments, the application of org. substrates under field conditions is influenced by a wider variety of factors. Worth mentioning in this context are climatic conditions (temperature and precipitation), soil properties like bulk density or clay content, and soil management. Furthermore, the already accumulated stocks of C and nutrients like N and P in soils are relevant to determine their long-term dynamics in soils. It is important to note that under field conditions, crops will accumulate nutrients and carbon and with the harvest, a part of the nutrients is removed. Residues like stubbles and roots will remain on the field and serve as a source of C input, and further as a source of nutrients which reenter the nutrient cycle. To close the gap between laboratory modelling and field conditions, one must answer the question:

(2): Are the turnover dynamics of org. substrates received from C incubation experiments scalable to the field scale, and beyond, are they sufficient to describe the SOC, SON, and Pav dynamics of arable soils?

Besides determining the quality of organic substrates, the question has to be considered:

(3): *How can the quantity of accruing crop residues in a field site be determined?*

P is, alongside N, another important macro-nutrient for plants, but to date, the P cycle has not yet been investigated as intensively and integrated into model calculations. This is partly due, to the complex behavior of P and the different forms of binding to the mineral and organic phases in the soil. For a holistic evaluation of organic substrates in terms of their nutrient availability in soils, P has to be considered to evaluate the fertilization use and adapt management practices. To be applicable with agronomic data and for a low entry threshold, simpler model structures are preferable, provided they are validated and deliver good results. From this deliberation arises the need to find out:

(4): *What degree of complexity does the modelling of the P cycle on arable soils need in order to adequately capture and predict the availability of P and its species*?

I.3 Structure & Objective of the Thesis

The three chapters have been published in international journals and build upon each other. The conceptualization of the thesis is depicted in Figure I-1. The data used are shown as dashed lines and were gathered from experimental conductors and aggregated in databases. In chapter II, a method to characterize the quality of organic substrates is introduced in which six commonly used mechanistic C models are applied to model the respiration curves of a variety of incubation experiments. Parameters describing the turnover process are optimized to those respiration curves. Furthermore, a method to describe the humus building efficiency is applied and the results of all six models are aggregated with a model averaging approach to generate an ensemble value for the humus building efficiency.

In chapter III, the parameters received from modelling of the incubation experiments (chapter II) are used to model the application of the investigated amendments in a field trial, using the CCB model. The study aimed at exploring the possibility of upscaling the parameters received from modelling C incubation experiments (from chapter II) to the field scale and predicting the C and N dynamics. Furthermore, methods of parameterizing the above-ground and below-ground residues were tested.

In chapter IV, the CCB model is expanded to include a P-module, taking into account all the modifications implemented in chapter II & III and the current literature. The model is labeled CNP-model, but the notation is not consistent; since the expansion was introduced in the third publication, it will be referred to as CNP-model. Nevertheless, the CCB-and CNP-model share the same structure, except for the CNP-model's additional P-module. Unless referring to P-related topics, they can be seen as identical. The P-module is tested on four field sites, using parameters from incubation experiments to describe the org. fertilizers, stubbles, and roots generated with the algorithm introduced in chapter II. The concept of modelling with parameters from incubation experiments applied in chapter III was also used to model the field experiments and to validate the P-module.

The overall goal was to create a method which allows to evaluate org. substrates in terms of their quality, and furthermore to establish a reliable method to parameterize the used model to generate parameters suitable to model the field dynamics of org. substrates in terms of their C dynamics and the connected soil N and P cycling.

The following hypothesis is derived: *The C-cycle and its turnover dynamics are the key drivers for the nutrient dynamics and plant availability of org. amendments.*

In this thesis the focus is set on ways to include all sorts of org. substrates into model calculations and to describe the C cycle and the dynamics of the plant nutrients N and P. This way, org. fertilizers can be investigated regarding their long-term effects and different fertilization purposes.

Here the following hypothesis is formulated that: *Organic amendments are very versatile, and to predict their dynamics they need to be parameterized separately to capture their behavior under field conditions.*

Finally, in chapter V, the results will be briefly summarized and discussed in their overall context. The synthesis section will contextualize the results and answer the question:

(5): *How can the results of this thesis support stakeholders in decision-making and evaluating management options, ultimately aiming at integrating the developed quality assessment into practical applications?*

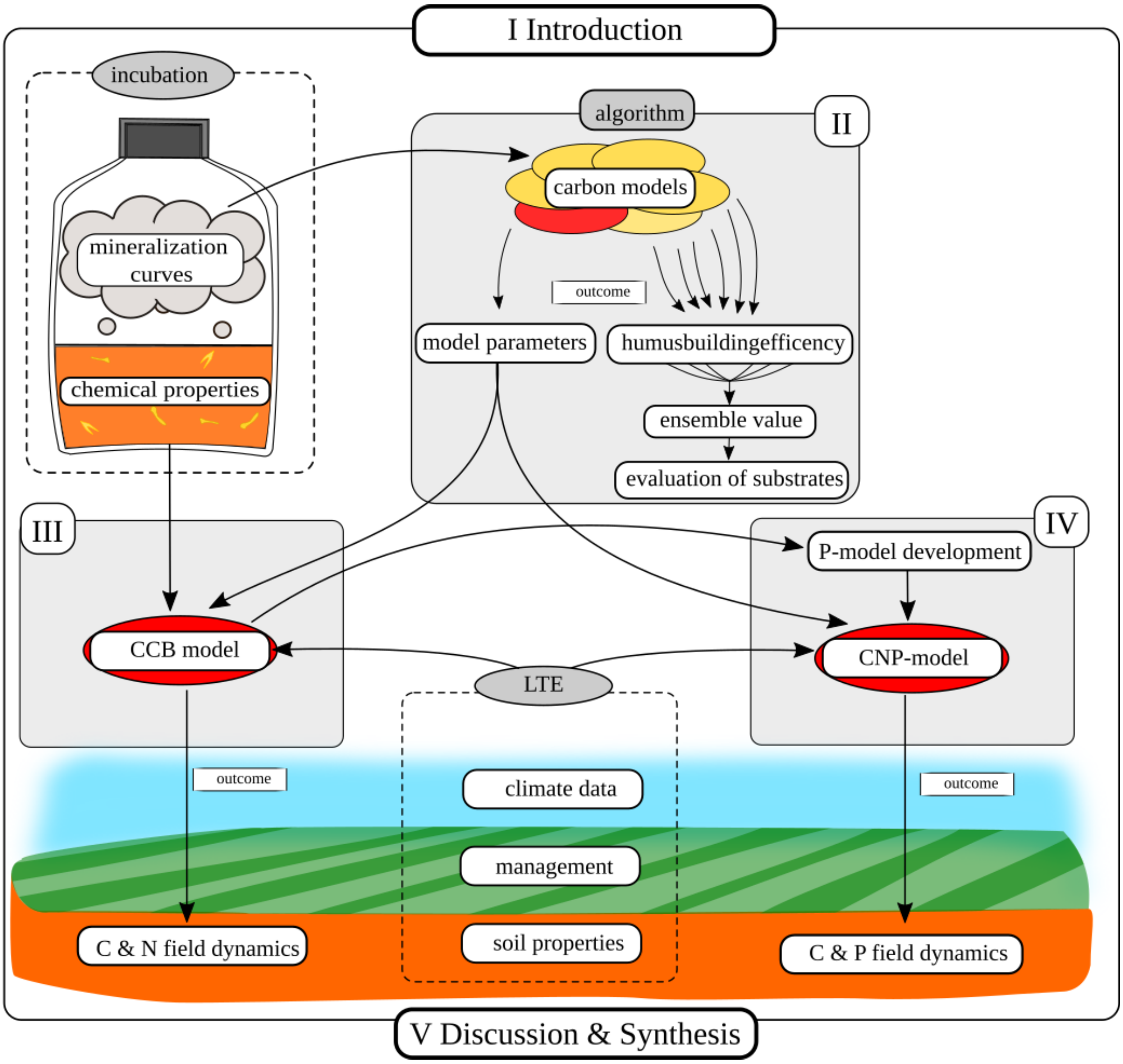

Figure I-1: Structure of the thesis. Dashed boxes represent the data sources which were aggregated from incubation experiments and LTEs. Grey boxes represent the chapters, arrows repesent the connection between chapters or data sources. Those three chapters are framed by the introduction, conclusion and the synthesis section.

I.4 Methodological Background

I.4.1 Incubation Experiments

Incubation experiments constitute a major basis for the thesis. The reported incubation experiments were aggregated from different experimental setups of different research projects and were conducted as a cumulative setup. In incubation experiments, a predefined amount of organic substrate is mixed with soil material. The water saturation is adjusted to 50-65 % to grant microbial growth. The mixture is sealed in vessels, which are opened at time of measurement. Over the study period, the cumulative release of CO_2, which is released by microbial cell respiration, is measured at defined times. Sodium hydroxide (NaOH) traps are placed within the vessel to capture the mineralized CO_2. The NaOH solution accumulates the CO_2, and at the measuring dates the solution is extracted and CO_2 concentration is analyzed. To ensure that the microbial respiration processes do not turn into an anaerobic environment, the vessels are regularly aerated. To differentiate between the turnover of SOM and the added organic material (AOM), soil is incubated without additives as control treatment. The respiration curve of the control treatments is subtracted from the AOM respiration curves. Besides the output of respiration curves, the incubated substrates are analyzed regarding their chemical composition. Thus, those amendments are analyzed in detail, providing a solid foundation to characterize those substrates (for details see Appendix VI.1).

I.4.2 Long-Term Field Experiments

A considerable challenge lies in the generalization from laboratory experiments' results to the dynamics and the behavior of org. substrates in soils under field conditions. In long term field experiments (LTEs), where turnover processes and crop production depend on seasonality, climate and soil properties, changes in soil dynamics need to be tracked for several years. Nevertheless, valuable knowledge can be gained from LTEs, where the long-term effects of fertilizer application and management practices are investigated. These can include different crop rotations, different amounts of fertilizer application as well as different mineral and organic fertilizers (Grosse et al., 2020). In general, a wide variety of data is gathered, including yields and the dates of seeding and harvesting as well as soil management procedures like plowing, irrigating, or fallowing. Furthermore, soil characteristics get determined like the soil bulk density, clay-, silt-, and sand-content, the pH value, water holding capacity etc. The soil is frequently tested regarding its organic and mineral C and N content, as well as the available and total P, but other elements can be targeted at the study site as well. The matter fluxes concerning inputs and outputs are well documented, making LTEs a good study system wherein many processes and management effects are well documented.

I.4.3 Soil Modelling

Experimental setups like LTEs and incubation experiments can be very costly and time-consuming. Model approaches can be used to fill the gap between laboratory- and field experiments and to extrapolate experimental findings to regional scales. This is based on the attempt to express physical, biological, and chemical processes in mathematical equations. Model concepts try to represent processes and sub-processes from systems with mathematical expressions. On the one hand, data-driven approaches can be applied, in which algorithms are used to search for correlations and relations from training data sets. Here, little or no knowledge of the underlying systems is necessary, rather, the information lies in the statistical correlation and in the amount of data. On the other hand, there are mechanistic mathematical model approaches. Here, physical, biological, and chemical processes are often expressed in differential equations. Their core component is a profound understanding of these processes, but a combination of mechanistic and statistical approaches is also not uncommon (Wu et al., 2021). If models are sufficiently validated and deliver reliable results, the influence of individual parameters on the investigated system can be verified and quantified. Through quantification, these processes can also be evaluated and characterized, which in turn makes it easier to translate model findings into practically relevant indices or to support political decision-making.

There is a variety of C-models, which differ in complexity with respect to their integration and combination with other process models (e.g. hydrological model), but also with respect to the required parameter input and the associated data basis. Further, these models differ in terms of their scale and spatial magnitude, which can range from molecular to global scale (Campbell et al., 2015). Those mechanistic C-models often have in common that C is distributed in defined pools, which have different residence times and interact with each other. These pools are often conceptual pools that are not directly measurable. An essential part of these models is that they describe the turnover of organic substrates and that their parameters describe the transfer of input C into different pools while CO_2 is released.

A major object and basic tool of this thesis is the CANDY Carbon Balance (CCB) Model by Franko et al. (2011), which is a simplified model of the CANDY model (Franko et al., 1995b). The CCB model comprises an active SOM pool (A-SOM) which represents the microbial biomass and serves as the driving pool for turnover processes. The A-SOM is in exchange with the stabilized SOM-pool (S-SOM) and the long-term stabilized SOM-pool (LTS-SOM). A detailed description of the model structure will be given in the following chapters as part of the thesis. In contrast to many other C models, the CCB applies unique characteristics to each FOM input into the modelled system. To do so, the CCB relies on a database with entries for each FOM input, which requires a certain amount of data. Some of those characteristics are easier to obtain than others, including the dry matter content, the C content and the C/N ratio of FOM inputs, which can be obtained from standard chemical analysis. Model-specific parameters need to be parametrized from some sort of experiment, or otherwise deviated. Those parameters are k_{fom}, which represents the decomposition of FOM, and eta (η), which is the synthesis coefficient. Eta describes the uptake of C by the A-SOM pool and consequently the growth of microbial biomass, while 1 - η describes the part of FOM that gets mineralized. Since incubation experiments investigate the mineralization of org. substrates, they constitute a solid foundation to acquire those parameters. To obtain all those FOM specific parameters, sizeable effort in data acquisition is required. Different approaches to obtain those parameters have been proposed and must be tested, depending on the availability of data.

II. A Model Ensemble Approach to Determine the Humus Building Efficiency of Organic Amendments in Incubation Experiments

S. ANTON A. GASSER, JULIUS DIEL, KERSTIN NIELSEN, PAUL MEWES, CHRISTOF ENGELS, UWE FRANKO

Abstract

Organic amendments are important to sustain soil organic matter (SOM) and soil functions in agricultural soils. Information about the contribution of organic amendments to SOM can be derived from incubation experiments. In this study, data from 72 incubated organic amendments including plant residues, digestates and manure were analyzed. The incubation data was compiled from three experimental setups with varying incubation times, soils and incubation temperatures, in which CO_2 re-lease was measured continuously. The analysis of the incubation data was performed with an approach relying on conceptual parts of C- TOOL, CCB, Century, ICBM, RothC and Yasso which are all well- approved first- order carbon models that differ in structure and abstraction level. All models are an approximation of reality, whereby each model differs in understanding of the processes involved in soil carbon dynamics. To accumulate the advantages from each model a model ensemble was performed for each substrate. With the ability of each carbon model to compute the distribution of carbon into specific SOM pools a new approach for evaluating organic amendments in terms of humus building efficiency is presented that, depends on the weighted model fit of each ensemble member. Depending on the organic substrate added to the soil, the time course of CO_2 release in the incubation studies was predicted with different accuracy by the individual model concepts. Averaging the out-put of the individual models leads to more robust prediction of SOM dynamics. The EHUM value is easy to interpret and the results are in accordance with the literature.

II.1 Introduction

The accumulation of soil organic carbon (SOC) is discussed as a possible solution to mitigate climate change (Minasny et al., 2017). Increasing SOC can rebuild soil fertility, reduce soil erosion, and increase yield stability (Bradford et al., 2019; Harden et al., 2018). The accumulation of SOC requires a reduced decomposition of SOC and/or an increased input of organic matter (OM), where the latter depends on the amount and quality of the OM input.

For an efficient agricultural management that sustains soil organic matter (SOM) and closes the nutrient cycle, it is important to know the specific contribution from different organic materials such as manure, plant residues and recently also from digestates of biogas reactors to SOM (Larney et al., 2012). SOM is a composition of compounds with different turnover times in soil. Therefore it is important to assess specifically the contribution of added organic matter to the long lasting part of SOM that is historically summarised under the term 'humus' and which demands certain attention within the debate about carbon sequestration. There are several attempts to use proxies like the C/N-ratio, hemicellulose or the lignin content to evaluate the contribution of OM to SOM. But those bio-chemical proxies have restricted capacity to predict the behaviour of OM reliable enough under microbial turnover (Lashermes et al., 2009; Morvan et al., 2005), since other factors like temperature, microbial communities etc. can influence the decomposition (Dignac et al., 2017).

Incubation experiments are a research tool to assess the quality of the added substrates with regard to humification and the microbial turnover within a certain time. Their results are often analyzed with statistical methods including different kinds of non-linear regressions where usually only the carbon loss is determined, whereas the transfer from the added organic material (AOM) to SOM generation is not quantitatively included (Cotrufo et al., 2013). Furthermore, there is no well approved solution to transfer the incubation results from statistical models to the field scale with regard to environmental conditions. Soil carbon models are usually developed for field conditions and reflect a complex understanding of the carbon turnover. The general model approach comprises a network of carbon fluxes between different pools which approximates in an abstract way the microbiological turnover processes in the soil. Consequently, carbon models are able to predict the retention of carbon in soils for specific site conditions. However, soil carbon models need to be parametrised in order to compute carbon fluxes and they require information about the quality of OM (Stockmann et al., 2013). Incubation experiments, where organic matter is mixed with soil and the resulting turnover is observed from the CO_2 evolution over time may contain this information (Jha et al., 2012).

The general understanding of carbon turnover includes several ‘unknowns’ and its expression in models follows different concepts. Each model has distinct strengths and weaknesses to project the examined processes (Sulman et al., 2018). Therefore, it may be risky to rely on only one specific model. Model ensembles/averaging are a common method to aggregate the prediction of several models into a single prediction, which is expected to be at least as good as the prediction of a single model and also compensates partial weaknesses of a single model (Diks et al., 2010; Hagedorn et al., 2005). In addition to improving the prediction, the calculated weights of a model averaging can be transferred to further purpose. The carbon models assign specific turnover characteristics to the underlying substrates, which can be used to evaluate the efficiency of a substrate to contribute to the long lasting SOM. Thus, the model averaging weights might be used to aggregate the humus building efficiency of a substrate into a single value depending on the performance of each ensemble member.

In this study the following questions were addressed:

i: How can soil organic carbon models be applied to incubation experiments?

ii: How can the humus efficiency of added organic matter be expressed with a single parameter based on the results of soil organic carbon models?

iii: Does a model ensemble increase the reliability of the quality assessment for organic amendments?

II.2 Materials and Methods

II.2.1 Incubation Experiments

In this study, data were compiled from three different incubation experiments with varying incubation time, soils and incubation temperatures (Table II-1). The first two data sets were obtained from the Institut für Agrar-und Stadtökologische Projekte Berlin (IASP) and are denoted by data1 and data2, the experimental setups vary in their incubation times. A data set that was already published by Sänger et al. (2014) is denoted as data3 and data4, each with the same substrates but with different soils. The third data set was derived from the Humboldt University Berlin and is denoted as data5 and data6 with different incubation periods.

In total, data from 72 incubated organic substrates including plant residues, digestates and manure were analyzed (Appendix A VI.1.1). The organic amendments were incubated together with soil in beakers. The moisture and the temperature were set to a constant state over the incubation time. In each experimental design the accumulated amount of CO_2 released was measured over the incubation period. Therefore, different sampling techniques were applied, see Appendix A VI.1.2, VI.1.3 and VI.1.4. What all methods had in common was that cumulative CO_2 released from the added organic matter (AOM) was differentiated from the soil born CO_2 released by reference samples, where only soil was incubated without any organic amendments, assuming no priming effects. Based on the amount of CO_2 C evolved in each substrate, the cumulative amount of total evolved C was calculated for each observation over the entire incubation period. The CO_2 C released from the organic substrates was calculated from the difference of CO_2 C released from the samples with and without AOM.

Table II-1: An overview of the experimental setups in this study for each data set (AOM = added organic matter)

	data1	data2	data3	data4	data5	data6
incubation time [d]	139.7	251.7	41	41	301	161
replicates	6	6	4	4	5	3
sampling interval [d]	1/24	1/24	1–20, 22, 24, 27, 30, 34, 36, 41	1–20, 22, 24, 27, 30, 34, 36, 41	1, 3, 7, 14, 21, 35, 56, 77, 98, 120, 162, 217, 301	1, 3, 7, 14, 21, 35, 56, 77, 98, 119, 161
temperature [°C]	20	20	25	25	22	22
soil pH	5.7	5.7	6.5	6.5	5.9	5.9
soil addition [g]	40	40	20	20	100	100
counts of substrates used	7	8	10	10	22	15
clay, silt, sand [%]	1, 9, 90	1, 9, 90	20, 75, 5	15, 39, 46	7 ,21, 72	7, 21, 72
soil water content (% of water holding capacity)	60	60	60	60	50	50
AOM type	digestates , manure	digestates , manure	digestates	digestates	roots, crop residues	roots, crop residues

II.2.2 Carbon Models & their Application to Incubation Data

In this study concepts of carbon models that follow first order kinetics and are well established on a field scale, namely C-TOOL (Taghizadeh-Toosi et al., 2014), CCB (Franko et al., 2011), CENTURY (Parton et al., 1987; Parton et al., 1994), ICBM

(Andrén et al., 1997), RothC (Coleman et al., 1999) and Yasso (Tuomi et al., 2011) are applied to the incubation data. Besides their handling of AOM, they differ in the number of conceptual SOM pools, their interconnection and texture dependencies of turnover time as well as in the depiction of environmental influences on turnover. A detailed description of each model is beyond the scope of this paper, but the adaptations made to apply the models to the incubation data are described in the Appendix A VI.1.5. Here it should be noted that the original model concepts are adapted to meet the requirements of modelling the incubation data. The adapted model concepts are referred to by their name with asterisk (*).

In order to apply the models to the incubation data with a unique algorithm and identical data structure, they were reduced to their core concept, as described in Appendix A VI.1.5. Assuming optimal water supply during the incubation period, only the respective temperature and soil texture functions (when available) were considered. For each model, a maximum of two AOM related parameters were fitted. All other model parameters were left constant at the values according to the individual model publications. Following Sierra et al. (2012), each model was implemented as a set of ordinary differential equations in R (R Core Team, 2019) that were solved using the deSolve package (Soetaert et al., 2010). The parameter fitting was accomplished by using the Levenberg-Marquardt algorithm implemented in the nls.lm function from the R package minpack.lm (Elzhov et al., 2016). The optimised parameters are described in Table II-2 for each soil carbon model for the observed cumulative net CO_2 production from AOM.

Table II-2: Overview of the models used and the fitted parameters; min/max describes the set thresholds for the parameters, the min value is numerically never truly = 0; FOM denotes fresh organic matter and AOM denotes added organic matter, for a description of the pools or the parameters see Appendix A VI.1.5 or the publications

model	considered FOM pool of the model	AOM assessment	fitted parameters	min/max

C-TOOL	*fom*	distribution	f_{hum}	≈0/1
		transformation	k_{fom}	0/10
CCB	*aom*	transformation	k10	0/0.5
			k12	0/2.5
CENTURY	*m*	distribution	f_{lig}	0/999
		transformation	k_{str}	0.24/4.8
ICBM	*y*	transformation	k10	0/0.3
			k12	0/3
RothC	*rpm*	distribution	f_{hum}	0.252/0.98
Yasso	*w*	distribution	p_w	0/1

II.2.3 Evaluating the Substrate Quality in Terms of Humus Efficiency

For a clear differentiation, italic miniscule is used to describe the original model pool names, whereas the concept applied here with more generalized pools to determine the humus efficiency are denoted with capital letters. AOM is defined as the substrate before incubation. FOM is denoted as the part of the substrate that still has the properties of AOM before microbial turnover and humus (HUM) that integrates all SOM pools after microbial turnover for a given time t.

$$HUM(t) = \sum_{i=1..p} SOM_i\,(t) \qquad 1$$

If a model does not include an explicit FOM pool, the most dynamic pool with the lowest turnover time is considered as FOM, this accounts for CENTURY, RothC and Yasso. Some substrates, especially manure, are subject to microbial turnover even before the material is added to the soil. Therefore, in several model concepts, a part of AOM is directly transferred to HUM without passing a FOM pool.

The models used express the quality of AOM as matter transformation into SOM with two general approaches:

1) Distribution: initial partitioning from AOM to one or two model pools

2) Transformation: efficiency for production of HUM

In the first case, at the beginning of the incubation experiment, a fraction or the total AOM is allocated between a FOM and SOM pool according to the structure of the specific model. In the second case, SOM pools are built up continuously.

During the simulation of an incubation experiment each model predicts the evolution of AOM into a designated FOM pool, one or more SOM pools and of course the amount of mineralized carbon (CO_2).

The data used represent the difference of CO_2 evolution between a treatment (soil + substrate) and the control vessel (soil only). In order to represent the net-mineralization, priming effects were neglected and each model was initialized with empty SOM pools that will fill up according to the individual model procedures. The amount of C which is lost from the added substrate (AOM in Eq. 2) during the incubation, is transferred into several SOM pools or is released as CO_2:

$$AOM - FOM(t) = \sum_{i=1..p} SOM_i\,(t) + C_{CO2}(t) \tag{2}$$

As mentioned above, the efficiency to build up HUM has to be quantified from two components. The first one is the quota (q) of added C that is immediately allocated to the SOM pools at the beginning of the incubation.

$$\mathrm{q} = \frac{\mathrm{HUM(0)}}{\mathrm{AOM}} \tag{3}$$

This reduces the amount of FOM for further decomposition to (1-q)*AOM.

The second component represents the dynamic transformation from FOM to HUM and is calculated as the relation between the rate of HUM production (dHUM) and the rate of FOM decomposition (dFOM). The sum of both components results in the humus building efficiency parameter E_{HUM}:

$$E_{HUM} = q + \max\left(\frac{dHUM(t)}{dFOM(t)}\right) * (1 - q) \tag{4}$$

For sufficiently small time steps the changes of HUM and FOM can be calculated with a negligible loss of SOM-C to CO_2:

$$dHUM(t) = \left(HUM(t) - HUM(t - \Delta t)\right);\ \ t > 0 \tag{5}$$

$$dFOM = \left(FOM(t) - FOM(t - \Delta t)\right);\ \ t > 0 \tag{6}$$

For all 72 substrates the variable parameters of each model were fitted to find the best agreement between observed and predicted CO_2 production. The obtained model parameters were then used to model the CO_2 mineralisation for small time steps of 10^{-4} d. In this way, E_{HUM} was calculated with each model for every substrate.

II.2.4 Model Averaging and Assessment

During the optimisation for some models, the optimized parameters adjoin their thresholds for certain substrates. In this case the models often insufficiently fit the data. To minimize the effect of parameters at their thresholds and to compensate individual weaknesses, the models were aggregated into an ensemble. Therefore, a model averaging method in analogy to the proposal of Bates et al. (1969) as described by Diks and Vrugt (2010) was applied, but instead of the variance, the mean squared error (MSE) was used to calculate the weights ($w_{i,s}$). With this method, models with the highest squared prediction error get the lowest weight with respect to the disproportional sensitivity to larger errors. For each combination of model i and substrate s the weight $w_{i,s}$ was calculated:

$$w_{i,s} = \frac{1/\mathrm{MSE}_{i,s}}{\sum_{j=1}^{n} 1/\mathrm{MSE}_{j,s}} \qquad 7$$

Where n denotes the number of models within the ensemble.

As performance measure of the incubation fit the root mean square error (RMSE) was used since it has the same unit. The individual model results were compared with the ensemble prediction in order to evaluate the ensemble performance to improve the prediction of the incubation data. Further on, the computed weights were applied to aggregate the model specific E_{HUM} values for each substrate to obtain $\overline{E_{HUM}}$ as a weighted ensemble value.

A model with a high weight for a substrate could provide the same information as others with lower weights, which is why another 6 ensembles were calculated, omitting one of the models each time. Afterwards the difference between $\overline{E_{HUM}}$ over all models and $\overline{E_{HUM}}$ with exclusion of the model i was calculated to get the influence of each model on the ensemble $\overline{E_{HUM}}$.

$$influence_{\ model=i} = |\overline{E_{hum(1,..,6)}} - \overline{E_{hum\ (1,..,i-1,i+1,..,6)}}| \qquad 8$$

II.3 Results

II.3.1 Model Fitting and Model Performance

It is possible to adapt the concepts of the used models to the incubation data and to parameterize the underlying substrates. Nevertheless, the quality of the model fit varies between models and substrates due to the characteristics of the incubation process. However, each model performs best in terms of minimizing the RMSE for at least one substrate. Some models have explicit incubation trends (e.g. rapidly decomposable or slowly decomposable substrates) where they perform superior to other models. Figure 1 shows three substrates, a digestate with a slow carbon mineralization, slurry with an intermediate mineralization and crop residue of sorghum with a fast mineralization. It is shown that some models have difficulties with stable substrates (Figure II-1 a & d) while others struggle with easy decomposable substrates (Figure II-1 c & f) and most models fit substrates with an intermediate mineralization sufficiently.

C-TOOL* fits the incubation data best when the measured mineralization rate reaches a constant state (Figure II-1 a). For substrates where the mineralization still rises continuously at the end of the incubation period, C-TOOL* fits the incubation data worse compared to other models (Figure II-1 b). Due to the combination of a distribution and transformation approach during the AOM turnover, C-TOOL* is able to model highly decomposed organic matter like digestates and rotten yard manure.

The model performance of CCB* is also relatively robust but, the model reaches its limits with highly decomposed AOM, since its AOM turnover is solely based on an efficiency approach (Figure II-1 a).

CENTURY* is challenged by strong mineralization rates at the beginning of the incubation and the approximation to the steady state, but works better on easy decomposable substrates (Figure II-1 a & b).

ICBM*, on the other hand performs best when C mineralization is rising fast at the beginning of the incubation (Figure II-1 f), but also lacks the ability to simulate a stagnating C mineralization due to the efficiency approach of AOM turnover (Figure II-1 d).

Initially, RothC* predicted the mineralization dynamics satisfactorily, but with advanced incubation time the predictions become almost linear (Figure II-1 e & f). Therefore substrates that show a pronounced saturation are not well represented.

Yasso* performs well compared to other models, when applied to highly decomposed materials (Figure II-1 d) like rotten farm yard manure or digestates. Due to the pre-distribution of FOM into the defined HUM pool, however, Yasso* lacks the ability to simulate easily decomposable AOM (Figure II-1 f).

During optimisation each model had reached its parameter limitation at least once. In this case the model fits are deficient and the incubation data is not well represented (Figure II-1). Relying solely on one model may, therefore, lead to an under- or overestimation of the incubation data.

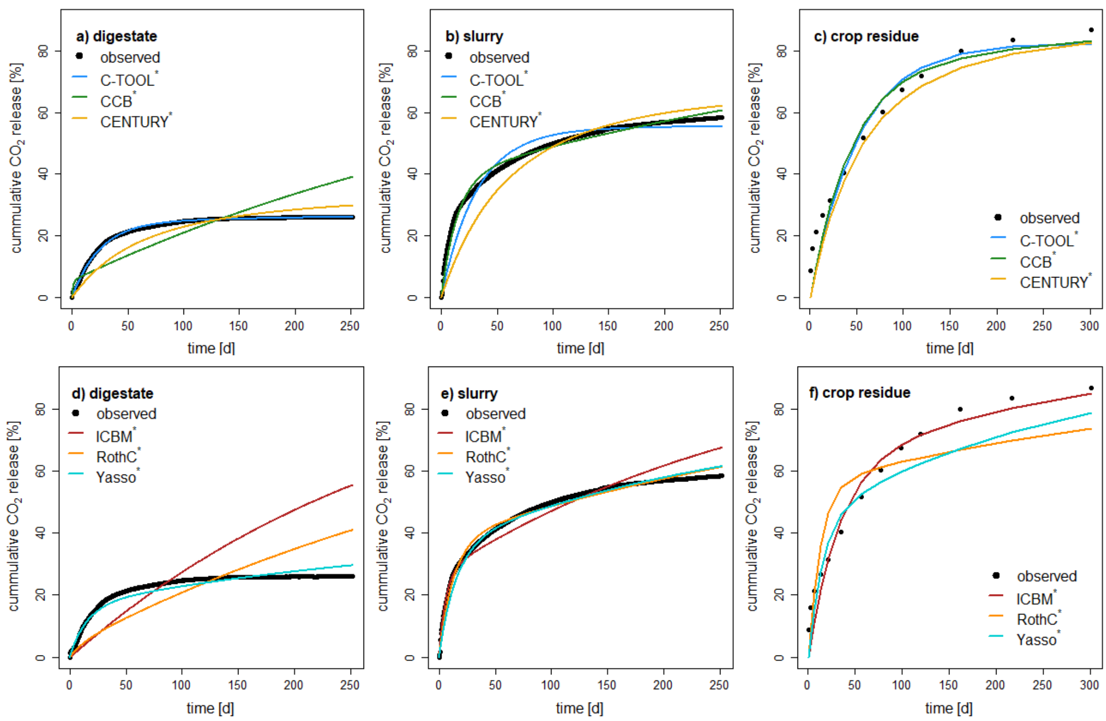

Figure II-1: Example of model results for the cumulative CO_2 release with three different substrates, (a, d) digestate (ID: 18), (b, e) slurry (ID: 22), (c, f) crop residue of sorghum (ID: 54), see Appendix A VI.1.1 for ID

II.3.2 Model Specific Diversity of E_{HUM}

Figure II-2 shows the distribution of calculated E_{HUM} values for each model. In general it shows very well how all model concepts designate high E_{HUM} values to already pre-composed materials such as manure and digestates and low E_{HUM} values to plant residues. But the model concepts differ in their overall conception of E_{HUM}. Models such as C-TOOL*, CENTURY*, RothC*, and Yasso* have a lower threshold of E_{HUM} unequal to 0 (Figure II-2), where the minimum E_{HUM} value is equivalent to the parameter describing the flux of the chosen FOM pool to CO_2. This parameter is texture dependent for C-TOOL* and RothC*, which leads to a slight shift in the possible flux from FOM to CO_2, to be observed by C-TOOL* (Figure II-2), where the E_{HUM} values align at a lower threshold, although with less clay content the values would be even lower (red line).

Model concepts without an AOM distribution, like CCB*, CENTURY* and ICBM*, lack the ability to fit highly decomposed substrates adequately with fitted parameters adjoining the parameter thresholds. This leads to an insufficient representation of the incubation data and results in E_{HUM} values of 1, even though more resilient substrates theoretically exist (like peat). In this case the max E_{HUM} is limited by the model structure.

Furthermore, the aggregation of all SOM pools into a HUM pool causes for RothC* information loss for high E_{HUM} values. The optimized parameter f_{hum} shifts C from *rpm* to *hum* for values higher than 0.772, but since both pools are considered as HUM pool E_{HUM} will reach its maximum at the parameter value $f_{hum} = 0.772$ (Dechow et al., 2019).

Only C-TOOL* and Yasso* have not adjoined the upper threshold of E_{HUM} whereas CCB*, ICBM* and RothC* have not adjoined their lower E_{HUM} threshold within the analyzed substrates. This demonstrates that each single model has its strength and weaknesses with regard to the substrates analyzed due to model structure and the intended purpose of the model. Nevertheless from each model concept follows a similar E_{HUM} value for a given substrate, with rotten yard manure and digestates as substrates with the highest humus efficiency and plant materials (except fine roots) with the lowest humus efficiency (Figure II-2).

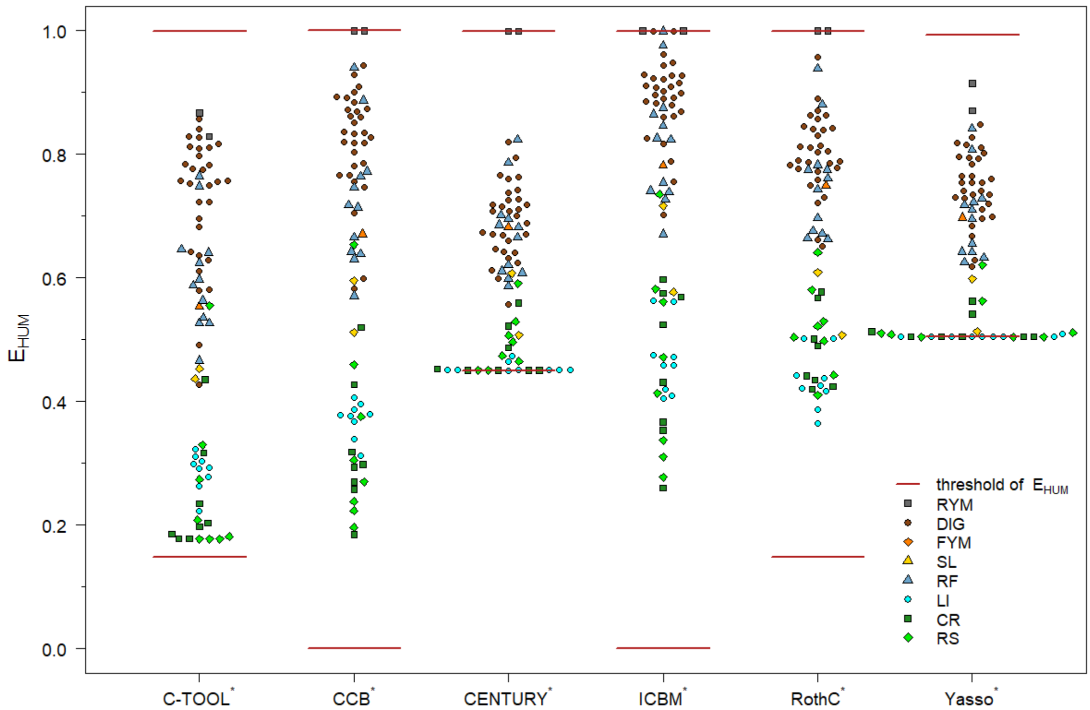

Figure II-2: E_{HUM} values for each model and substrate, line: model specific thresholds of E_{HUM} considering texture dependency, RYM: rotten yard manure, DIG: digestate, FYM: fresh yard manure, SL: cattle slurry, RF: fine roots, LI: litter, CR: crop residue, RS: coarse roots, classes don't consider material composition e.g. different plant residues

II.3.3 Ensemble Performance

The averaging method applied leads to an overall robust performance of the ensemble in displaying the incubation data. Compared with the single models, the ensemble scores 32 times the lowest RMSE for the underlying substrates and never has the highest RMSE compared to a single model. The average RMSE over all 72 substrates was calculated, which is for C-TOOL* = 2.39, CCB* = 2.48, CENTURY* = 4.59, ICBM* = 4.30, RothC* = 4.11, Yasso* = 3.62, ensemble = 1.92.

Furthermore, the calculated weights were applied to the E_{HUM} value each model supplies for a substrate. The average weight of the ensemble $\overline{E_{HUM}}$ value, is compiled out of the analyzed 72 substrates is, C-TOOL* = 28.4 %, CCB* = 28.7 %, CENTURY* = 7.9 %, ICBM* = 13.3 %, RothC* = 10.3 %, Yasso* = 11.4 %, which demonstrates that every model used contributes to the ensemble $\overline{E_{HUM}}$ values.

Since the E_{HUM} value varies between models, the influence of a model on the ensemble $\overline{E_{HUM}}$ for each substrate was calculated. As a result one model was omitted and a new ensemble $\overline{E_{HUM}}$ value was calculated, without the regarding model. The effect that the omission of one model has on the ensemble $\overline{E_{HUM}}$ calculation is shown in Figure II-3. The most influential model for the ensemble $\overline{E_{HUM}}$ value compilation is C-TOOL*, followed by CCB*, ICBM*, CENTURY*, Yasso* and RothC*. Rather than the fitting performance, as described before, the information that one model provides to the $\overline{E_{HUM}}$ value and the information that one model concept provides which is redundant and can be compensated by other models is shown in Figure II-3. The most influential model for the ensemble $\overline{E_{HUM}}$ value compilation is C-TOOL*, followed by CCB*, ICBM*, CENTURY*, Yasso* and RothC*. The average divergence of $\overline{E_{HUM}}$ for one substrate, occurring when one model is left out of the ensemble $\overline{E_{HUM}}$ calculation, is for C-TOOL* = 2.91 %, CCB* = 1.42 %, CENTURY* = 0.749 %, ICBM* = 1.131 %, RothC* = 0.429 %, Yasso* = 0.659 %, indicating that this is a rather robust concept.

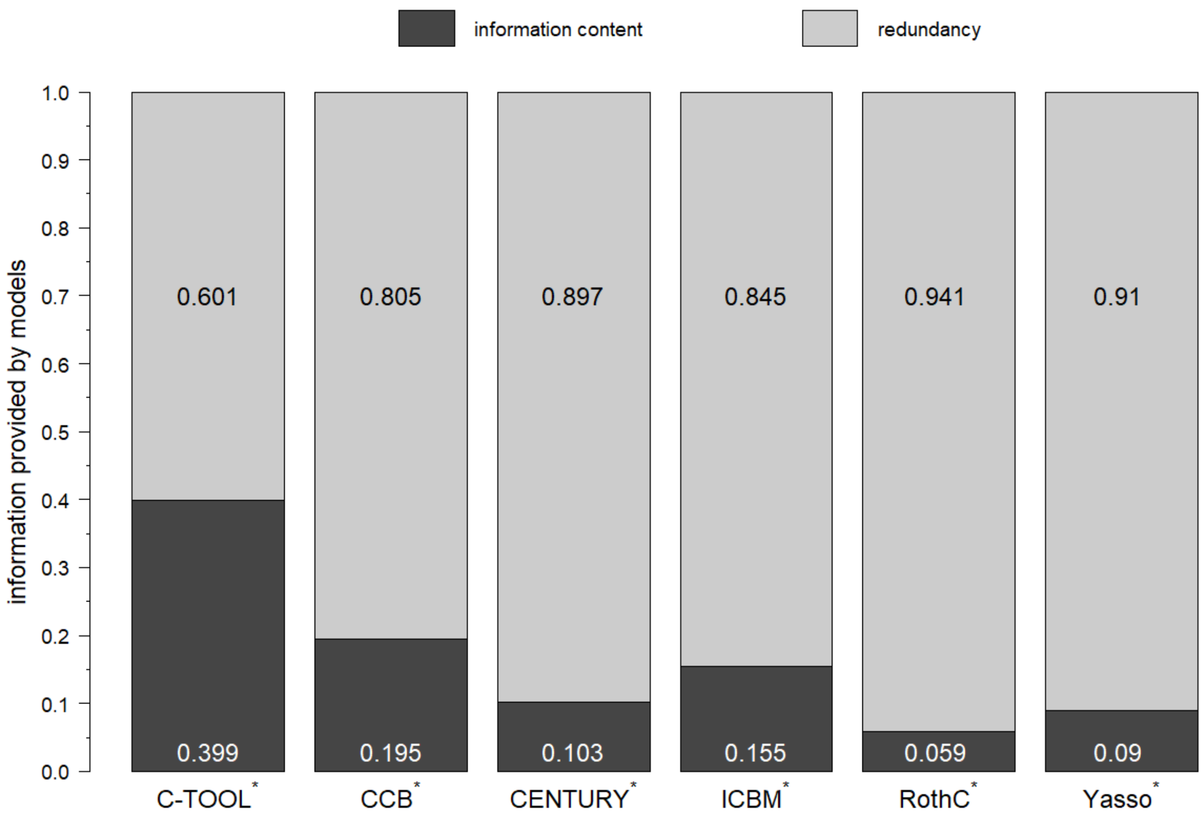

Figure II-3: The relative change of $\overline{\mathbf{E}_{\mathbf{HUM}}}$ for 72 substrates without the considered model, high redundancy means that the E_{HUM} values of a model is similar to the E_{HUM} values of other models and model fits to the incubation data are worse than other models

II.3.4 Humus Efficiency of Organic Substrates

For a practical application, the ensemble $\overline{E_{HUM}}$ concept with model averaging was applied to substrate classes. The classes were aggregated by their material origin, while differences in species for plant material and composition among digestates were not taken into account.

Figure II-4 demonstrates the weighted $\overline{E_{HUM}}$ values for different substrate types. Rotten yard manure and digestates show the highest $\overline{E_{HUM}}$ values followed by fine roots. Untreated animal feces like slurry and yard manure have medium $\overline{E_{HUM}}$ values whereas plant materials like coarse roots, crop residues and litter show the lowest $\overline{E_{HUM}}$ values and cannot be distinguished statistically.

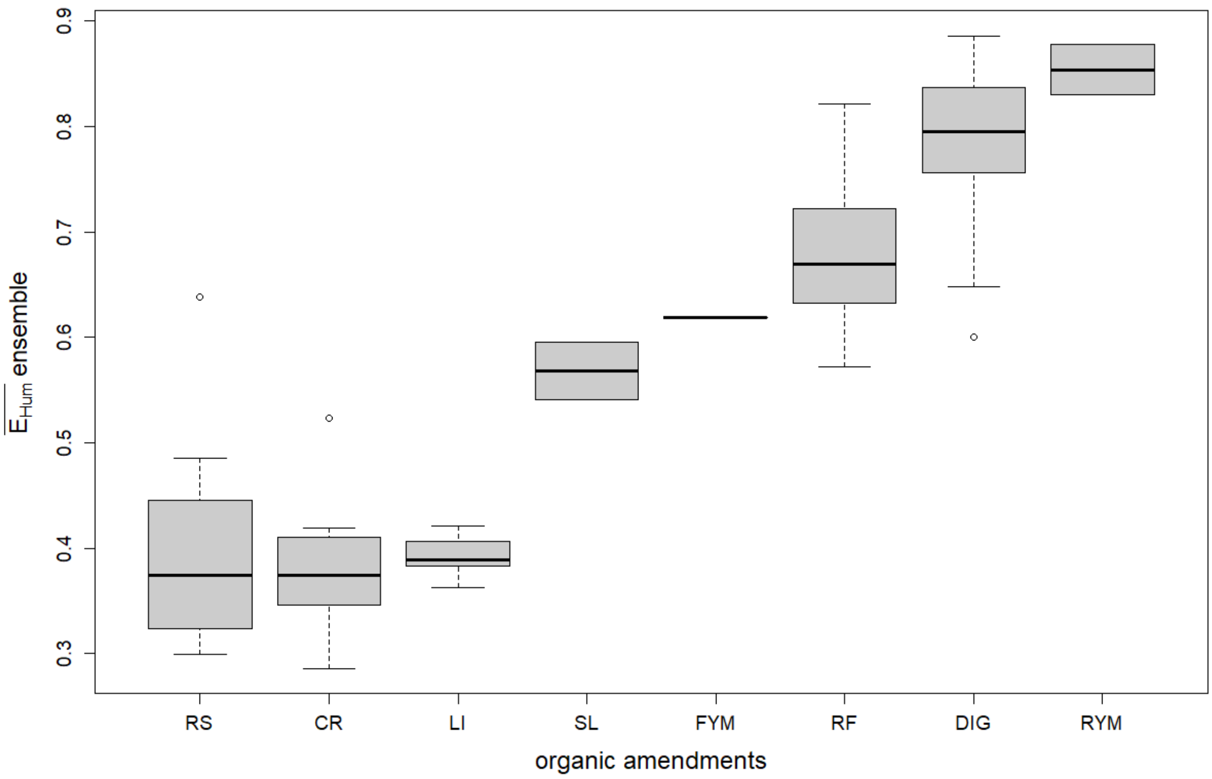

Figure II-4: Ensemble $\overline{\mathbf{E_{HUM}}}$ values for substrates by class; RS: root stock (coarse root), N= 8; CR: crop residues, N=8; LI: litter, N=9; SL: cattle slurry, N=2; FYM: fresh yard manure, N= 1; RF fine roots, N =12; DIG: digestates, N= 30; RYM: rotten yard manure; N=2, N: count of group members

II.4 Discussion

II.4.1 Carbon Model Adaptation to Incubation Data

Despite being developed for field application, the chosen model concepts were applied successfully to the incubation data while preserving the core concept of the models under the application of the same algorithm and data structure. Nevertheless, some models can be better adapted to the incubation data than others due to model complexity and the model structure. This especially accounts for the handling of AOM, where a higher flexibility was required to deal with a bigger variety of substrates as by some models intended.

Commonly in incubation studies the incubation data gets analyzed with some sort of regression where the results are presented as mineralization in percent or as amount of mineralized C over the incubation time (Sänger et al., 2014). Those regressions are not transferrable to other substrates and serve only a descriptive purpose. Rather than developing models to predict the incubation data, the here used models are already successfully used in field studies and most parameters are derived from field experiments. This gives the models a high credibility, as well as involving more sophisticated pool interactions and SOC processes. Furthermore, a maximum of two parameters describing the decay were optimized thereby minor equifinality is expected compared to other approaches (Tang et al., 2020).

As a further advantage of using SOM models for incubation, the results from the model fitting can be used to transfer observations from incubation experiments to field scale. Thus the calibration results for models on field scale can be validated and possibly improved.

II.4.2 Model and Ensemble Performance

The method applied for model averaging considers the results of model fits to the cumulative CO_2 released, giving higher weights to models with a lower MSE. The MSE is sensitive to larger errors due to the squaring, therefore the influence of models with high prediction errors gets minimized.

The model averaging leads to a better prediction accuracy and the ensemble has the lowest RMSE for 32 substrates, 27 times the second lowest, 11 time the third lowest and two times the fourth lowest RMSE. Also the average RMSE over all 72 treatments demonstrates that the ensemble is more robust in predicting incubation results than a single model concept and that some model concepts don't vary as much as others in their prediction accuracy.

In hydrological and meteorological forecasting, model ensembles are a common tool, to reduce model uncertainties (Li et al., 2017) whereat this technique is not fully established in SOC modeling yet. A recent study by Riggers et al. (2019)

successfully used the same model compilation like this study in an ensemble approach on a field scale. In this study the ensemble members were not weighted, rather the combination of models and different initialization processes were reduced to minimize the prediction error and to find a robust ensemble. The application of several models as an ensemble can help to balance the prediction errors of the individual models which result from the specific structure of their embedded processes, as well as from their individual parametrization or scope and the scale the models were developed for (Martre et al., 2015; Tebaldi et al., 2007).

II.4.3 Concept of E_{HUM}

In this study a method addressing the humus building efficiency of AOM is presented, that evaluates the CO_2 mineralization of AOM and then allows to draw conclusions about the substrate quality. Several carbon models were fitted to the cumulative mineralization and the resulting pool dynamics of each model was used to evaluate the substrate quality. The obtained E_{HUM} value describes the efficiency of a substrate to generate new humus with a time independent metric that considers the incubation temperature during calculation, which allows the comparison of incubation experiments with different time spans and different incubation temperatures. Nevertheless a certain incubation period is required for the models to predict the incubation trend. There are several other methods which describe the humification processes like the E4/E6 ratio which is determined by the optical density of humic and fulvic acids, the Humification Index (HI) and other methods which mostly rely on chemical and physical properties of the substrates (Klavins et al., 2008). Additionally there exist also field experiments in which the application of organic substrates is compared to a control plot with no application of organic substrates (Kätterer et al., 2011). The focus of the presented approach is based on the incubation curve characteristics and the behavior of SOM pools. In contrast to chemical analysis, E_{HUM} also considers microbial turnover and incubation experiments are less costly and time consuming than field experiments. Some of the applied ensemble members even employ mineralization processes with regard to soil properties. Therefore this new concept could be a valuable addition to existing methods.

Each model employed represents a slightly different understanding of the soil processes involved in soil carbon dynamics, which is why their model structure and interpretation of SOM generation varies. Aggregating several SOM pools into a single, conceptional HUM pool influences the E_{HUM} value for each model differently. Thus, each model comes to slightly different predictions of E_{HUM}. Some models show a restricted range for E_{HUM} whereas others are theoretically able to display the complete expected scale of E_{HUM} from 0 to 1. This depends on the model structure and the selected approach of only one FOM pool, which was defined in this study to be the one with the fastest C turnover.

Based on the robust ensemble performance, the calculated weights are not applied in the first place to improve the overall prediction, but rather to evaluate the substrate quality in terms of the humus building efficiency using a model ensemble. The influence of model concepts, which are not suitable for certain substrates, is thereby minimized in the calculation of the ensemble $\overline{E_{HUM}}$ value. The averaging therefore leads to a more trustworthy prediction of the C dynamics from the incubation data and also prevents over-and underestimation of the E_{HUM} value when model parameters reach their limits during optimisation.

Computing power is hardly a limiting factor and it is possible to calculate complex models within a very short time. Nevertheless it is important to know how much information a model contributes to the results of an ensemble and if a model can be left out of the ensemble formation. It was shown (Figure II-3) that every model contributes to the ensemble $\overline{E_{HUM}}$ value. Within the combination of these six models, C-TOOL* has the biggest influence on the ensemble $\overline{E_{HUM}}$, followed by

CCB*, ICBM*, CENTURY*, Yasso* and RothC* which can be compensated for the most part by other models. Whether a model can be omitted from the ensemble calculation is within the discretion of the user.

II.4.4 Application of the Ensemble $\overline{E_{HUM}}$

The 72 substrates analyzed were classified by their origin in order to evaluate the E_{HUM} value for practical applications. The values for each substrate class are in an expected order where more mature substrates have a higher E_{HUM} and therefore a stronger resilience to microbial depletion (Bernal et al., 1998). Ajwa et al. (1994) found similar results for the mineralization of organic material in soil. Where C of plant material had a half-life between 39 and 54 days, animal manure had a half-life which ranged from 37 to 169 days, and for sewage sludge the half-life was 39 to 330 days.

E_{HUM} characterizes the humus efficiency of a substrate in one single value and is therefore easy to interpret. All mature substrates and animal feces show a higher humus building efficiency compared to plant materials except fine roots (

Figure II-4). Digestates or animal feces on the other hand, undergo microbial turnover either in the digestive system and/or in a bioreactor and therefore, the substrate contains more fungal and bacterial necromass as well as decomposition products, which are considered to be a main component of stable SOC (Kallenbach et al., 2015; Liang et al., 2017). An explanation for the higher humus building efficiency of fine roots compared to the other plant materials analyzed, can be found in Rasse et al. (2005), who pointed out, that the high resilience of roots against carbon turnover is due to the physicochemical protection caused by the steady contact of roots to soil particles.

Alongside the chemical analysis of organic amendments like the C/N ratio, Lignin content etc. the E_{HUM} value delivers an easy to interpret assessment to evaluate the quality of the organic amendments based on their behavior in soils under controlled conditions.

For field management that aims at retaining or increasing carbon stock the ensemble $\overline{E_{HUM}}$ value can deliver valuable information about management options concerning the choice of organic amendments. Knowing the humus efficiency, the quantity of newly applied organic amendments can be adjusted to cover the C demands and to conform to possible restrictions in terms of carbon dioxide mitigation goals. An organic amendment with lower E_{HUM} value could be replaced by one with a higher E_{HUM} value, which needs a lower application rate to reach an equal soil carbon stock. Nevertheless such a decision is complex and other nutrients like nitrogen and phosphorus have to be considered as well.

II.5 Conclusions

This study demonstrates that carbon models developed for field scale with different target environments and time scales are a suitable tool to predict carbon incubation data, derived from laboratory experiments. The pool structure of those models can be used to derive information about the efficiency of a substrate to build humus and be displayed in a single value which is easily comparable, which is not possible in the same manner with statistical models. Nevertheless some adaptations to the model concepts had to be made to cover the wide scope of organic amendments. Furthermore, substrate and model specific parameters derived from incubation experiments can be used to improve modelling of SOC turnover at field scale with regard to the modifications of the model concepts made in this approach. This could be a cost and time efficient alternative to long-term field experiments and could give insights into the dynamics of organic amendments which are not fully analyzed yet. The presented approach could help to close the gap between laboratory experiments under controlled conditions and field applications where much more influential factors need to be considered to evaluate the substrate quality. Furthermore, every model incorporates different mechanisms, with a different scope of application. This diversity cannot be covered by a single model and therefore, ensemble approaches can be a useful tool for future SOC modeling challenges.

Contextualization

In chapter II the E_{HUM} value was introduced as advisory metric to characterize org. amendments, and their ability to build up humus. Therefore, soil properties and microbial turnover were considered. Besides that, an algorithm was implemented to optimize six C turnover models to the mineralization curves and receive the according turnover parameters. Of particular importance is the parametrization of the CCB (CNP) model. In chapter III those parameters and the chemical properties of incubated org. amendments will be used, to model the field dynamics of C and N with the CCB model. This allows to model the dynamics on a field scale without further parametrization and also serves as validation of the approach presented in chapter II.

III. Transfer of Carbon Incubation Parameters to Model the SOC and SON Dynamics of a Field Trial with Energy Crops Applying Digestates as Organic Fertilizers

ANTON A. GASSER, KERSTIN NIELSEN, UWE FRANKO

ABSTRACT

The fertilization with organic amendments and digestates from biogas plants is increasingly used to increase carbon stock and to improve the soil quality, but little is still known about their long-term effects. A common method to analyze organic amendments and their mineralization is incubation experiments, where amendments get incubated with soil while CO_2 release is measured over time. In a previous study, carbon models have been applied to model the carbon dynamics of incubation experiments. The derived parameters describing the carbon turnover of the CCB model (CANDY Carbon Balance) are used to simulate the SOC and SON dynamics of a long-term field trial. The trial was conducted in Berge (Germany) where organic amendments like slurry, farmyard manure or digestates were systematically applied. To grant a higher model flexibility, the amounts of crop residues were calculated for roots and stubble separately. Furthermore, the mineralization dynamics of roots and stubble are considered by the model parameters for each crop. The model performance is compared when using the dry matter and carbon content received from the field trial and the incubation experiments, to evaluate the transferability. The results show that the incubation parameters are transferable to the field site, with rRMSE $< 10\%$ for the modelled SOC and rRMSE between 10% and 15% for the SON dynamics. This approach can help to analyze long-term effects of unexplored and unusual organic fertilizers under field conditions, whereat the model is used to upscale the C dynamics from incubation experiments, considering environmental conditions.

III.1 Introduction

With a rising demand of renewable energy, the number of biogas plants is growing continuously. The hereby accrued digestates are commonly applied to cropland to increase the carbon storage, recycle nutrients and improve soil fertility and soil quality. The long-term effects on soil properties are hard to determine, since the physical and chemical properties of digestates can vary significantly due to the substrates and their composition, the technical processing in the biogas plant etc. (Barduca et al., 2020; Nielsen et al., 2020; Zirkler et al., 2014). Due to this variety, there is a need to evaluate the long-term behavior of those substrates, whereat methods which are less time intense than long-term field experiments need to be developed.

Besides chemical properties of organic amendments, the soils to which they are applied can have a decisive impact on the carbon turnover, due to pH, soil texture, bulk density etc. (Gami et al., 2009; Roy et al., 2014). Incubation experiments are a common method to analyze the behavior of organic amendments in soils under controlled conditions, with constant temperature and pre-defined water saturation. The CO_2 that is released during the microbial turnover is measured continuously. Commonly several regression approaches or mineralization models are used to derive information from the incubation data, but the dynamics cannot be upscaled. The necessary transfer of those information to the field scale is quite difficult and not clear (Sleutel et al., 2005).

Long-term field experiments are conducted, amongst other things, to analyze organic amendments and their long-term behavior, which are influenced by climate, field management, water supply etc.; these experiments generate the most application-related data. However, those experiments are time and cost consuming and significant results cannot be retrieved until a certain time span is reached.

Furthermore, the results of those experiments are site specific, since they are influenced by climatic and soil specific parameters.

The modelling of field experiments, can be a possible approach to evaluate the soil organic carbon (SOC) and soil organic nitrogen (SON) dynamics of organic amendments. Still, the modelling poses a number of challenges for the operator. These include the choice of an appropriate model, which vary in complexity and scope. There are several models developed for arable lands like Century (Parton et al., 1987), RothC (Coleman & Jenkinson, 1999), ICBM (Andrén & Kätterer, 1997), C-TOOL (Taghizadeh-Toosi et al., 2014), CCB (Franko et al., 2011), just to mention some. Further the operator faces the collection of data, the parameterization of the model, the handling of changing measurement analytics, the choice of the initial value for the modelling, the validation of the model results and as well a method to determine mineralization behavior of organic substrates within the model concept.

Especially new or seldom applied organic amendments cannot be explored within field experiments to their fullest extent. A plausible method to study the quality of organic substrates is the modelling of incubation, as shown by Gasser et al. (2021b). The authors used the carbon turnover concepts of six mechanistic models to model the C dynamics of 72 incubated substrates. The hereby received parameters, which describe the mineralization are assumed to be transferred to model the SOC and SON dynamics on field scale.

The hypothesis that the results from incubation experiments can be used to model the turnover of organic substrates on field scale is proposed. To validate this hypothesis a result dataset from an incubation study (Gasser et al., 2021b) is used to parameterize the CCB model accordingly, and applied on a field experiment where the same organic materials that were studied during incubation are applied as organic amendments. The data of incubated roots and stubbles are used to parameterize the residues used to model the field trial. The implemented N turnover in the CCB model depends on the carbon turnover, therefore the suitability of carbon incubation data is evaluated to calculate the N turnover of the field sites as well.

The following questions are addressed:

i: Are the chemical properties required to characterize the organic substrates like C-content, N content, dry matter content collected during incubation experiments, sufficient to cover the variability of those properties during a field trial?

ii: How to calculate the Masses of roots and stubble in dependence of the main product, to evaluate the input in the SOC cycle?

iii: Are the parameters describing the mineralization, received from modelling incubated organic amendments, roots and stubble with the CCB model transferable to the field site?

III.2 Materials and Methods

III.2.1 Field Site of Berge

The field site was situated in Berge near Nauen, an agricultural experimental station of the Institute of Agricultural and Urban Ecological Projects at the Humboldt-Universität zu Berlin (IASP) (52°37'11"N and 12°47'16"E, and 51°49'N, 45 m above sea level), Germany.

Basic material for the soil generation of the site is glacial cover sand over boulder clay. The boulder clay on the trial area has different depths, which results in a heterogeneous soil texture from sand to loamy sand. The topsoil (0-20 cm), has a clay content of 1.1 %, silt 9 %, sand 88.9 %. The bulk density is between 1.5 and 1.6 g/cm^3 while the pH value of the soil is 5.54.

The field trial was set up in March 2011 with a one-factorial randomized block design, with four replications. The crop rotation was: Winter rye as whole crop silage followed by maize and in the next year winter rye as whole crop and silage–sorghum. Fertilisers are applied twice a year before the sowing of either rye or maize/sorghum. Furthermore it is to be noticed that all treatments have been cultivated with winter wheat and mustard as intercrop with an N fertilization of 100 kg N ha^{-1} as pre-management.

Five different digestates (DG) as well as farmyard manure (FYM) and cattle slurry (SLY) were used as organic fertilisers. In addition, there was also an unfertilized control (CRL) and one treatment receiving only mineral fertilizer (calcium ammonium nitrate (CAN)).

The fertilizer quantities are based on the amount of applied carbon of a standard farmyard manure (FYM) application of 12.5 t ha^{-1} a^{-1}. (7.5 t ha^{-1} before maize or sorghum and 5 t ha^{-1} before winter rye). The amount of the other organic fertilisers is determined by the amount of organic carbon (Corg) spread by the manure at every application date, so that the amount of Corg is the same for all applied organic fertilisers. The resulting differences in applied nitrogen are balanced by mineral fertilization (CAN). The treatments FYM and DG D-l start a year later compared to the other treatments (2012).

Average inputs and operating parameters of the biogas plants providing the digestates are given in Table III-1.

Biogas plant D uses liquid-/solid-separation of the digestate as subsequent treatment. The cattle slurry that serves as substrate in plant A as well farmyard manure from plant D is used as a reference treatment in the field trial.

The climate data required for the modelling were obtained from a weather station of the German Meteorological Service which is located next to the experimental field.

Table III-1: Input material and operating parameters of the four biogas plants included in the study, DG = Digestates, DG D is separated in liquid (l) and soil (s) components.

Plant	DG A		DG B		DG C		DG D-l DG D-s	
Average Input	50 % 30 % 15 % 5 %	cattle slurry corn silage grass silage fodder remains	43 % 46 % 10 % 1 %	pig slurry corn silage grass silage grain	86 % 14 %	corn silage rye silage	30 % 30 % 30 % 10 %	cattle slurry grass silage corn silage farmyard manure
Operating temperature	mesophile		mesophile		thermophile		mesophile	
Retention time	70 days		60 days		50 days		80 days	

III.2.2 Soil Sampling and Analysis

At each plot five soil samples were taken to a depth of 20 cm two times a year (2011-2020), once after the harvest of green rye in May and then after the harvest of either sorghum or maize in October. The soil was air-dried, sieved (<2 mm) and analyzed for soil organic carbon (SOC) and nitrogen (Nt) content (Dumas method). From September 2015 on, the carrier gas in the analytics was changed from helium to argon. This leads to differences between the measurement results and a systematic offset for the Nt measurements. To correct this, a regression was calculated between comparative measurements with an adjusted $R^2 = 0.9993$ (Appendix B VI.2.1). This regression was used to convert the values carried out with helium to the values carried out with argon.

III.2.3 CCB Model Description

The used CCB model, which is a simplified version of the carbon dynamic model in CANDY (Franko et al., 1995b) is used. It describes the turnover of decomposable carbon in monthly time steps for average site conditions depending on crop yields and input rates of fresh organic matter (FOM). A specific characteristic of the CCB model is the handling of FOM as a list of specific pools from which the C is released to atmosphere or used to build up new SOM. The decomposition is controlled by the FOM specific parameters k_{fom} describing the breakdown of a specific FOM and eta (η) describing the part of carbon that is transferred to SOM. First FOM is moved into the pool of active SOM (A-SOM) which is interacting with the pool of stabilized SOM (S-SOM). Additionally, the model concept includes the long-term stabilized pool (LTS-SOM) where SOM is considered as physically protected (Figure III-1). The nitrogen turnover is linked to carbon turnover via the C/N ratio for each FOM pool, while the C/N ratio of A-SOM and S-SOM are set to 8.5 and the C/N ratio of the LTS pool is calculate with the initial Nt value and the carbon content of all SOM pools. The CCB does not consider a mineral N pool. The microbial-driven matter dynamics in the easily decomposable pools (A-SOM and S-SOM) are simulated in monthly time steps. This process, as well as the FOM turnover, is controlled by site conditions like soil texture, air temperature and rainfall. These conditions are aggregated into a Biologic Active Time (BAT in days [d]) expressing the part time interval under the assumption that no environmental restrictions are in place. Additionally, a matter transfer between A-SOM and LTS pool is considered. A part of the newly built SOM (C_{rep}) is captured inside micropores and thus shielded from decomposition, whereas a part of C-LTS is released from protection and exposed to microbial turnover. Details about the CCB modelling approach and its applications to describe SOM topsoil dynamics were already published (Franko et al., 2011).

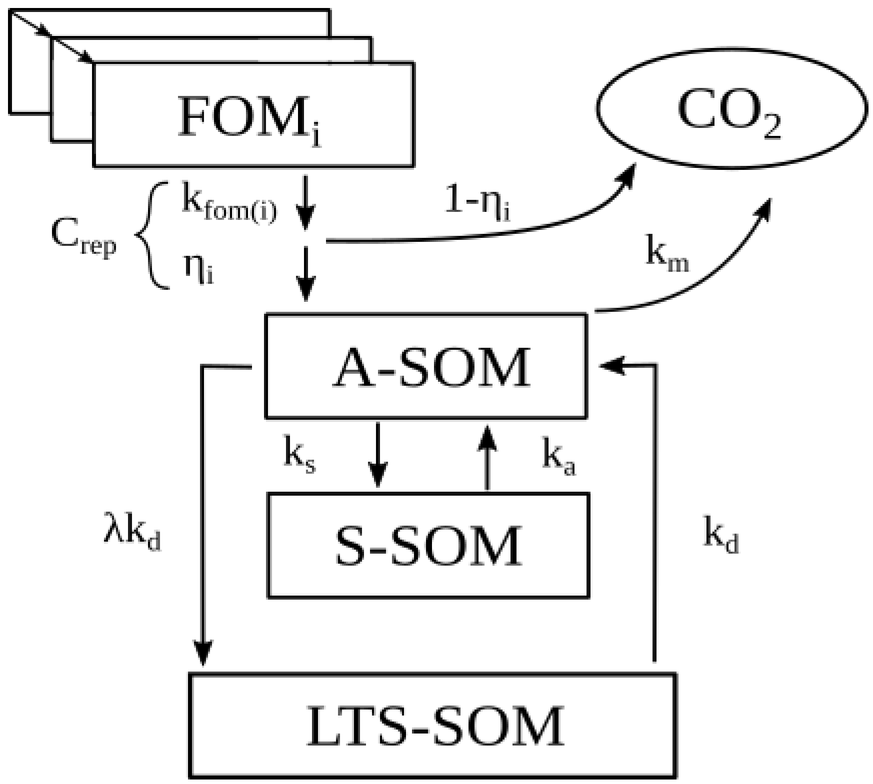

Figure III-1: Scheme of the carbon turnover in CCB, organic matter in soil is subdivided into four compartments: (1) fresh organic matter (FOM) including roots, stubble and organic amendments, (2) biological active soil organic matter (A-SOM), (3) stabilized soil organic matter (S-SOM) and (4) long-term stabilized soil organic matter (LTS-SOM), the fluxes are indicated as lines with the corresponding parameters

III.2.4 Statistical Analysis and Model Initialization

The yields, calculated stubble and root masses of the treatments, were tested for significant differences using the ANOVA, and in the case of significant differences, a post hoc Tukey test was performed. The normality of the data was tested with the Shapiro-Wilk-Test, in case of not normal distributed data the Kruskal-Wallis-Test was performed. The homogeneity of variances were tested with the Levene-Test. The significance level was set to $\alpha = 0.05$.

The goodness of fit was compared by the root mean squared error (RMSE, Equation 9) and furthermore the relative RMSE (rRMSE, Equation 10) was calculated to characterize the differences between observed values (O), $\bar{O}$ as mean of the observations and predicted values (P):

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(O_i - P_i)^2}{n}} \quad 9$$

$$rRMSE = \frac{100}{\bar{O}} \sqrt{\frac{\sum_{i=1}^{n}(O_i - P_i)^2}{n}} \quad 10$$

The choice of the appropriate starting value for modelling is not straightforward. There are different approaches that all show advantages and disadvantages. In this approach the mean error (ME, Equation 11) was used to define the start value of each treatment.

$$\mathrm{ME} = \frac{\sum_{i=1}^{i=n}(O_i - P_i)}{n} \quad 11$$

All analyzes were performed with R statistics (2019).

III.2.5 Parametrization of the CCB Model

Besides the climate data (air temperature [°C] and precipitation [mm]), the CCB model requires, data on soil properties as well as k_{fom} and η values, which describe the mineralization for the organic amendments, roots and stubble. Furthermore, chemical properties, such as C, dry matter and N content of those substrates have to be determined. Besides the quality parameters the quantity of the organic substrates like organic fertilisers or roots and stubble is necessary to calculate the C and N input into the soil cycle.

III.2.5.1 Root and Stubble Quantity Parameters for Berge

The stubble and root mass in the CCB are calculated by a linear equation using the dry matter main product (MP_{dm}) to estimate ether the root (RT_{dm}) or the stubble dry mass (ST_{dm}) (Franko et al., 2021):

$$RT_{dm} = FIX_r + BIX * MP_{dm} \tag{12}$$

$$ST_{dm} = FIX_s + RIX * STIX * MP_{dm} \tag{13}$$

The intercept of the linear equation describes a constant amount of root (FIX_r) or stubble mass (FIX_s) which is yield independent, while the slope describes a yield dependent root (BIX) and stubble (RIX) factor. The part of stubble related to the above ground crop residue e.g. straw, is expressed with STIX. Since all crops are harvested as whole plant, stubble are the only above ground residues and therefor STIX is set to 1.

The root and stubble masses that are needed for the parametrization are derived from Höcker (2017), who analyzed these masses for different crops under different N supply in field trials. The retrieved masses of yield, stubble and roots are used to calculate the parameters which describe the quantity dependency of roots and stubble on the yield of the main product.

The parametrization of the root and stubbles quantity is evaluated, by comparing two approaches. The first method (R1) includes a yield independent part, FIX_r and FIX_s unequal to 0 (Figure III-2 R1) with a lower sensitivity to the yield, while for the second method (R2), FIX_r and FIX_s are set to 0 assuming the stubble and root masses are proportional to the yield (Figure III-2 R2). The control (CRL) and the mineral fertilized plot (CAN) are used to compare and evaluate both approaches.

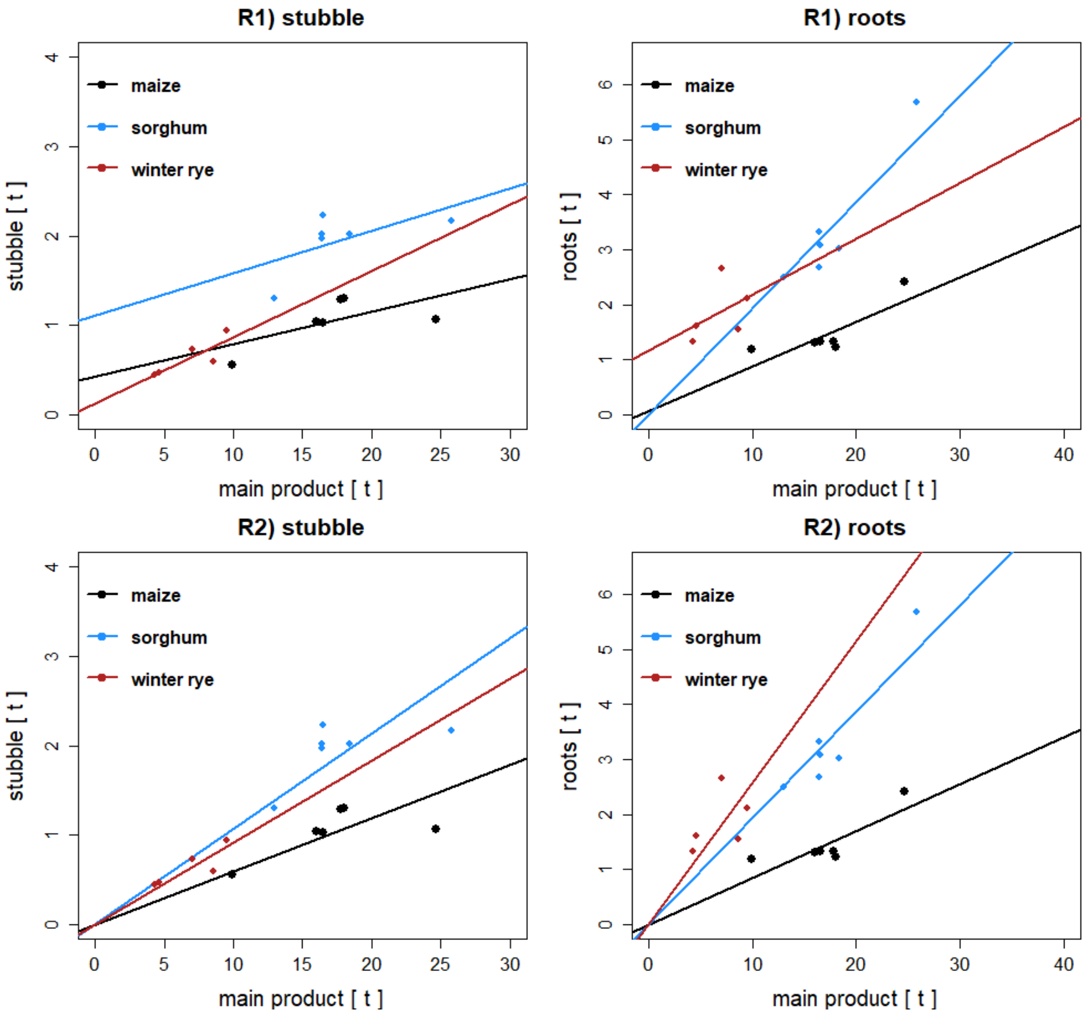

Figure III-2: Linear regression of main product dry matter and the stubble or root dry matter of crops; a) linear regression with yield independent part (intercept) and yield dependent part (slope)(R1); b) linear regression with solely yield dependent part (intercept=0)(R2); data (Höcker, 2017)

It should be noted that the regression describing the amount of sorghum roots are strongly influenced by one data point, which causes a negative intercept (Figure III-2, R1 stubble). In this case, the intercept (FIX_r) was forced through 0 and therefore there is no yield independent part for the sorghum roots. The parameters are displayed in Table III-2.

Table III-2: Linear regression of main product dry matter and the stubble or root dry matter of crops; a) linear regression with yield independent part (intercept) and yield dependent part (slope)(R1); b) linear regression with solely yield dependent part (intercept=0)(R2); data (Höcker, 2017)

Plant residues	RIX (R1)	FIX_s (R1)	BIX (R1)	FIX_r (R1)	RIX (R2)	FIX_s (R2)	BIX (R2)	FIX_r (R2)
Maize	0.0364	0.42	0.081	0.07	0.059	0	0.085	0
Sorghum	0.0475	1.1	0.194	0	0.107	0	0.194	0
Winter rye	0.074	0.13	0.102	1.16	0.092	0	0.258	0

III.2.5.2 FOM Quality Parameters from Incubation Data

The CCB model distinguishes between FOM inputs as organic amendments (in this case organic fertilisers), the incorporation of by-products and the remaining of stubble and roots after the harvest. Those inputs have substrate specific mineralization behavior which are received in this context from incubation experiments.

III.2.5.2.1 Incubation Experiments

The organic fertilisers were incubated at 20 °C and one batch over a period of 139.7 days while the second batch was incubated over 251.7 days, each with 6 replicates. They were incubated in 40g soil with a clay content of 1 %, loam 9 % and 90 % sand with a water saturation of 60 %.

The plant roots and stubble were incubated for 165 (3 replicates) and 300 (5 replicates) days at 22 °C in 100g soil (7 % clay, 21 % loam and 72 % sand) with a water saturation of 50 %. Detailed information about the experimental setup and procedure can be found in the Appendix B VI.2.3.

Gasser et al. (2021b) demonstrated in a model ensemble approach amongst other models, the application of the CCB to incubation data. In this context k_{10} and k_{12} were fitted to the mineralization of 72 different organic substrates. Those substrates include the organic amendments, which are applied on the field experiment in

Berge, as well as roots and stubble substrates of the same crops as grown in Berge. In the approach by Gasser et al. (2021b) the parameters k_{fom} and η of the CCB model had been transformed to k_{10} and k_{12} to unitize the pool flows, which can be retransformed by the following equations:

$$k_{fom} = k_{10} + k_{12} \tag{14}$$

$$\eta = \frac{k_{12}}{k_{fom}} \tag{15}$$

The parameters (k_{10} and k_{12}) were optimized to the incubation curves, using the *Levenberg-Marquardt* algorithm, an example is shown in Figure III-3. The hereby achieved model accuracy varied between a RMSE [%] of 0.6 and 3.5 for the organic fertilizer and between 1.5 and 6.7 for the plant residues (roots and stubble). The parameters have been retransformed to k_{fom} and η as required by the CCB model and are now labelled as such. The incubation experiments were carried out with different temperatures and soils textures, those were considered accordingly by the model, while the water saturation was assumed to be optimal.

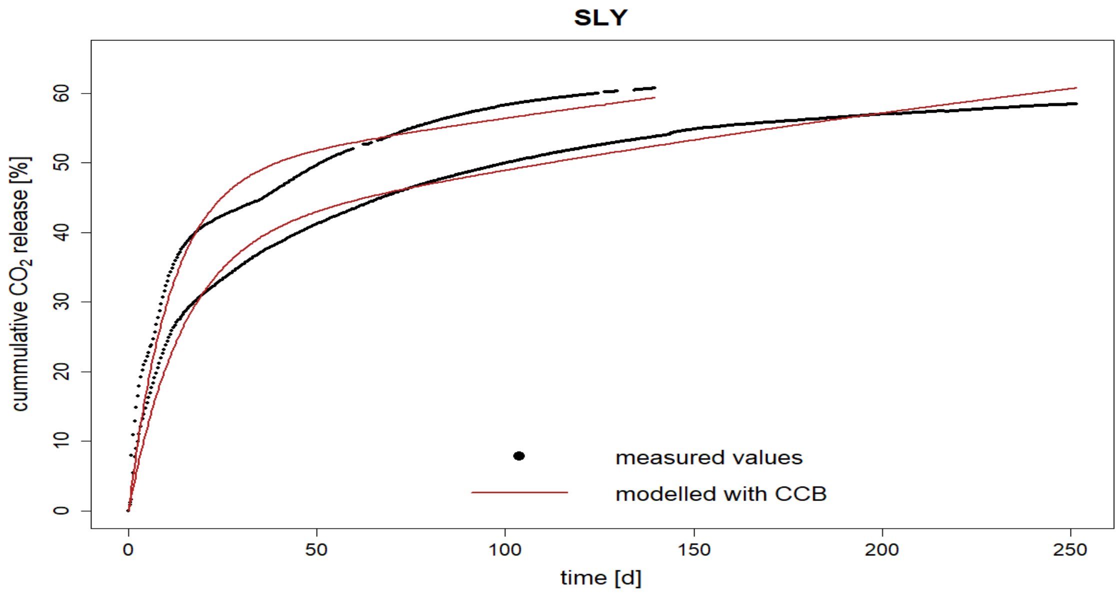

Figure III-3: Optimisation of the CCB model to the mean respiration curves of the organic amendment slurry (SLY) with the Levenberg-Marquardt algorithm (k_{10} & k_{12}), for two batches with 6 replicates, with a period of 140 days (RMSE = 2.38) and 252 days (RMSE = 1.45); the measured respiration (black) and the model prediction (red)

III.2.5.2.2 Quality Parameters for Organic Fertilisers

During optimisation for some organic fertilisers the algorithm reached the parameter limits of the CCB model for k_{fom} and η resulting in no valid solution of k_{fom} and η predicting the incubation trend. In this case only the valid parameters of the batch (N=2) where the limits were not reached are used. This accounts for FYM and DG D-s (N=1). The C/N ratio, dry mass, k_{fom} and η values of the organic amendments, which result from the analysis of the incubated organic fertilisers are presented in Table III-3.

Table III-3: k_{fom} and η vaules, as well as chemical properties like C/N ratio, dry matter content and C content of the organic amendments, roots and stubble, derived from the incubation experiment (N=2, * N=1) and the mean RMSE [%] of the model fit to the respiration curves of the organic substrates

Organic substrates	k_{fom} [d-1]	η [-]	C/N [-]	Dry matter [%]	C content [%]	Mean RMSE [%]
SLY	0.2445	0.55403	10.4	9.2	41.5	1.91
FYM	0.0951*	0.67062*	12.8	23.7	32.1	0.68*
DG A	0.32917	0.81297	5.8	6.7	37.7	1.68
DG B	0.10606	0.5913	5.6	4.1	39.6	2.14
DG C	0.33322	0.74272	5.4	6.7	47.4	2.67
DG D-l	0.26218	0.76117	5.2	7.1	39	1.65
DG D-s	0.2146*	0.80332*	13.5	21.3	40.3	1.16*
Maize stubble	0.067	0.313	73.0	-	42.0	3.78*
Maize roots	0.124	0.418	55.7	-	37.8	2.86
Sorghum stubble	0.073	0.258	57.0	-	41.0	6.13
Sorghum roots	0.112	0.456	43.4	-	33.4	2.72
Winter wheat stubble	0.070	0.258	86.0	-	42.0	5.2
Winter wheat roots	0.139	0.579	34.7	-	35.6	2.14

When transferring the incubation results to field scale, the question arises how comparable the laboratory results are with those measured in the field trial. The CCB model calculates the amount of added carbon by multiplying the dry matter with the carbon content of organic amendments. Both properties vary over time and different batches of organic amendments. Figure III-4 shows the carbon concentration of the organic amendments on the field trial (C1) and the carbon concentration of the incubation experiment (C2). Both values are tested for the SOC modelling and the results are compared in a later section (III.3.2).

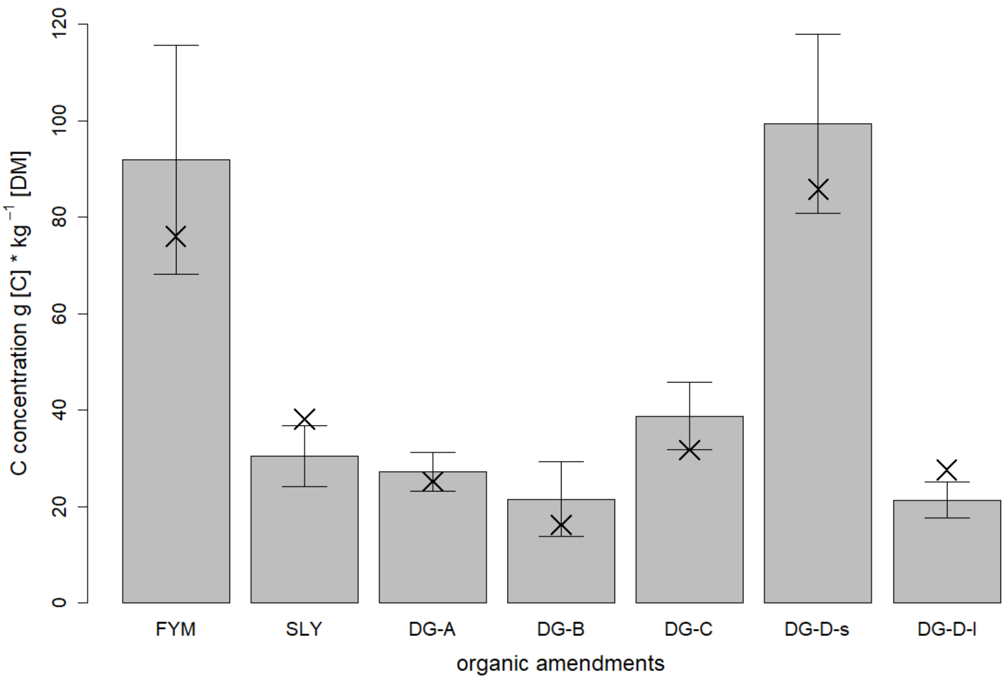

Figure III-4: Carbon concentration of the organic amendments from the field trial (histogram) and incubation experiment (X) (N=2); bars represent standard deviation (N=9).

III.2.5.2.3 Quality Parameter for Plant Residues (Roots and Stubble)

The values for k_{fom} and η (k_{10} & k_{12}) for the plant residues were also obtained from Gasser et al. (2021), whereby the analyzed incubation experiments were conducted for fine and coarse roots separately. Due to the different mineralization behavior of coarse roots (relatively fast) and fine root (relatively stable)(Gasser et al., 2021b), k_{fom} and η were weighted according to their ratio, derived from Höcker (2017) (see Appendix B VI.2.3.2). For green rye no incubation data was available, therefore the incubation data of winter wheat was used instead. The k_{fom} and η values of roots and stubble used for the simulation of the field site in Berge are shown in

Table III-3. The C/N ratio of the plant material was taken from Mewes (2017) who conducted the incubation experiments for the plant residues.

III.3 Results

III.3.1 Analysis of the Field Experiment

The mean yields for each treatment are displayed in Table III-4. Yields for winter rye have a normal distribution, whereas yields for maize and sorghum are not normally distributed. Hence the Kruskal-Wallis test was performed, which shows no significant differences between yields and treatments, maize p-value = 0.6186, sorghum p-value = 0.8446. The analysis of variance homogeneity showed that the variances are homogeneous for all crops. For winter rye, the ANOVA showed significant differences between the treatments (p-value = 0.0003), which is why the post hoc Tukey-test was performed. The CRL treatment was significantly different from CAN (p-value = 0.0004), SLY (p-value = 0.0011), DG A (p-value = 0.0356) and DG C (p-value = DG D-s (p-value = 0.0026), while all other treatments showed no significant differences.

Table III-4: Mean yields [$t*ha^{-1}$] and standard deviation for crops and treatments, within the year 2011 (*2012) -2020

treatment	winter rye	sorghum	maize
CRL	8.436 ± 7.75	19.644 ± 9.44	24.600 ± 11.96
CAN	26.426 ± 9.25	33.084 ± 17.51	33.587 ± 17.05
FYM*	20.964 ± 8.35	28.699 ± 16.38	33.653 ± 13.52
SLY	25.443 ± 8.54	32.642 ± 17.39	39.673 ± 16.36
DG A	21.237 ± 8.06	27.520 ± 14.66	38.246 ± 14.73
DG B	18.748 ± 7.88	28.920 ± 14.69	37.599 ± 16.06
DG C	21.426 ± 7.68	29.137 ± 16.24	41.492 ± 11.51
DG D-s	24.515 ± 6.91	32.295 ± 18.27	38.562 ± 11.55
DG D-l*	15.090 ± 8.89	22.893 ± 9.49	34.167 8.28

Root and Stubble Quantity Parametrization

The two methods R1 and R2, which describe the quantity parametrization for roots and stubble are compared in Figure III-5. R1 with a yield independent part and therefore a lower yield dependency and R2 without a yield independent part and a higher yield dependency were tested at the CRL plot.

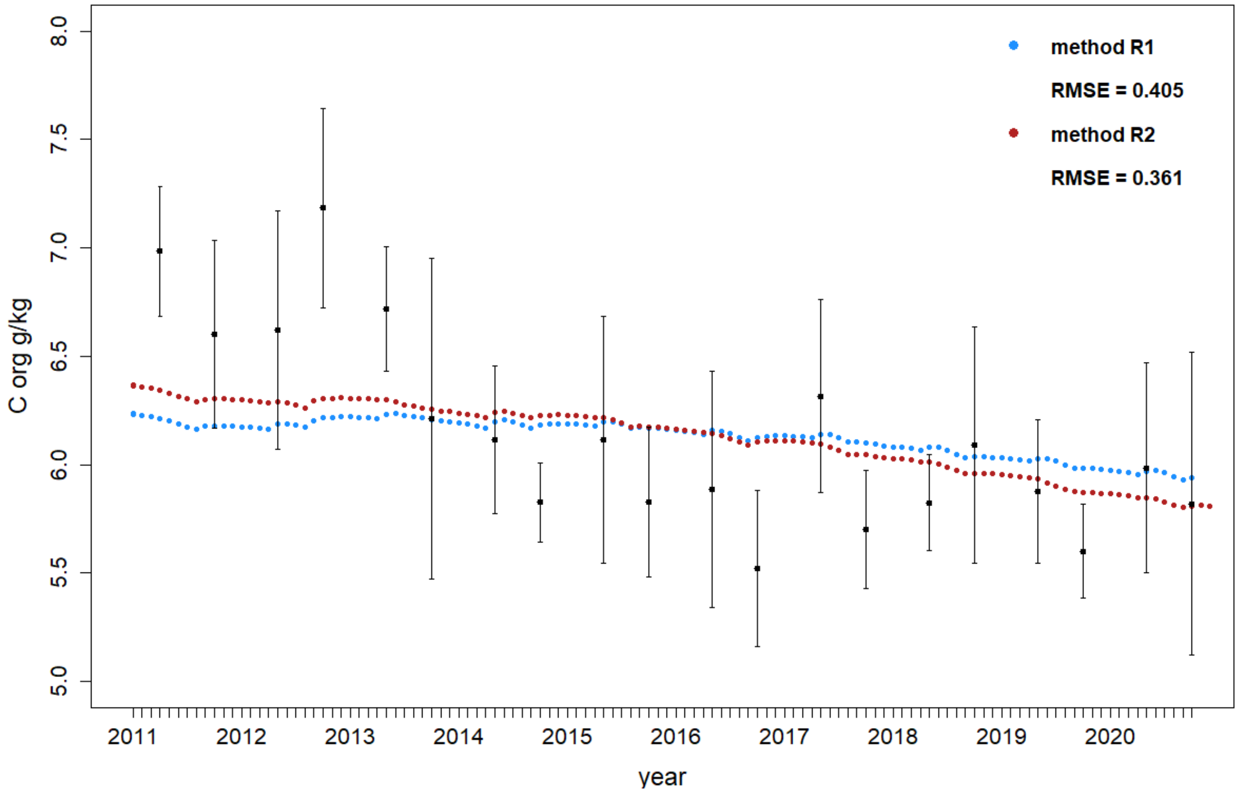

Figure III-5: Mean measured Corg (markers) and sd (N=4) for CRL treatment, output of the model with parametrization of root and stubble dry mass from linear equation considering yield dependent and yield independent part (blue, R1) vs. equation considering only yield independent part (red, R2), initialized with ME

The model fit can be improved with method R2, with a reduction of the RMSE by 0.045 g/kg (for the CAN treatment the RMSE gets reduced by 0.004 g/kg). Thus method R2 has been used for further calculations.

The resulting masses of stubble and roots which were calculated with the R2 method are displayed in Appendix B VI.2.3.2. No significant differences between the treatments and corresponding stubble or root masses of the crops have been detected after the described procedure in the section III.2.4, except for the control treatment of winter rye roots and winter rye stubble.

III.3.2 Organic Amendments Quality Parametrization

The comparison of the model results, using the carbon concentration measured during the field trial C1 and for the incubation experiments C2, shows no superior performance for one of the applied methods. For FYM, SLY, DG B, DG D-s the used dry matter and carbon concentration measured in the field improve the RMSE [g/kg] while for DG C, and DG D-l the properties measured for incubation experiment reduce the RMSE (Table III-5). The difference between the two methods is very small that it does not lead to a clear preference of one method over the other.

Table III-5: RMSE [g/kg] of the CCB output (Corg) using the mean dry matter content and carbon content of organic amendments from the field trial (C1) and the incubation experiment (C2), residual mass calculate with method R2, initialization with ME

	FYM	SLY	DG A	DG B	DG C	DG D-s	DG D-l
RMSE C1	0.584	0.401	0.401	0.366	0.429	0.446	0.511
RMSE C2	0.600	0.409	0.406	0.375	0.425	0.456	0.503

III.3.3 CCB Model Results and Validation

The final modelling of the field trial was conducted with the FOM quantities of stubble and roots calculated with the method R2 and the C concentrations of the organic amendments are taken from the incubation experiments (C2). Figure III-6 shows the mean values with standard deviation for the Corg measurements, the corresponding regression and the results of the CCB model for all treatments. The corresponding RMSE, rRMSE and sd of the observed Corg values are displayed in Table III-6. The CRL and the CAN treatment show a negative trend over the observed period, this trend is captured by the regression as well as by the CCB model. Nevertheless the CCB model overestimates and shows a much smaller decrease in Corg for CRL and CAN treatments compared to the regression. In contrast, the regression and the CCB model display an increase in SOC for the other treatments. The CCB model estimates a smaller increase in Corg for the FYM treatment compared to the regression, this accounts especially for later years.

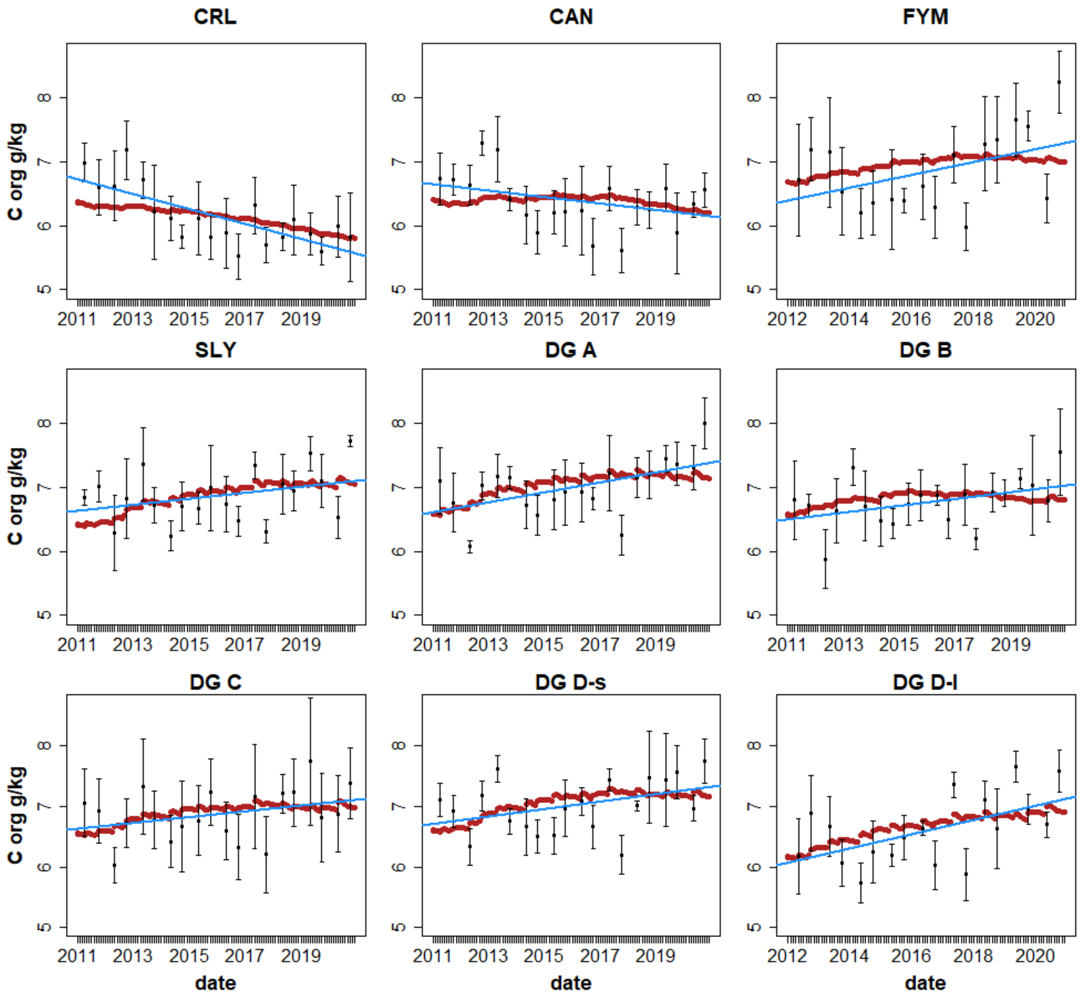

Figure III-6: Mean measured Corg (markers) with sd (N=4, 0-30 cm), CCB simulation (red line), CCB initialized with ME for each treatment, parametrization of residues R2, and chemical properties from incubation experiments (C2), regression (blue line), CRL = Control, CAN = mineral fertilizer, FYM = farm yard manure, SLY= slurry, DG = Digestates, s = solid fraction, l = liquid fraction

Table III-6: RMSE [g/kg] and rRMSE (%) for the modelled treatments with CCB and the mean (N=4) observation of the treatments, mean standard deviation (sd) for Corg and Nt measurements (N=4)

treatment	RMSE SOC	sd Corg	rRMSE SOC	RMSE SON	sd Nt	rRMSE SON
CTR	0.361	0.416	5.87	0.077	0.054	13.35
CAN	0.422	0.359	6.62	0.073	0.053	12.25
FYM	0.600	0.537	8.76	0.98	0.064	14.96
SLY	0.409	0.345	5.96	0.081	0.048	12.52
DG A	0.406	0.349	5.81	0.077	0.048	11.64
DG B	0.375	0.375	5.54	0.074	0.063	11.66
DG C	0.425	0.587	6.17	0.065	0.059	10.12
DG D-s	0.456	0.350	6.48	0.072	0.053	10.90
DG D-l	0.503	0.371	7.61	0.095	0.043	14.99

Figure III-7 shows the Nt turnover of Berge. The regression indicates a negative trend of Nt for the CRL and CAN treatment, while the CCB model predicts a slightly decrease for Nt in the CTL treatment and stable Nt dynamics in the CAN treatment for the given period. For all treatments with organic amendments the data shows stable or slightly increasing Nt concentration. The CCB prediction indicates a slight increase for those treatments.

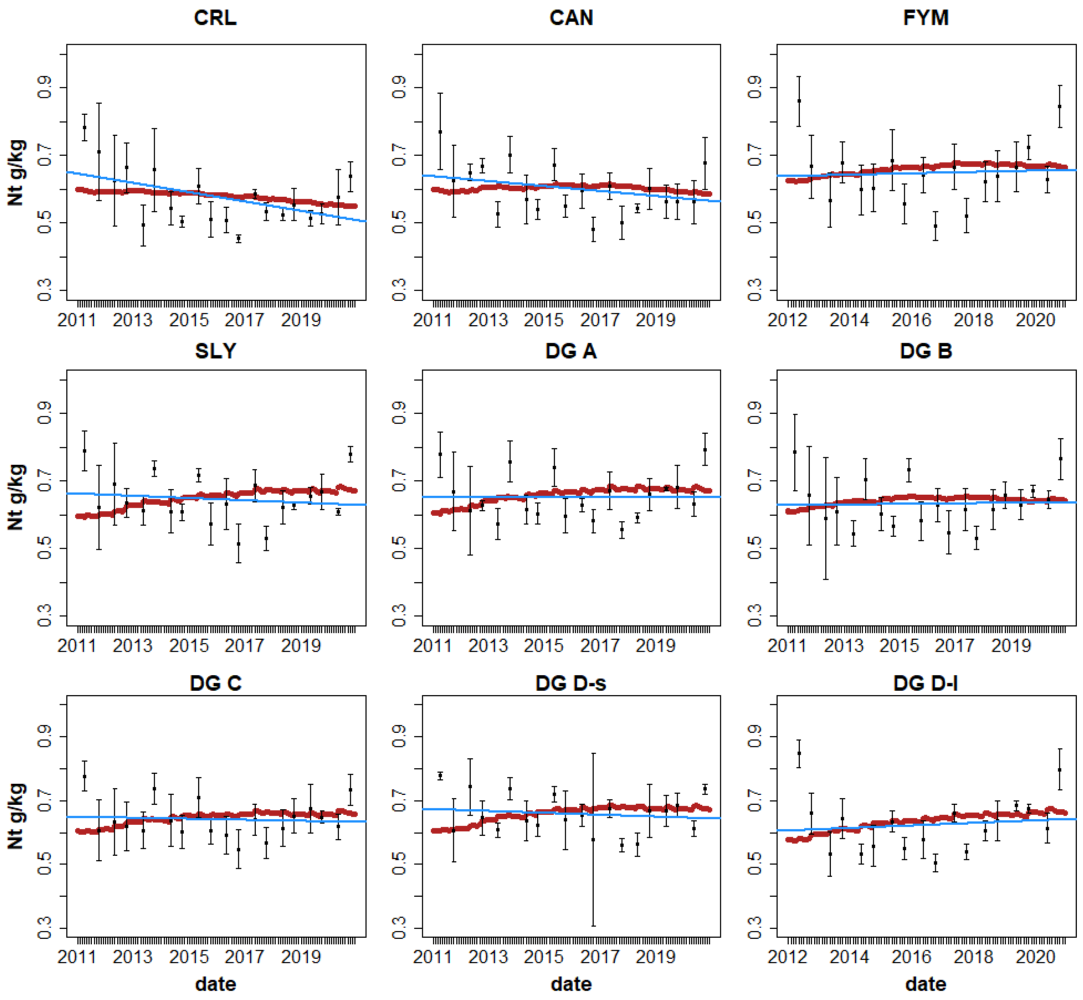

Figure III-7: Mean measured Nt (markers) with sd (N=4, 0-30cm), CCB simulation (red line), initialized with ME for each treatment, parametrization of residues with R2, and chemical properties from incubation experiments (C2), regression (blue line), CRL = Control, CAN = mineral fertilizer, FYM = farm yard manure, SLY = slurry, DG= Digestates, s = solid fraction, l = liquid fraction

III.4 Discussion

In mechanistic carbon models, commonly at least one parameter describing the carbon turnover or the pool sizes gets calibrated to fit the field measurements (Benbi et al., 2002). In this study no model parameter was optimized to the field data expect for the initial value, instead the CCB model was fitted to the carbon turnover of incubation experiments, including organic amendments, roots and stubbles, with substrate specific k_{fom} and η values. The modelling of the respiration curves showed overall good results (Table III-3) only for sorghum stubble and winter wheat stubble the RMSE was slightly higher, which can be caused by fluctuating respiration curves. Uncertainties arise from the incubation data for green rye, since it is sowed every year on the field site but no incubation data for the stubble and roots of green rye were available. Instead, the incubation results of winter wheat were used which are assumed to be the most similar to green rye and do not differ in chemical properties vital from green rye (Edmisten et al., 2008).

Further uncertainty can arise from the variability of the organic amendments applied on the field site. The physical and chemical properties for the organic amendments vary over the time, depending on the batch, while the CCB model uses constant parameters, which can lead to an over or under estimation of dry mass, C and N content. The comparison of the average chemical parameters of the organic amendments applied to the field (C1) and those derived from the laboratory (C2) vary only slightly. Moreover, for two treatments the chemical parameters derived from incubation are not within the standard deviation of the field values (Figure III-4). Also the RMSE for the modelled SOC values does not show big differences between method C1 and C2 and for the here considered field trial the chemical properties of the organic substrates received from the incubation experiments can be used to model the field trial with good results.

The model outcome of the CCB slightly underestimates the SOC loss of the Control treatment but the results are still within the standard deviation of the observed Corg values and the rRMSE with 5.87 is in a good range. The separate implementation of roots and stubble in the CCB and the parameterization of their dynamics in the laboratory enable the observation of the influence of roots, stubble and organic fertilizers on the SOC dynamics in the field in much greater detail. Levavasseur et al. (2020) used IROC values to parametrize the AMG model, with overall good results except for the control treatment, their explanation are the inappropriate allometric coefficients for roots. The here presented methods R1 & R2 were explicitly tested on treatments without the influence of organic amendments, which lead to an improved model accuracy and RMSE values which are smaller than the sd of the observed Corg values. Nevertheless the observed data still indicate a linear trend, which is due to the short period of the field trial and a longer period would lead to more pronounced dynamics. The CRL and the CAN treatments receive no addition of organic amendments and both treatments show a decrease in Corg and Nt. The calculated amounts of stubble and roots don't vary significantly across treatments. Hence, rise in Corg for the treatments with addition of organic amendments depends mainly on the input of Corg throughout the amendments and is not caused by the increase of net primary production and therefore more residues. The CAN treatment has the highest yields among others but still shows a decrease in Corg, Maltas et al. (2018) found similar results in their research, where the increase in crop does not induce an significant increase in Corg. Furthermore the statistical analysis of the yields shows that there are only significant differences in the yield between the treatments, of winter rye between the CRL and some treatments with organic amendments. Most likely the field trial needs to be continued for several years to observe significant effects.

Overall, the modelled SOC values show a good fit (Figure III-5) with rRMSE between 5.8 and 8.7 %, which is comparable to other studies (Begum et al., 2017; Franko et al., 2021; Levavasseur et al., 2020). Furthermore the RMSE and the mean sd of the observed Corg values are in a comparable range, thus the measuring errors and the variability of the plots is in the same scale as the model error. The reason why the FYM and DG C-l treatment shows a higher rRMSE compared to other treatments could be due to the optimization to the incubation data where one incubation batch could not be modelled because the CCB model reached its parameter limits since its mineralization was too low. Therefore incubation experiments should be conducted on different batches of organic material to cover their variability, due to the composition of parent material, the processes in gas plants and other influencing factors. Furthermore, the parameter limits could be extended to model more resilient substrates in the incubation experiment. While for the modelled SON values the rRMSE is above 10 % and the RMSE ≈ 0.01 [g/kg] for each treatment, the parameters might not be as easy transferable, since the SON calculation in the CCB model depends on the dynamics of carbon turnover and the mineral nitrogen pool is not considered. Furthermore the Nt data shows high variability, the first data points had to be adjusted due to the change in analytics, which can lead to inaccuracies. Further studies with N incubations as a basis could be a solution to improve the model accuracy.

III.5 Conclusions

This study successfully demonstrated how model parameters and chemical properties derived from incubation experiments can be transferred to model field experiments without many adaptations or optimisation of parameters to the field site. Those site-independent parameters are particularly important for scenario calculations and regionalization and can help to predict the behavior of organic amendments under field conditions. They are transferable to other sites with different environmental conditions, because the climate and soil functions implemented in the model can be adapted to the new sites. Also more uncommon substrates could be analyzed with incubation experiments and combined with model predictions, be a cheaper and less time intense approach to evaluate the long-term behavior of selected substrates compared to field experiments. While the N dynamics which rely on the C dynamics are not as easy transferable to the field site and needs further investigation.

III.6 Acknowledgements

Sincere gratitude is expressed to Paul Mewes and Sven Höcker for their research on the quality and quantity of roots and stubbles published in their Ph.D thesis. Furthermore, the authors express their appreciation to Martin Volk for critical reading and to Samira Kalemba for proof reading.

Contextualization

In Chapter III the upscaling of the parameters from incubation experiments was demonstrated and approved to be valid. Further methods to parametrize the residues according to their quantity were tested and applied. Those approaches will be further used in chapter IV to generate the parameters for org. amendments. Moreover, the CCB model will be re-established as the CNP-model with a novel P-module. The P-module comprises mineral P pools, as well as organic P turnover dynamics. The methods introduced in chapter II and III allow to account for diverse org. amendments, considering their specific turnover dynamics and nutrient compositions. P is one of the most important plant nutrients, it has an economic and environmental impact and the modelling of its dynamics can help to improve management strategies and be used to guide policy making. The inclusion of the P-module therefore is a consequent step towards a holistic view of soils and fertilization practice.

IV. Simulating the Soil Phosphorus Dynamics of Four Long-Term Field Experiments with a Novel Phosphorus Model

S. ANTON A. GASSER, KERSTIN NIELSEN, BETTINA EICHLER-LÖBERMANN, MARTIN ARMBRUSTER, INES MERBACH, UWE FRANKO

Abstract

Phosphorus is a non-renewable resource which is required for crop growth and to maintain high yields. The soil P cycle is very complex, and new model approaches can lead to a better understanding of those processes and further guide to research gaps.

The objective of this study is to present a P-submodel which has been integrated in the existing Carbon Candy Balance (CCB) model that, already comprises a C and N module. The P-module is linked to the C mineralization and the associated C-pools via the C/P ratio of fresh organic material. Besides the organic P cycling the module implies a plant available P-pool (P_{av}), which is in a dynamic equilibrium with the non-available P-pool (P_{na}) that comprises the strongly sorbed and occluded P fraction.

The model performance was tested and evaluated on four long-term field experiments with mineral P fertilization, farm yard manure as organic fertilizer and control plots without fertilization. The C dynamics as well as the P_{av} dynamics were modelled with overall good results. The relative RMSE for the C was below 10% for all treatments while the relative RMSE for P_{av} was below 15% for most treatments.

To accommodate for the rather small variety of available P models, the presented CNP-model is designed for agricultural field sites with a relatively low data input, namely air temperature, precipitation, soil properties, yields and management practices. The CNP-model offers a low entry threshold model approach to predict the C-N and now the P dynamics of agricultural soils.

IV.1 Introduction:

In the last decades a lot of effort has been made to analyze carbon and nitrogen cycling in soil and to develop models which represent those processes. A further key element for plant nutrition is P which is responsible for plant growth, reproduction and energy transfer within the plant. In agriculture, mineral P is used as fertilizer but P reservoirs are limited and depleting (Sulieman et al., 2021; Yan et al., 2022). Therefore, P cycling gains a rising interest in agricultural praxis. Hereby the application of organic amendments can be an essential part in closing the P cycle. Besides fertilization, P occurs naturally in bedrock and is slowly released through weathering of P-bearing minerals (Dzombak et al., 2020). For some regions, P input through deposition can play an important input factor (Vet et al., 2014), however erosion and leaching processes are an important output pathway where P can get lost into hydrological systems (Alewell et al., 2020).

In soils, P occurs in different species. Water dissolved P, which is directly plant available, while weakly adsorbed P can be made available by plants e.g. through root exudates. Furthermore, P can be bound to aluminum (AL) or iron (FE) complexes or organic compounds. The organic bound P is linked to the C cycle and occurs in biomolecules, such as nucleic acids, phosphoproteins, sugar phosphates, and inositol phosphates (Wang et al., 2021). There is a wide variety of analytical extraction method for different P species like calcium acetate extractable P, double lactate extractable P, Olsen P, Mehlich 3, just to mention some (Wuenscher et al., 2016).

While those measurable P species represent the extraction method, in model approaches P species often get aggregated in conceptional pools which interact with each other. The choice of pools has to be adapted to the complexity of the analyzed system, the data input, the evaluation between complexity and sufficient accuracy. There are some models addressing P turnover in soils: the DDPS model (dynamic phosphorus pool simulator) comprises two pools on spatial scale with annual steps

(Sattari et al., 2012; Zhang et al., 2017), whereas the APLE (Annual P Loss Estimator) model calculates the P dynamics on annual scale with three inorganic P-pools and an organic one (Vadas et al., 2012). The LePA (legacy phosphorus assessment) model considers three inorganic P-pools with P fluxes on annual steps (Yu et al., 2021). However, none of these models considers the organic P cycle separately. In DDPS, organic P is assumed to be part of the labile and stable P-pools but it is not considered that P gets released during mineralization of C or bound during the building up of soil organic matter (SOM). APLE assumes a fix rate of organic P which is not mineralized at the end of the year, not considering, environmental conditions, the date of application nor chemical composition of the organic amendments. Neither do they calculate the crop P uptake, rather fix numbers are assigned (DDPS) (Sattari et al., 2012) or the soil P content is used to calculate crop uptake with linear regressions, which are site specific (LePA.)(Yu et al., 2021)

The P model approach presented in this paper is integrated into the existing CCB model (Franko et al., 2011), which already comprises C and N modules and targets arable soils requiring small data input on a monthly time scale. From now, on this model is labeled as CNP-model. In addition to the mineral P fractions, the new P-module also deals with an organic P fraction, where the P turnover is coupled to the C mineralization of the three SOM-pools of the CNP-model. Notably, each fresh organic matter (FOM) input is characterized by specific mineralization parameters and a FOM specific C/P ratio. Furthermore, the P-module describes an easily available P (P_{av}) fraction, which is considered as plant available pool. The P_{av}-pool acts as active pool which is responsible for the translocation of P into other pools and serves as first sink for P inputs. The P_{av}-pool is in a dynamic equilibrium with the non-available pool (P_{na}) which represents the bound and occluded P species. All P associated to the SOM pools, the P_{av}-pool and the P_{na}-pool, form together the total P fraction.

Long-term field experiments (LTE) are most suitable for examining P fertilization management on the soil P status. They enable studying complex fertilizer turnover processes in soils operating on long time scales under environmental conditions. Thus they provide an overview of the effectiveness of fertilizer management on nutrient mobilization, transformation, translocation, and uptake by crops (Siebers et al., 2021). Furthermore, LTEs provide sufficient data to validate model concepts for P dynamics which are not as easy predictable as C and N dynamics due to high complexity.

For this study four LTEs where used to evaluate the P model. The LTEs are located across Germany with different soil types and have different crop rotations. The input data requirement for the CNP-model is relatively low needing air temperature, precipitation, crop yields and management (e.g. ploughing, irrigation, time of seeding and harvest), fertilizer inputs, as well as soil properties like clay and silt content, bulk density and initial values for C and P. The model validation was performed on control plots without fertilizer amendments, mineral fertilized plots and plots with farm yard manure (FYM) as organic fertilizer. Thus, common mineral and organic treatments are used to evaluate the model performance. Moreover, the model is tested on non-fertilized plots to conclude about anthropogenic unsupplied P soil processes.

Agricultural process models can serve as tool to conclude about nutrient dynamics and can help to identify research gaps and provide practical support for farmers and stakeholders. Therefore, the aim of this study is to present the P soil model approach, to validate its performance and to test the model concept on different soils, and management practices.

The main objectives of this study were:

i: Introduce and describe the P model concept.

ii: Validate the P-module on four long-term field experiments with control plots, mineral fertilization and organic fertilization, with different soil properties.

iii: Evaluate the model performance compared to the field measurements.

IV.2 Material and Methods

IV.2.1 Field Trials

Four different field trials were considered for the model evaluation. The field trials were situated across Germany, in Bad Lauchstädt (BL) in Saxony-Anhalt, Berge (BG) in Berlin, Speyer (SP) in Rhineland-Palatinate and Rostock (RO) Mecklenburg Western Pomerania. The required weather data was received from the closest weather station to the test site.

The validation of the P-model was conducted on the control plots (CRL), plots with mineral fertilization (MIN) and plots with farmyard manure (FYM) application. A brief overview is given in Table IV-1.

Table IV-1: Soil properties of field trials for the upper 30 cm, the considered period of the trial and fertilizer application

Field trial	**Clay [%]**	**Silt [%]**	**Sand [%]**	**Soil pH**	**Period [years]**	**CRL [kg ha-1 a-1]**	**MIN [kg ha-1 a-1]**	**FYM**	**Location**
BL	21	68	11	7	1950-2019	No fertilizer	N: 40-170 , P: 0-60	30 t ha-1 biennially No P and N	51°23'25.8" N 11°52'49.1" E
BG	1.1	9	89.9	5.54	2011-2022	No fertilizer	N ~ 250, no P	12.5 t ha-1 a-1 No P and N	52°37'11"N 12°47'16"E
RO	7.65	24.5	67.85	5.64	1999-2014	N: 160, no P	P: 21.8, N:150- 200	30 t ha-1 triennially No P and N	54°03'41.6" N 12°05'07.2" E

SP	9	20	71	6	1984-2018	No N, P: 30	P: 30, N: 200-240	30 t ha-1 triennially, P 30 kg ha-1 a-1, No N	49°21’40’’N 8°25’14’’E

In the LTEs of BG, BL and RO the available P species was measured as double lactate soluble P (DL-P), since this is common for the northern part of Germany. Due to the replacement of the DL-P Method, the values were transformed to calcium acetate lactate soluble P (CAL-P) following van Laak et al. (2018) using the equation:

$$CAL_P[mg * kg^{-1}] = 8 + 0.61 * DL_P[mg * kg^{-1}] \qquad 16$$

IV.2.1.1 Berge (BG)

The field trial was set up in March 2011 with a one-factorial randomized block design, with four replications. The crop rotation was: Winter rye as whole crop silage followed by maize and in the next year winter rye as whole crop and silage–sorghum. Fertilizers were applied twice a year before the sowing of either rye or maize/sorghum. Furthermore, it is to be noticed that all treatments have been cultivated with winter wheat and mustard as intercrop with an N fertilization of 100 kg N ha^{-1} as pre-management.

The fertilizer quantities were based on the amount of applied carbon of a standard farmyard manure (FYM) application of 12.5 t ha^{-1} a^{-1} (7.5 t ha^{-1} before maize or sorghum and 5 t ha^{-1} before winter rye). The amount of the other organic fertilizers is determined by the amount of organic carbon (Corg) spread by the manure at every application date, so that the amount of Corg is the same for all applied organic fertilizers. The resulting differences in applied nitrogen were balanced by mineral fertilization.

At each plot five soil samples were taken to a depth of 20 cm two times a year (2011-2020), once after the harvest of green rye in May and then after the harvest of either sorghum or maize in October. The soil was air-dried, sieved (<2 mm) and analyzed for soil organic carbon (Dumas) and phosphorus content (double lactate method).

IV.2.1.2 Bad Lauchstädt (BL)

The Static Fertilization Experiment in Bad Lauchstädt was set up in 1902 on an area of 4 ha, divided into 8 fields of which the third was used. The experiment has a systematic design without replications. The analyzed plots were fertilized with organic manure donation of 30 t/ha every second year. Further, a plot series without any addition of manure was established. Besides the organic fertilization the plots were further subdivided into plots with mineral fertilization with the addition of NPK and without mineral fertilization. The level of mineral fertilization has been geared to breeding progress from the very beginning. Farmyard manure, P and potassium (K) are applied every two years after the harvest of cereals. Cereals receive two mineral N applications: at the beginning of vegetation and at the beginning of tillering. Silage maize is N-fertilized before sowing. N is fertilized as calcium ammonium nitrate, P as triple superphosphate (TSP) and K as 60 % potash. The harvested crop, including the by-products, is driven off the field. The crop rotation was sugar beet-spring barley-potato-winter wheat until 2014. In 2015, the sugar beet and potato were replaced by silage maize.

The soil samples were each taken after harvesting with a grooved auger at a depth of 0-20 cm, dried, sieved (2 mm) and analyzed (SOC after dry burning -elemental analysis, P double lactate (DL)-extract with photometry/F-AAS). Details can be found in Körschens (2000).

IV.2.1.3 Rostock (RO)

In autumn 1998 the field trial was established as randomized slit-plot with four replication. Rather than having a fix crop rotation, the field trial was cropped with varying crops, starting in 1999 with spring rape followed by spring barley (2000), spring wheat (2001), spring rape (2002), winter wheat (2003), winter barley (2004) winter rape (2005), maize (2006-2008), sorghum (2009, 2010), sunflower (2011), winter rye (2012) and maize (2013, 2014). Furthermore, intercrops have been cultivated in the years 1999, 2000, 2001, 2002 with an intercrop mix, 2006 with buckwheat, 2007 with mustard, 2008 with a rye mix, and 2009 with green rye.

For this study the control treatments with no addition of P, the mineral plots with fertilization of TSP, and the plots with cattle manure where chosen. TSP was applied annually at a rate of 21.8 kg P ha^{-1} while the manure was applied every three years at about 30 t ha^{-1} (1998, 2001, 2004, 2007, 2010, and 2013) (Zicker et al., 2018).

The soil sampling was carried out twice per year in February/March and September in the upper soil layer (0–30 cm) with four spatial replications (samples from each spatial repetition consisted of ten to 15 subsamples). Soil samples were air-dried and sieved (2 mm) and plant available P was extracted with double-lactate solution.

IV.2.1.4 Speyer (SP)

The test site is located in the Upper Rhine valley north of Speyer (Germany) at 99 m above NN. The soil is a cambisol developed from loamy sand with a low field capacity of 10 %. The average annual rainfall is 600 mm and the average annual temperature is 10 °C. Due to the low water capacity the trial is irrigated if necessary.

The field trial was performed within the International Organic Nitrogen Fertilization Experiment (IOSDV) to investigate the interaction of a combination of organic and mineral fertilization. The experiment with a three year crop rotation of sugar beet, winter wheat, and winter barley was established in 1983. Additionally, since 2004 different soil tillage methods were investigated.

The different fertilization treatments were set up based on a full-factorial design on plots with a size of 6 m * 7.5 m with three replicates for each treatment but with a shifted crop rotation. The chosen plots were fertilized with mineral N application of 0 and 240 kg N ha^{-1} yr^{-1} for sugar beet, 0 kg N ha^{-1} yr^{-1} for winter wheat and 200 kg N ha^{-1} yr^{-1} for winter barley. All plots received P fertilization, therefore there is no real control plot (CRL*). Farmyard manure was applied at a rate of 30 t ha^{-1} ahead sugar beet. The intercrop received 50 kg ha^{-1} mineral nitrogen fertilizer.

Mineral fertilization with basic nutrients is carried out in all variants in a uniform manner with an average (1984-2018) of 30 kg P ha^{-1} yr^{-1}, 118 kg K ha^{-1} yr^{-1} and 32 kg Mg ha^{-1} yr^{-1}. Details about the field experiment can be found in Körschens (2000).

IV.2.2 Model Description

IV.2.2.1 Carbon Module

The CNP-model is an enhancement of the CCB model (Franko et al., 2011) where a new P-module is coupled to the C-model of the CCB. The C-module describes the turnover of decomposable carbon in monthly time steps depending on site conditions, crop yields and input rates of FOM. A specific characteristic of the CCB model is the handling of FOM as a list of specific pools from which the C is released to atmosphere or used to build up new SOM. Each FOM entry in that list also comprises a specific C/P ratio. The decomposition is controlled by the FOM specific parameters k_{fom} describing the FOM breakdown and eta (η) describing the part of carbon that is transferred to SOM. First, FOM is moved into the pool of active SOM (A-SOM) which behaves like the microbial biomass that is interacting with the pool of stabilized SOM (S-SOM) and acts as the mineralization driving pool.

Additionally, the C model includes the long-term stabilized pool (LTS-SOM) where SOM is considered as physically protected. All this processes, as well as the FOM turnover, are controlled by site conditions like soil texture, air temperature and rainfall. These conditions are aggregated into a Biologic Active Time (BAT in days [d]) expressing the part time interval that would be required under optimal conditions in the laboratory to produce the same C-turnover as under real conditions in the field. Additionally, a matter transfer between A-SOM and LTS pool is considered. A part of the newly built SOM (C_{rep}) is captured inside micropores and thus shielded from decomposition, whereas a part of C-LTS is released from protection and exposed to microbial turnover. Details about the CCB modelling approach and its applications to describe SOM topsoil dynamics were already published (Franko et al., 2021; Franko et al., 2011).

IV.2.2.2 P-module

The new P-module links the organic P cycle to the C-pools A-SOM, S-SOM and LTS which are aggregated to P_{SOM} in Figure IV-2. When FOM enters the system, a part gets transferred into the SOM-pools (Figure IV-2 [2]), while another part gets mineralized and P is released ($P_{FOM(min)}$) and transferred to the P_{av}-pool (Figure IV-2 [3]). During C mineralization of the SOM-pools the C assimilated P moves through these pools. The C/P ratio for the SOM-pools is assumed to be 186 (Cleveland et al., 2007). A-SOM ether controls the release of organic P during the mineralization of SOM ($P_{SOM(min)}$) (Figure IV-2 [4]) or the sequestration into a SOM-pool with a longer detention time (S-SOM or LTS for detail description see section 2.2.1).

Additionally the P-module comprises an available P-pool (P_{av}), which represents the plant available P species including dissolved P and easily sorbed P. The P_{av}-pool is in an equilibrium with the non-available P-pool (P_{na}) (Figure IV-2 [9, 10]). This pool represents the P which is strongly sorbed to the mineral phase of the soil.

The equilibrium is described by the function:

$$PS = 0.6226 + P_{av} * 0.0131 + clay * 0.0214 - SOC * 0.0621 - \ln(silt) * 0.2085 \quad 17$$

Where the function is influenced by the current state of P_{av} and SOC content as well as by the clay and the silt content of the soil. PS represent the relation between P_{av} and P_{na}:

$$PS = \frac{P_{av}}{P_{na}} \quad 18$$

Where P_{na} can be calculated:

$$P_{na} = P_t - P_{av} - P_{SOM} \quad 19$$

The observed PS value can be received from measurements with formula 3 and 4 with given Pt, Pav and SOC values assuming SOM has a C/P ratio of 186. The calculated PS value can be obtained from formula 2, the relation between those approaches is displayed in Figure IV-1 which match the identity line.

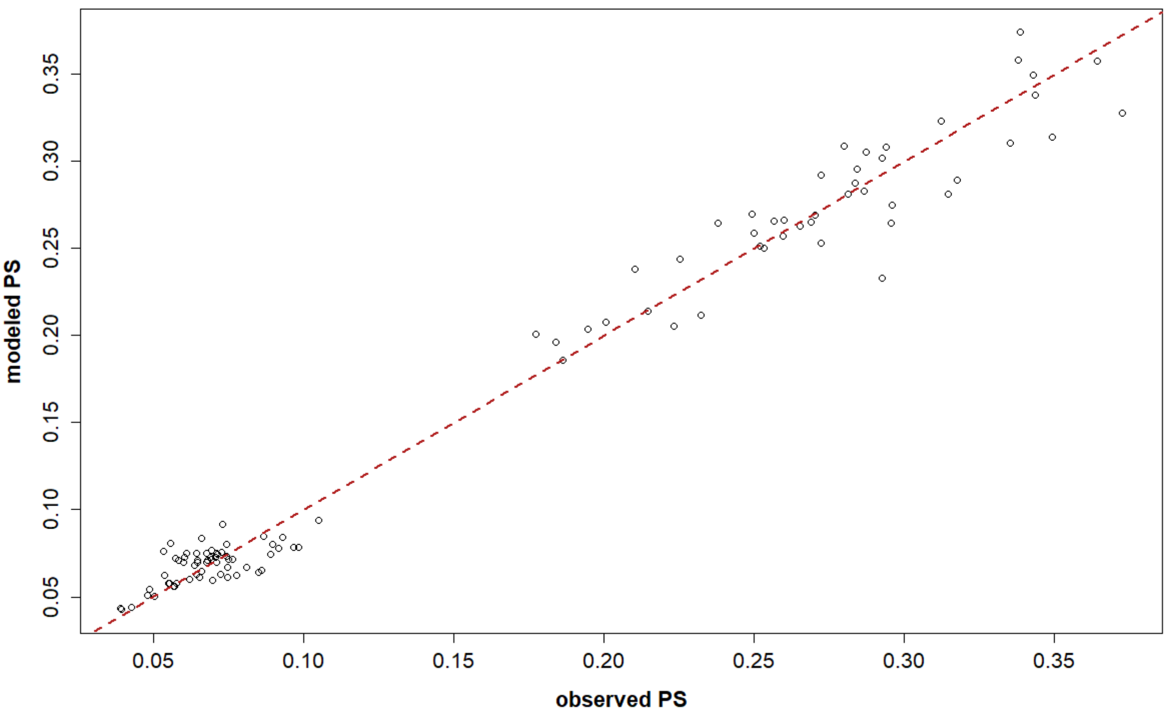

Figure IV-1: Observed PS calculated with formula 3 and the modelled PS received with formula 2, red: the identity line (1:1)

The plant uptake is withdrawn from the P_{av}-pool (Figure IV-2 [11]), while the amount is calculated trough the production of biomass, distinguishing between main product, by product, stubble and roots. With the harvest of crops, P (P_{crop}) gets removed (Figure IV-2 [13]) from the system while stubble and roots enter the P cycle as FOM (Figure IV-2 [12]). Mineral P fertilizer (P_{fert}) enters with 80 % into P_{av} and with 20 % into P_{na} (Figure IV-2 [7, 8]), while a constant amount of P enters through weathering (P_w) or deposition directly into the P_{av}-pool (Figure IV-2 [6]).

On a monthly base (i), the state of the P_{av}-pool is calculated as:

$$P_{av(i+1)} = P_{av(i)} + P_{SOM(\min(i))} + P_{FOM(\min(i))} + P_{w(i)} + 0.8 * P_{fert(i)} + P_{na(i)} * \kappa - P_{av(i)} * \kappa * z_i - P_{crop(i)} \quad 20$$

Where ϰ represents a constant site specific parameter and z is expressed as:

$$z = \frac{1}{PS} \tag{21}$$

And the corresponding P_{na} value is calculated with equation 7:

$$P_{na(i+1)} = P_{na(i)} - P_{na(i)} * \kappa + P_{av(i)} * \kappa * z_i + 0.2 * P_{fert(i)} \tag{22}$$

The total Phosphor (P_t) comprises the P_{av}, P_{na} and P_{SOM} pools:

$$P_{t(i+1)} = P_{av(i)} + P_{na(i)} + P_{SOM(i)} \tag{23}$$

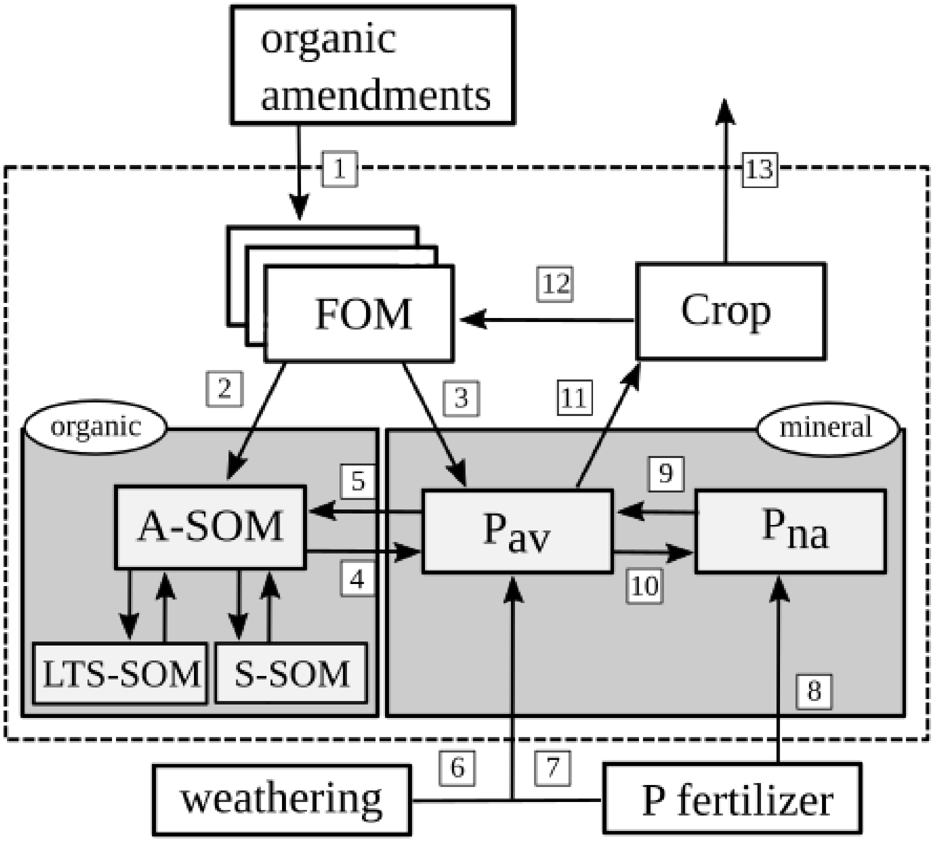

Figure IV-2: Visualization of the P fluxes in the CNP-model; 1: External input of organic amendments like farm yard manure; 2: P transferred from FOM-pools to SOM (A-SOM), 3: P transfer into P_{av} during C mineralization depending on the C/P ratio of FOM; 4: P release during C mineralization of SOM; 5: P uptake of SOM from P_{av} during the buildup of SOM (details in the description of the C module); 6: P input into P_{av} trough weathering; 7: 80% mineral P input into P_{av} through mineral fertilizer; 8: 20 % mineral P input into P_{na} through mineral fertilizer; 9: ϰ, the flux from P_{na} to P_{av} (site specific); 10: the flux from P_{av} to P_{na}, ϰ *z (z depends on PS); dark grey boxes: total P; 11: Crop P uptake into main product, by-product, stubble and roots; 12: FOM-P input trough stubble and roots of the crop; 13: P removal with main product and by-product

IV.2.2.3 Initialization

The P dynamics depends on the C turnover of the examined soil system. Therefore the C mineralization has to be initialized first with feasibly good results, to improve the P modelling results. The C-module was initialized by minimizing the mean error, with the integrated function of the CNP-model.

For the initialization the P-module requires a $\varkappa$ value which is site specific and was chosen to fit the CRL plot as well as possible, with respect to good results of the other plots. Furthermore, a start value for the P_{av}-pool is required and a P_t value which gets calculated internally if not provided where P_{na} can be calculated from P_{av} and PS:

$$P_{na} = \frac{P_{av}}{PS} \qquad 24$$

P_{SOM} gets calculated according to the distribution of C into the C-pools. The weathering rate was assumed to be 1 kg ha^{-1} a^{-}1 except for BL which was set to 5 kg ha^{-1} a^{-1}.

Table IV-2: The $\varkappa$ values for each plot received by optimization and the initial P_{av} and P_t values for the plots

		CRL initial value		MIN initial value		FYM initial value	
LTE	$\varkappa$	P_{av}	P_t	P_{av}	P_t	P_{av}	P_t
BG	0.009	10	48	10	51	10	46
BL	0.002	4	50	4	40	4	63
SP	0.0035	20,23,27	43,42,44	16,20,20	42,48,50	23,20,26	37,40,42
RO	0.011	3.2	60	3.2	58	3.2	60

IV.2.2.4 Parametrization

The C-model requires on the one hand parameters to determine the quality of FOM as well as parameters which describe the quantity of FOM in terms of the amount of crop residues at a certain yield. The quality of each FOM unit is defined by the dry matter content and the C content, separating FOM into organic fertilizers, by-products which remain on the field, stubble and roots as well as the incorporation of catch crops. Furthermore the quality is described by the FOM specific mineralization parameters of the CNP-model. With k_{fom} which is the turnover coefficient of FOM and η the synthesis coefficient which describes the relation between CO_2 release to the composition of A-SOM. Furthermore, the C/P ratio of each FOM unit is required. The quantification of Crop input is described by linear functions between the main product and the corresponding amount of by-product, stubble and roots (Franko et al., 2021; Gasser et al., 2021b; Gasser et al., 2022). This is of importance for the SOM cycle as well as for the organic P cycling in the model. The input of each FOM unit needs to be specified and can have different parameters for the mineralization as well as for the chemical composition, resulting in different qualities for each FOM input. Furthermore, for each FOM input the C/P ratio of the stubble and roots needs to be defined. An overview of the used parameters is given in Table IV-3.

Table IV-3: the main crop parameters required by the CNP-model, with the dry matter (dm_{mp}), as well as the C and P content (%) of the main product (mp), stubble (st) and roots (rt); C/P ratio of stubble and of the roots; Stix, Fix_s and Rix are the parameters to calculate the amount of stubble in dependence of the main product; Bix and Fix_r describe the amount of roots in dependence of the main product, η_{st} and $k_{fom(st)}$ describe the decomposition of the stubble and η_{rt} and $k_{fom(rt)}$ of the roots

Crop	Main Product	Dm_{mp} [%]	P_{mp} [%]	C_{mp} [%]	C_{st} [%]	C_{rt} [%]	C/P_{st} [-]	C/P_{rt} [-]	Stix [-]	Fix_s [dt]	Fix_r [dt]	Bix [-]	Rix [-]	η_{st} [-]	$k_{fom(st)}$ [-]	η_{rt} [-]	$k_{fom(rt)}$ [-]
maize	plant	32.9[c]	0.187[b]	42[e]	42	37.8	182.6[f]	317.9[g]	1	0	0	0.0851	0.059	0.313	0.067	0.419	0.124
potato	tuber	20.6[a]	0.22[a]	40.4[h]	33	40.7	194.1[h]	145.8[h]	1	0	3.2	0.28	0.14	0.39	0.12	0.54	0.17
sorghum	plant	35.1[c]	0.22[bc]	41	41	33.8	136.6[c]	355.4[c]	1	0	0	0.1935	0.107	0.257	0.073	0.456	0.112
sunflower	plant	21.6[b]	0.32[ab]	40	43	34.9	165.4[a]	132[g]	1	0	27.9	0.4	0.27	0.39	0.12	0.54	0.17
spring barley	grain	86	0.35[b]	40.6	45	35	1006.7[e]	368.4[e]	0.1	0	7.2	0.125	0.85	0.39	0.12	0.54	0.17
spring rape	seeds	92.3[a]	0.74[ab]	60	44.9	35	748.3[f]	472.9[g]	0.1	0	13.2	0.19	1.47	2.4	0.71	0.54	0.17
spring wheat	grain	86	0.37	44	45.8	35.5	915[f]	593	0.1	0	6	0.088	0.87	0.57	0.2	0.55	0.125
sugar beet	tuber	23	0.17	39	31.4	37.9	84.9[a]	222.6[a]	0	5.3	4.7	0	0.55	0.62	0.67	0.54	0.17
winter barley	grain	86	0.35[b]	44	45	35	1006.7[e]	368.4[e]	0.1	0	9.3	0.13	0.84	0.39	0.12	0.54	0.17
green rye	plant	22.9[c]	0.44[b]	43[d]	42	35.6	330.7	273.8	1	0	0	0.257	0.097	0.257	0.07	0.57	0.139
winter rape	seeds	92.3[a]	0.60[b]	60	44.9	35	748.3[f]	472.9[g]	0.1	0	4.6	0.179	1.58	2.4	0.71	0.17	0.54
winter wheat	grain	86	0.31[b]	40.6[e]	45.8	35.5	915[f]	593.3[e]	0.1	0	11.6	0.16	0.93	0.57	0.2	0.55	0.125
oil radish	catch crop	15	0.168	43	43	35	256[j]	208[j]	0	4.68	7.0	0	0	0.39	0.12	0.54	0.17
mustard	catch crop	15	0.35	43	43	35	198[i]	194[i]	0	4.1	7.6	0	0	0.39	0.12	0.54	0.17
buckwheat	catch crop	15.9[a]	0.24[a]	43	43	35	179[a]	145	0	4.4	6.6	0	0	0.39	0.12	0.54	0.17

Source: a: ("Feedipedia - Animal Feed Resources Information System,"); b: measurements LTE RO; c measurements LTE BG, d: (Mewes, 2017); e: measurements LTE BL; f:(Max et al., 2022); g calculated with formula 8; h:(Chea et al., 2021) i:(Hallama et al., 2022); j:(Mann et al., 2021)

The total P content of the stubble and the roots of four crops where harvested and analyzed internally in a laboratory. This was done for winter wheat and spring barley in BL and for sorghum and green rye in BR. The linear regression is shown in Figure IV-3 and equation 25 (residual error = 0.47 [g/kg]). For plants with lacking information about the P content in roots the regression was used as approximation to calculate the amount of P in the roots in accordance to the amount of P in the stubble.

$$P_{root\,[g/kg]} = 0.17186 + P_{stubble\,[g/kg]} * 0.9472 \qquad 25$$

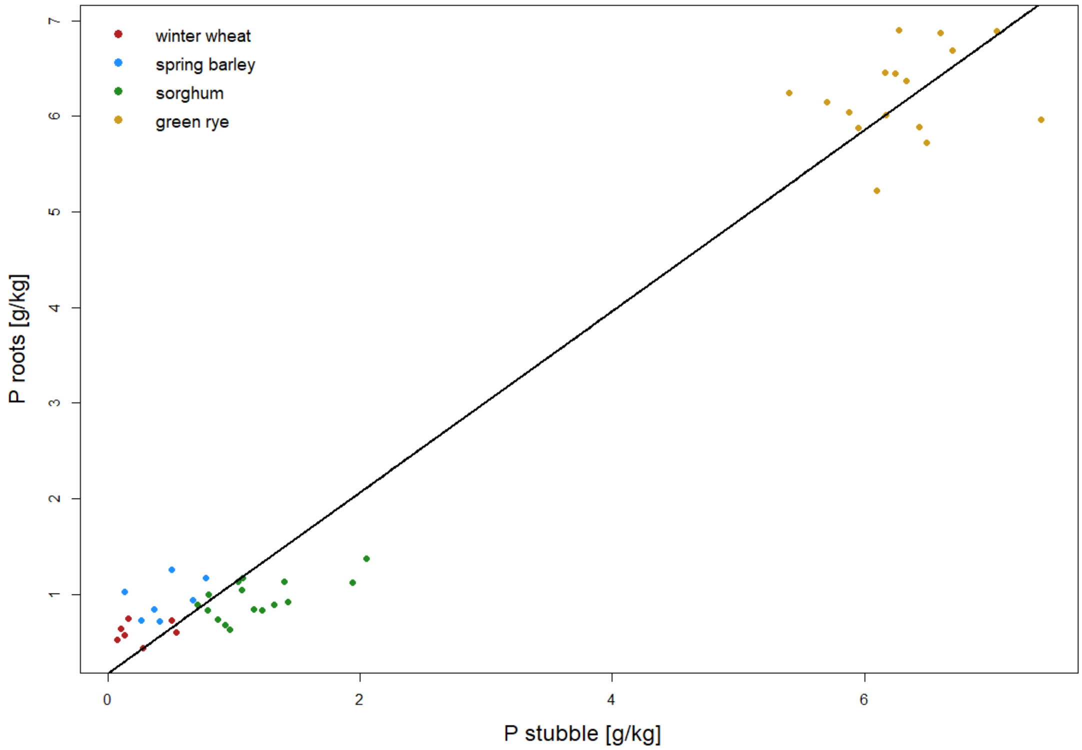

Figure IV-3: Relation between P in stubble and roots of four crops (red: winter wheat, blue: spring barley, green: sorghum, orange: green rye)

The k_{fom} and η values where determined by the modelling of incubated organic material, where the CO_2 release was measured over time, for details see Gasser et al. (2021b); Gasser et al. (2022). If no incubation data for a specific crop residue or roots was available, the average of either all available stubble or roots was used. The average parameters for stubble are, $k_{fom(st)} = 0.12$ and $\eta_{st} = 0.39$ (N = 13), while for roots the average was used of incubate fine roots (N = 12) and coarse roots (N = 7) with $k_{fom(rt)} = 0.17$ and $\eta_{rt} = 0.54$.

The farm yard manure was parametrized according to the data of the average FYM applied on the corresponding LTEs.

Table IV-4: Model parameter for FYM, the dry matter content [dm], carbon content, the C/P ratio and the mineralization parameter k_{fom} and η for all LTEs

LTE	dm [%]	C [%]	C/P ratio	k_{fom}	η
BG	23.7	32.1	45.1	0.095	0.67
BL	27	37.9	56.3	0.114	0.64
RO	28	39	53.5	0.123	0.67
SP	31	39	79.6	0.123	0.67

IV.2.3 Statistical Analysis

The goodness of fit was evaluated by the root mean squared error (RMSE, Equation 26) and furthermore the relative RMSE (rRMSE, Equation 27) was calculated to characterize the differences between observed values (O) and predicted values (V), with $\bar{O}$ as mean of the observations:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(O_i - V_i)^2}{n}} \tag{26}$$

$$rRMSE = \frac{100}{\bar{O}} \sqrt{\frac{\sum_{i=1}^{n}(O_i - V)^2}{n}} \tag{27}$$

IV.3 Results

IV.3.1 Available P Dynamics

The model results are displayed in the following section. In BG the overall trend for P_{av} shows a decrease over the observed period. The CRL plot shows higher P_{av} values than the MIN plot which can be attributed to the higher removal of P_{av} due to higher crop yields.

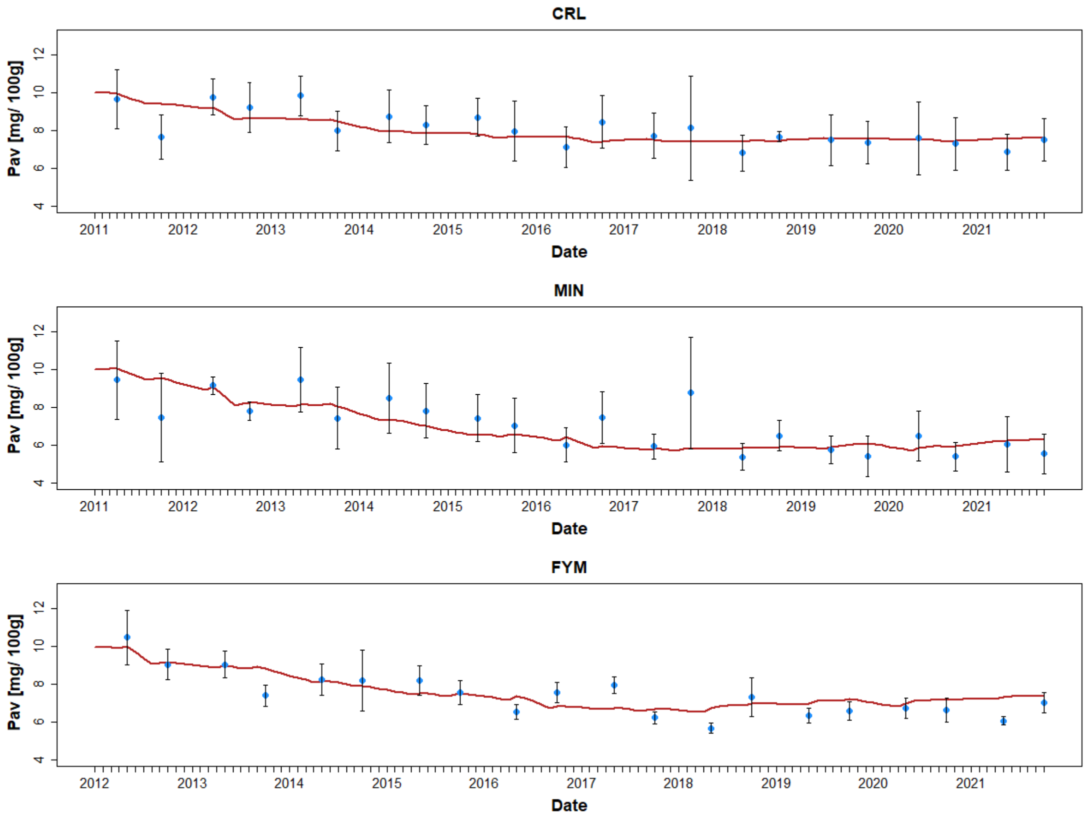

Figure IV-4: P_{av} dynamics for BG, blue mean of transformed DL-P to CAL-P measurements with standard deviation (N=4), red modelled P_{av} values.

In BL the difference between P_{av} at the CRL and FYM plot are relatively (4-15 mg/100g) big compared to the other LTE, which can be due to the long experimental setup. Especially in the early years of the LTE the model overestimates the P_{av} dynamics. On the MIN plot the P-CAL dynamics stay constant despite continuous P fertilization.

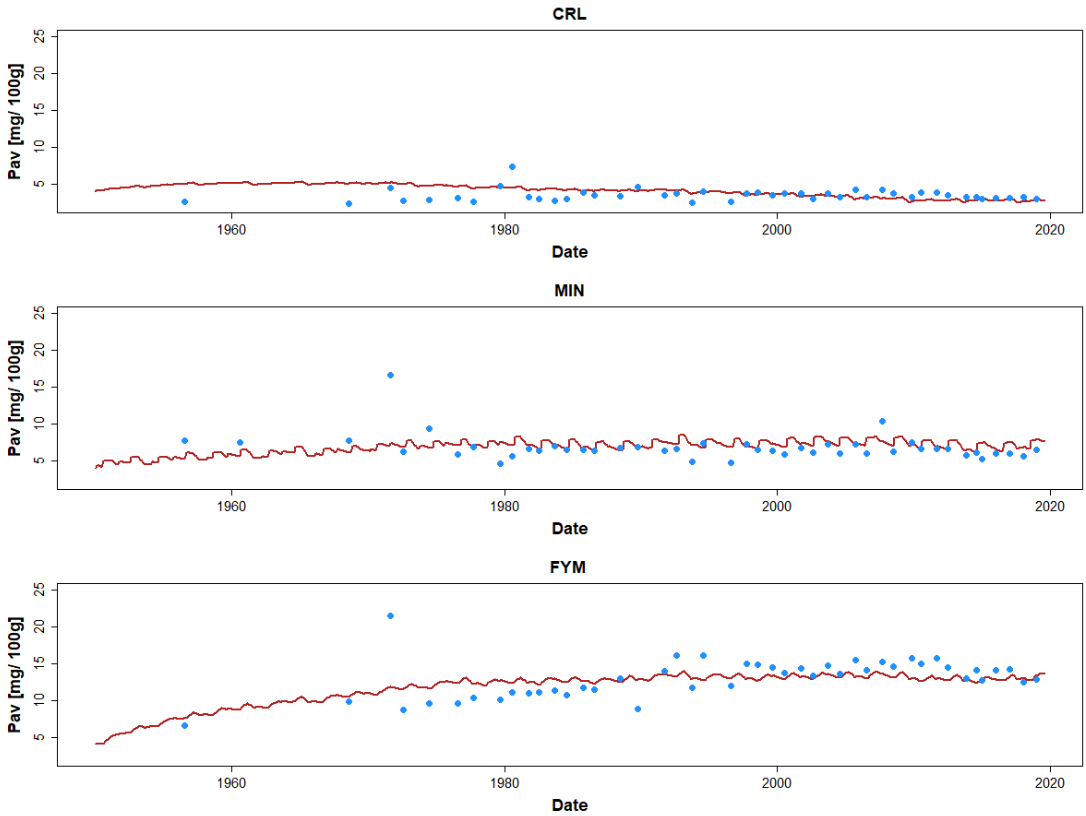

Figure IV-5: P_{av} dynamics for BL, blue transformed DL-P to CAL-P values (N=1), red modelled P_{av}

The plots in RO show the lowest P_{av} values, while P_{av} seems to decrease at the CRL plot it stays at the same level for MIN and FYM and no big differentiation between the plots is visible.

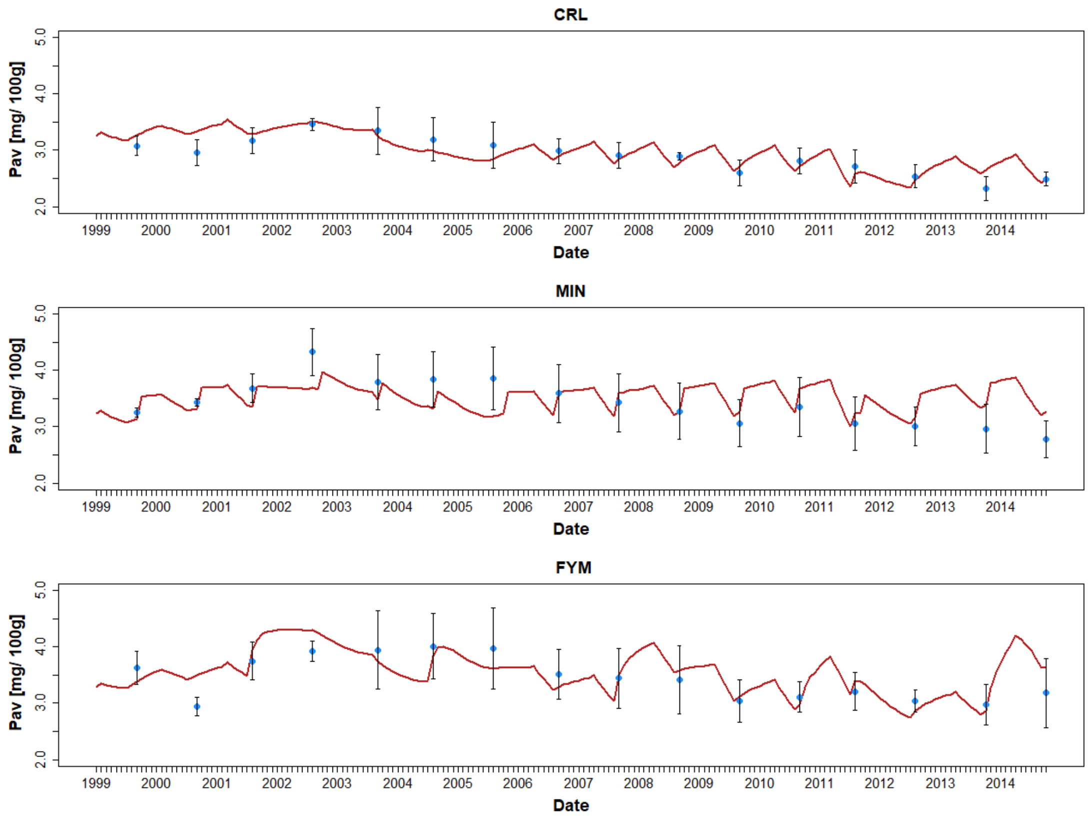

Figure IV-6: P_{av} dynamics of RO, blue mean transformed DL-P to CAL-P measurements with standard deviation (N=3), red modelled P_{av}

The CRL* plot in SP shows higher P_{av} and P-CAL values compared with the MIN plot, this could be due to the higher yield and the corresponding P uptake achieved with N-fertilization. The FYM plot shows the highest P_{av} and P-CAL values since it receives mineral P fertilization and organic P fertilization.

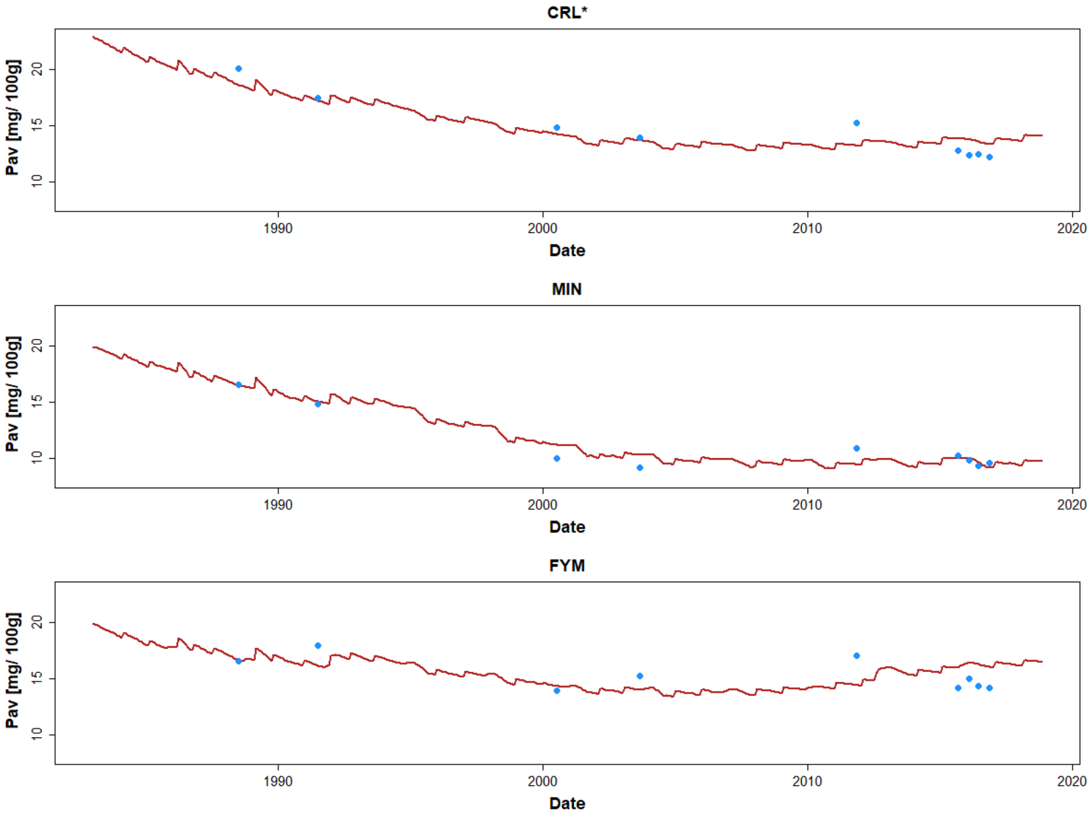

Figure IV-7: P_{av} dynamics of SP, blue CAL-P measurements (N=1), red modelled P_{av}

The model performance for all analyzed plots for P_{av} and Corg are displayed in Table IV-5. If replicates were available, the RMSE to the mean was calculated. Since SP has a shifted crop rotation in the treatments, each plot was simulated separately and the mean of the RMSE and rRMSE was used over all plot with the same fertilization. The RMSE for P_{av} increases with soil high in P_{av} values.

Table IV-5: Aggregated statistics, RMSE of P_{av} values [mg/100g], the standard deviation (sd) of P-CAL measurements [mg/100g] if replicates are available and the relative RMSE [%]; RMSE [mg/100] and relative RMSE [%] for Corg

Plot	LTE	RMSE P_{av}	rRMSE P_{av}	sd P-CAL	RMSE Corg	rRMSE Corg
CRL	BG	0.68	8.42	1.26	0.04	5.83
MIN	BG	1.04	14.65	1.29	0.04	6.8
FYM	BG	0.7	9.43	0.66	0.06	8.75
CRL	RO	0.18	6.08	0.23	0.04	2.72
MIN	RO	0.35	10.34	0.40	0.03	2.11
FYM	RO	0.26	7.7	0.42	0.03	1.93
CRL	BL	1.11	31.93	-	0.13	9.02
MIN	BL	1.87	27.73	-	0.12	6.57
FYM	BL	2.27	17.46	-	0.13	6.10
CRL*	SP	1.6	8.87	-	0.05	8.46
MIN	SP	1.15	9.38	-	0.05	6.15
FYM	SP	2.43	12.86	-	0.07	9.51

IV.3.2 Total P Dynamics

Besides the plant available P, the P-module calculates the P_t dynamics. Due to limited timelines of P_t measurements only two plots were evaluated, namely the CTR and MIN Plot of RO (Figure IV-8). The corresponding RMSE for CRL is 1.0 and the rRMSE = 1.8 and respectively RMSE = 2.5 and rRMSE = 4.2, for the MIN plot.

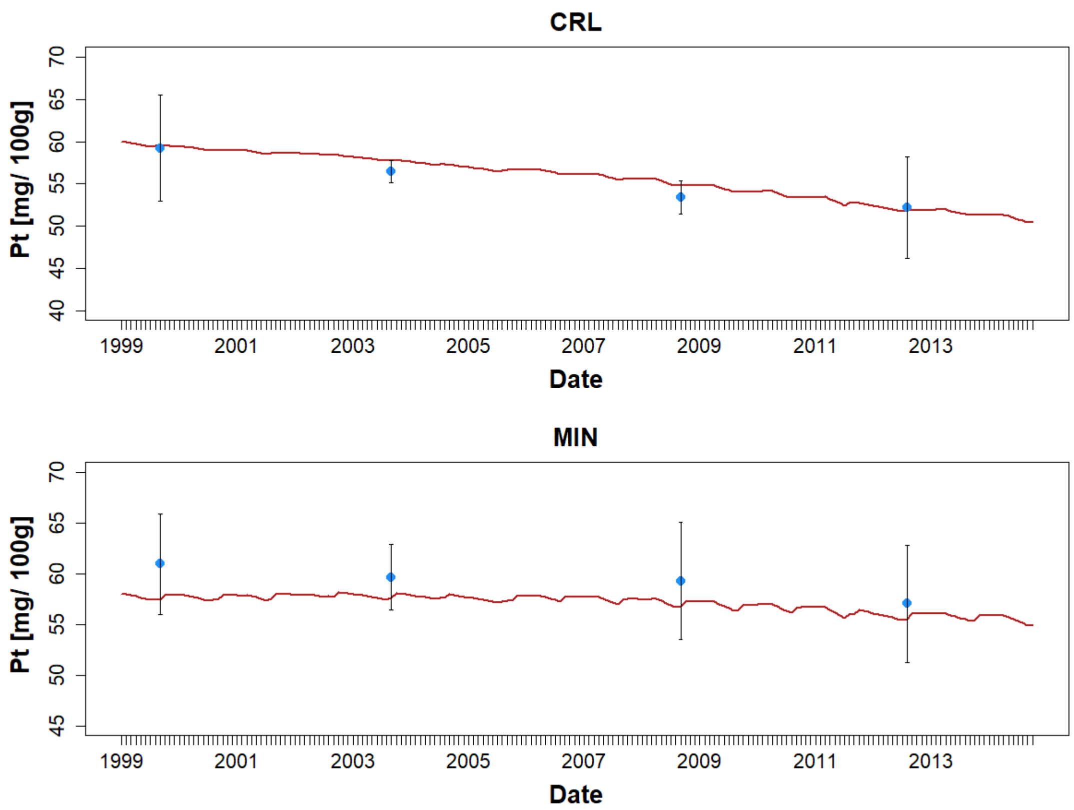

Figure IV-8: Total P dynamic, blue: aqua regia digested P of the CRL and MIN plot of RO with standard deviation (N=3), red modelled P_t

IV.4 Discussion

To make statements about the performance of the P-module, the model results of the carbon module have to be in an adequate range. For all analyzed plots of all LTEs the rRMSE for Corg is below 10%, which lies in a good range compared to other studies (Begum et al., 2017; Guillaume et al., 2021).

The P-model shows a rRMSE of around 10% for most plots. To mention is that in BL the P-model is worse in terms of the rRMSE, comparted to all the other LTEs. The reasons for that are amongst others the high variability in the measurements between two years. Furthermore, BL shows the highest silt and SOC (1.5-2 %) content of all LTEs, which might result in soil P processes which aren’t fully covered by the CNP-model. The measured CAL-P values of the CRL plot in BL stays constant over the observed period with no entry of P fertilizer. Either the total P-pool is declining over time strongly, or there might be a bigger P input of unknown sources or plant uptake is withdrawn from deeper soil layers (Pothuluri et al., 1986; Siebers et al., 2021). In the LTE of BG and RO, where replicates were available, the RMSE is lower than the standard deviation of the measured CAL-P values.

For most plots a time series for P_t was not available, solely a single measurement, where the modeled P_t values are in a close range. For RO the P_t timeline is modeled with good results, representing the trend with low RMSE and rRMSE. This enables the evaluation of the total P stock of soils and to determine if the P stocks are increasing or declining, and provides information about the potentially available P resources in the soil.

Several studies have shown that P cycling is influenced by erosion and leaching into deeper soil layers (Andersson et al., 2015; Ulén et al., 2007). Subject of the CNP-model is the cultivation layer, the upper 25 cm of the soil. The model does not consider transport mechanisms into deeper soil layers and comprises no water model or an erosion estimate like the Universal Soil Loss Equation which would be essential for erosion and leaching processes (Reid et al., 2018). In favor of simplicity and a low-threshold model approach, leaching and erosion was not considered yet, because more data input and parametrizations would be required and eventually lead to equifinality.

Yet another influential factor on P sorption and desorption processes is the pH value of the soil. With an increasing pH value P gets sorbed to Ca^{+} Ions, while with deceasing pH value the Ca bound P gets released again and at pH values of around 5 sorption processes to Fe^{-} and AL^{+} complexes gain more importance (Haynes, 1984; McLaughlin et al., 2011; Nobile et al., 2020). Agricultural soils are highly managed soils where the pH value gets regulated to maintain optimal productivity. Therefore changes in pH value don't play a decisive role for the model scope and have not been considered in the first version of the P-module.

Cleveland and Liptzin (2007) reported a mean global C/P ratio of microbial biomass of 60. Other studies assume that the C/P ratio in microbial biomass is not homeostatic, due to population size dependent scaling, habitat and ecosystem differences, or shifts in microbial community composition (McConnell et al., 2020). For the current model version the C/P ratio of all SOM-pools is assumed to be 186, but since the CNP-model comprises the A-SOM-pool which behaves like microbial biomass the C/P ratios could be further distinguished.

The PS formula is derived from the four experimental sites, which comprise four soils. Under certain conditions, especially with high silt and SOC contents and low P_{av} and clay contents the PS formula can get negative and lead to an undefined PS value. Further experiments are required to validate and improve the PS formula. Moreover, with diverse soil properties further influential parameters might be required to cover all soils with their attributes. Nevertheless, the two-pool model presented here can be used to model the P dynamics on different sites, with varying soil properties, diverse crop rotations and management practices such as intercropping, organic or inorganic fertilization. As organic bound P can have a decisive influence on the P turnover processes the C dynamics have to be considered and the modeling of the C dynamics have to be precise to grand good results.

The CNP-model can be initialized with the measurable P values P-CAL and P_t. Furthermore, the model output is equivalent to those measurable P species and can be directly compared. While other models like APSIM (Agricultural Production Systems Simulator) and EPIC (erosion-productivity impact calculator) include a sophisticated organic P cycling, but the plant available P-pool does not correspond to a measurable P species (Das et al., 2019) or does not even show a correlation to measurable P species (Raymond et al., 2021). This lowers the predictive use as well as the practical application of such models to consult farmers or other stakeholders.

Compared to APLE, DDPS and LePA the CNP-model differentiates in detail between the FOM inputs (organic amendments/fertilizer, byproducts, stubbles, roots and catch crops). Every input can be characterized in terms of quality like P content or mineralization characteristics. This is also considered in the organic P cycling of the CNP-model, where P release during mineralization of SOM as well as fixation during SOM build up is considered. This grants a high model flexibility and an overall wide application range. As stated by Damon et al. (2014) crop residues can have a significant influence on P availability by high amounts and high concentration. Furthermore, the application of a higher variety of organic fertilizers, like digestates or composts is expected, which have a different mineralization behavior and P availability.

The CNP-model can model the P dynamics of different soil with varying management. This demonstrates the potential of the model to simulate different scenarios. Those scenarios may include different management strategies, like intercropping, the use of digestates or sewage sludges as organic fertilizers or even a reduction of P fertilizers and the long-term effects on soil P.

IV.5 Conclusion

The CNP-model is a model with few data inputs and the possibility to model the C, N and now the available and total P dynamics of arable soils. The data input is kept low enough that the required data can be provided by farmers from their management practices and yields. The two-pool model presented can be used to model the P dynamics on different sites, with varying soil properties, diverse crop rotations and management practices such as intercropping, organic or inorganic fertilization. As organic bound P can have a decisive influence on the P turnover processes, the C dynamics must be considered, and the modeling of the C dynamics have to be precise to grand good results. The P model initialization and output is equivalent to measurable P species, which makes the output easy to interpret and comparable to measurements. Moreover, a comprehensive list of model parameters comprising common crops is presented. Nevertheless, further field trials need to be modeled and used to validate the P model concept and to improve model processes.

IV.6 Acknowledgements

This project was funded by the Agency of Renewable Resources (FNR) on behalf of the German Ministry of Food and Agriculture, thank you.

V. Discussion & Synthesis

V.1 Summary of the Main Results

The method presented in chapter II proposes an overall approach on how to implement an algorithm to calculate a value representing the contribution of a substrate to humus formation, considering the microbially induced turnover dynamics. The so called E_{HUM} was generated by modelling the C respiration curves of incubation experiments, with the concepts of six field scale C-models. The E_{HUM} value is calculated from the allocation mechanisms of FOM to SOM depending on the model-specific pool interactions. The following aggregation of the results with an averaging method into the ensemble E_{HUM} leads to an elimination of weak model performances and enables a model-overarching substrate quality assessment.

In this context, the CCB model was applied, amongst other models, to the incubation experiments. The parameters describing the turnover process were successfully extracted and used to simulate the C dynamics of these org. amendments in LTEs (chapter III and IV). This transfer is a useful method to model the field scale dynamics under consideration of environmental conditions, like soil properties, climate conditions, and management options. Furthermore, in Chapter III, the SON dynamics could be successfully modeled in the field using those parameters. By integrating a P-module into the CCB model as introduced in chapter IV, the parameters from incubation experiments are also reliable to model the P_{av} and P_t dynamics of LTEs where the organic P cycle was integrated similarly to org. N through the stoichiometric coupling to the C cycle.

Besides the substrate quality assessment, a major issue is the quantity of applied org. amendments. While the amount of org. fertilizers can be accessed in the agronomic data, the amount of accruing residues can vary strongly depending on the yields and crops. In addition to the input of external organic fertilizers, the fields' own C and nutrient cycles play an important role, in which C is added to the system by crop residues and nutrients are released during mineralization. Here, the method for the determination of the arising residues could be successfully revised and the data of field experiments were used to set up relations between yield and residual masses, as well as the stubble to root ratio of crops.

The introduced P-model was successfully integrated into the CCB model structure, with an organic P cycle which was linked to the C pools via the C/P ratio and the occurring matter fluxes of the C-pools. Moreover, P has a complex mineral P cycle, which is composed of different strong binding forms, weathering processes, plant-specific extractions, leaching etc. Here, the mineral matter flux is calculated by an equilibrium function between the two mineral P pools (P_{av} & P_{na}), which considers the clay, silt, and SOC concentration and its dynamic changes in the soil. The presented model approach was sufficiently accurate to determine the P fluxes on different arable soils and complement the model matter fluxes of C and N.

V.2 Discussion

V.2.1 Substrate Quality

Mineralization is a nonlinear process and methods which consider this nonlinearity must be developed to characterize org. amendments. There are approaches which try to use chemical proxies to determine the substrate stability during mineralization, but the quality evaluation of org. substrates can only be accessed to a certain degree by chemical analysis of the org. substrates. Those analyzes may include parameters such as the C/N ratio, cellulose -, lignin-, and hemicellulose-contents from which conclusions about the resilience and degradability can be drawn. Nevertheless, the explanatory power of said approach is limited (Lashermes et al., 2009) since the microbial interactions and environmental conditions, such as temperature, moisture or soil texture, and the interaction with the soil phase are not considered (Coonan et al., 2020).

A proper classification and differentiation between FOM inputs can increase the model accuracy and support the evaluation of different management strategies and their outcomes. Consequently, model approaches could be a useful tool to account for microbial turnover and create a taxonomy of organic substrates to classify them accordingly to their fertilization purpose and beneficial effects for soils. Expressing the nutrient availability and interactions of org. substrates, with regard of microbial turnover processes, is extremely complex. Here, the presented approach describes the turnover processes of the org. substrates with the addition of soil and the initiated microbial mineralization. The advantage of this approach is that there is no direct time component in the representation of the E_{HUM}, provided that the incubation was long enough for the mineralization dynamics to develop. Further, the texture of the soil and the temperature of the experiment are also taken into account, which allows the evaluation of different incubation experiments with the E_{HUM} method. In addition, the E_{HUM} method is based on a variety of model approaches created by different research groups, and therefore considers different model pool approaches and interactions between the pools (Farina et al., 2020). Such cross-model procedures can improve the results, cover a higher variety of model structures, and be a step towards community-based development approaches (Yeluripati et al., 2015). By subsequent model averaging, weaker model performances can be automatically eliminated from the calculation of the ensemble E_{HUM} value. Thus, the reliability can be increased and the robustness of the result can be improved. Comparisons with the literature can confirm the significance, for e.g., Kätterer et al. (2011) and Berti et al. (2016) used the humification coefficient (H) which describes the fraction of total C input remaining after 50 years. Those results are comparable with the findings of this thesis, showing that above ground residues and green matter have the lowest H, followed by slurries, manures and roots, which is in alignment with the ranking achieved with the E_{HUM} value.

Furthermore, the E_{HUM} considers different soil types so that it is applicable across different regions. Such substrate evaluations can be a tool to adapt agricultural management to regionally predominant crop types and, consequently, differences in accruing org. amendments used as fertilizers.

(1): The aggregation of nutrient availability and interaction into advisory numbers is extremely complex. The presented E_{HUM} value constitutes such an advisory score, which characterizes the ability of an org. substrate to contribute to humus formation.

V.2.2 Methodology

In addition to a numeric quality assessment, the parameters describing the turnover dynamics of org. substrates in incubation experiments are shown to be applicable to predict the dynamics on field scales. These parameters were used in chapter III and further in chapter IV to model the C-, N-, and P-dynamics of org. residues and amendments on LTEs, with good results for predicting the dynamics of the mentioned elements. This shows that the parameters are scalable to the field scale and sufficiently generalized to be used on different field sites with varying soil properties and climatic conditions. The successful application of the parameters to the field scale in chapter III and IV allows the further conclusion that the method developed in chapter II is valid and precise enough to describe the turnover dynamics of org. amendments and that field scale models are an appropriate tool to determine the substrate quality. Therefore, the proposed approach is a reliable tool to assign laboratory findings on to agronomical scales, where a multitude of environmental impacts occur.

The temperature during the incubation was considered by the BAT function (biologic active time). This approach splits the annual time into the time during which microbial turnover is only limited by the substrate while environmental conditions are optimal, and into a non-BAT time during which no turnover occurs

(Franko et al., 1995a). The climatic and site conditions (air temperature, precipitation and aeration), which influence the microbial turnover, are aggregated into a time in which microbial processes would occur under optimal conditions (Franko & Oelschlägel, 1995a), which can be assumed for incubation experiments where temperature and hydration are adjusted and kept constant. The BAT concept is therefore an eligible method for the transfer of incubation experiments to model field site turnover dynamics and can help to close the gap between laboratory and field approaches. It should be noted that during incubation, the mineralization was not inhibited by lack of nutrients such as P and N, and an optimal supply was ensured. Relying on parameterizations from incubation experiments could lead to an overestimation of turnover dynamics on undersupplied croplands. However, in cropland management it is not common to omit fertilization, thus, the issue is more of theoretical interest, e.g. in unfertilized LTEs.

Besides the quality assessment, a further issue of the constituted method is the evaluation of occurring residual quantities to account for the field internal SOC and nutrient cycles. Those quantities differ between the grown crops and further in dependence of the yield. As discussed in chapter II, fine roots show an E_{HUM} value comparable to the E_{HUM} of digestates, which makes them one of the most resilient org. amendments (Zhang et al., 2015). Their input can account for 30-90 % of C input in agricultural soils, making them one of the most driving factors in soil dynamics (Hirte et al., 2018). Within the framework of the thesis, the CCB model by Franko et al. (2011) was expanded and modified. This includes the separation of the crop residues into above ground residues (e.g. stubbles) and below ground residues (e.g. roots). This division was introduced by Franko et al. (2021) to achieve an improved differentiation of crop parts regarding their C and N (and P) contents as well as their turnover behavior. While Franko et al. (2021) introduced the functions to calculate the amount of below and above ground residues in dependences of the main product, the used parameters were based on the division of the former CCB crop residues unit, which included the above- and the below-ground residues and treated them as on single FOM input. The division was achieved by a fixed ratio between the above- and below-ground residues. A major issue of this division is that no data was given for the proportion between above and below ground residues. Furthermore, the nutrient composition of the above- and below-ground residues was also not sufficiently clear and was divided between the two with no data basis. In chapter III, all data required to describe the above and below ground residues were aggregated from experimental setups and the correlations to describe the above- and below-ground masses are derived from field measurements. Different approaches to attain those parameters and residual properties were described in chapter III and tested. Still, the data concerning crop roots are often scarce, and methods and correlations need to be investigated to parameterize those residues accordingly and to set up a comprehensive database. The underlying database sets the foundation of reliable model results, and the presented approaches offer guidance to parameterize the quality and quantity of occurring residues and applied org. amendments. Only if the databases keep up with the model development, reliable results can be produced and changing trends in farming practices can be faced.

(2): In summary, the presented methods can be used to determine the substrate quality (E_{HUM}) and compare substrates to another. Furthermore, parameters can be gained which describe the quality and successfully predict the turnover dynamics of C, N and P on arable soils, which allows a distinctive application of the model to varying org. amendments. The model approaches serve as an interscale tool which can help to close research gaps between laboratory and field scales. (3): Moreover, the occurring quantity of residues must be parameterized accordingly to receive reliable results about the turnover dynamics, where more research is needed to investigate root residues.

V.2.3 C-N-P Matter Fluxes

After a phase of high P surpluses and low P use efficiencies, industrialized countries nowadays set a stronger focus on P use efficiency of crops and adapted fertilizing strategies (Mogollón et al., 2018). Here, P-models can help to calculate the current state of plant-available P to adapt P fertilizer applications. Furthermore, the accumulated soil P stocks (legacy P) can be tracked and the P reservoirs can be integrated into fertilizer strategies (Rowe et al., 2015). Here, models can track the release of P stocks and help to implement precise fertilizing strategies, which allows planning over decades rather than for one crop rotation, especially when using org. amendments as fertilizers with a long retention time.

The P cycle has proven to be very complex and influenced by a lot of biological, chemical, and physical factors and their interactions, as elaborated in the introduction. Model development always requires an estimation of sufficient precision and complexity regarding the availability of data and the scope of the model. The here-established P-module was successfully integrated into the existing model structure and kept a low data threshold. The overall CNP-model structure and pool interactions between C, N, and P are shown in Figure VI-1. Particularly the SOC dynamics drive and determine the dynamics of the N and P fluxes. P is not only allocated to the organic pools and released during turnover of FOM and SOM into the P_{av} pool, but the equilibrium function between the mineral P_{av} and P_{na} pools is also adjusted in dependence of the current SOC concentration for each time step (for details see chapter IV). At the current state, the C- and the N-module are applicable to field sites without any parameter optimization or adjustment, except for the choice of the start value for each. In contrast, the P-module requires the P_{av} and P_t starting value as well as the optimization of the $\varkappa$ parameter which influences the dynamic equilibrium between P_{av} and P_{na}. Nevertheless, the $\varkappa$ parameter was shown to be site-specific and only needs to be adjusted for one field, regardless of the management regime. This allows for the model to be used for a wide range of applications with little effort, but also highlights the need for further research into the binding forms and their intensities of P to the mineral phase of the soil.

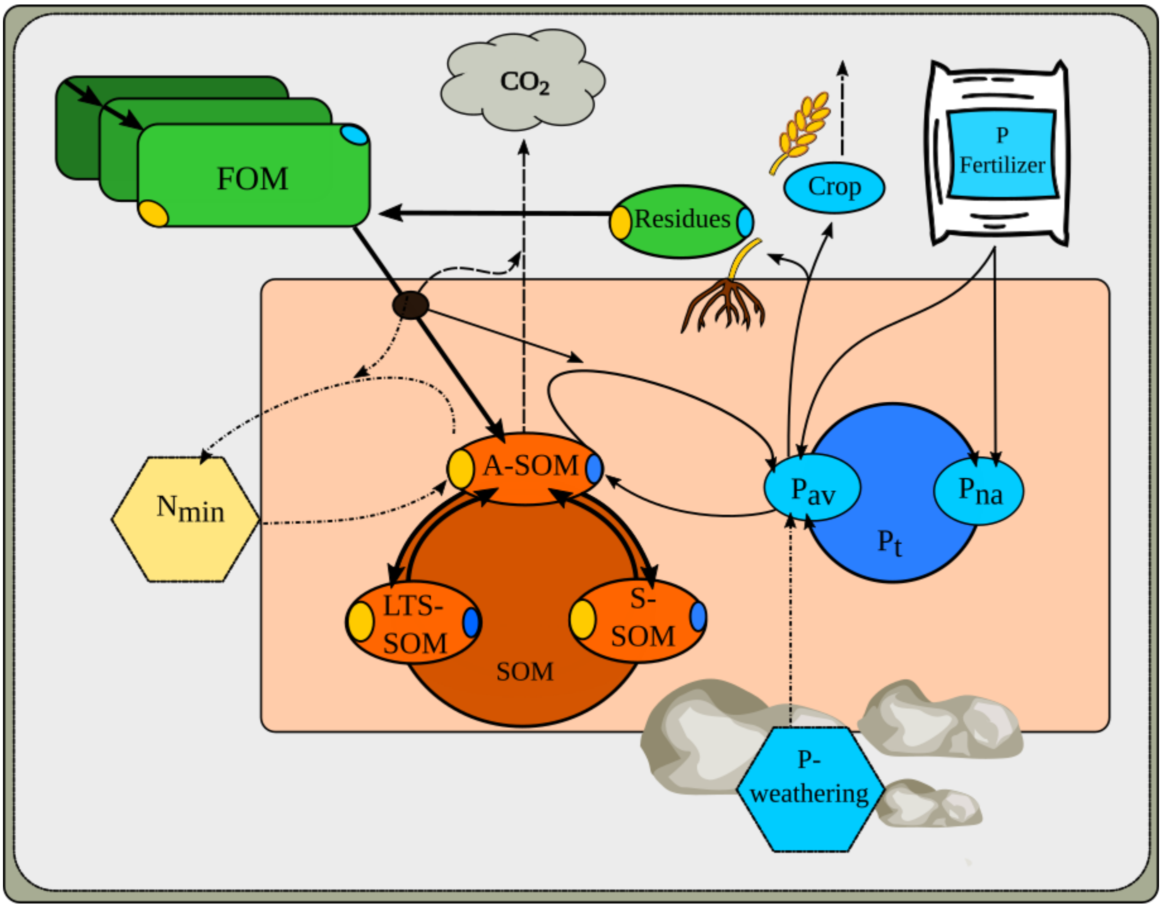

Figure V-1: Scheme of the CNP-model; the big arrows represent C, N & P fluxes, brown ovals represent C-pools, yellow ovals represent the org. N associated to C-pools via C/N ratio, blue ovals represent P-pools with organic P associated to the C-pools via C/P ratio; the circles represent the total elements of the connect pools (P_t also includes the organic P); green elements represent organic matter not integrated into soil matrix; the dotted arrows and the hexagons represent fluxes from non-Pool sources with no mechanistic background, the dashed lines represent fluxes leaving the system.

The comprehensive differentiation between the FOM inputs with varying properties like specific turnover dynamics and nutrient compositions empathizes the significance of the C-cycle. The acquisition of FOM inputs with separate turnover properties and chemical compositions allows to parameterize any type of org. substrate, including manures, slurry, composts, digestates, roots, stubble, and other org. amendments which are not yet very common. This recommends the CNP-model for versatile use, especially if a wider pallet of organic fertilizers is used and the nutrient cycle and circular economy are targeted as future developments (Prays et al., 2018). Thus, the long-term and large scale changes in soil cycles of all these org. amendments can be investigated with the application of the CNP-model, which is of particular importance in the field because a large number of org. amendments can be actively in circulation at the same time, e.g., plant residues can occur during the application of org. fertilizers. Thus, the CNP-model can serve as a holistic tool for farmers or stakeholders to choose and compare appropriate org. amendments for their management goals. Furthermore, in areas where no constant soil measuring is conducted, the application of org. amendments can be investigated using the CNP-model to evaluate the current and targeted management practices. The integration of a new P-module further allows a broader analysis of org. amendments and their fertilization potentials and can help to achieve a comprehensive understanding of soil cycles and the interactions of SOC and plant nutrients. Furthermore, a rather simple model approach can be an accessible tool to help operators to track nutrient dynamics and promote the increasing use of org. amendments as an alternative to mineral fertilizers.

(4): The elaborated model concept is able to model the P_{av} and P_t dynamics on arable soils with relatively little data input and a simple model structure. In favor of simplicity, some known P mechanics that play a major role in the P cycle are not yet implemented. Rather, a strong focus was set on the interactions between the C cycle, the P cycle, and the field internal matter cycling. Nevertheless, the chosen approach was proven to be sufficiently accurate for different arable soils.

V.3 Synthesis

Compared with mineral fertilizers, organic fertilizers are composed of a variety of nutrients that can be integrated into different fertilization strategies and the impact of which is much more complex than that of mineral fertilizers. This is mainly due to the binding forms to SOM and the release of nutrients in the course of turnover processes. With an adequate parametrization, models can be an advantageous method to predict the impact of org. amendments where laboratory experiments exclude too many environmental impact factors and LTEs are very cost- and labor-intensive. The use of org. amendments as org. fertilizers is one way to achieve closed nutrient cycles and circular economies, provided it is possible to successfully track the nutrient inputs and outputs. Nevertheless, the application of org. substrates from off-site production needs to undergo a full life cycle assessment to evaluate the C-emissions of production, transport as well as the biomass removal (Paustian et al., 2016). Furthermore, an evaluation of hazardous constituents (heavy metals or pathogens) must be considered (Epelde et al., 2018). The E_{HUM} can help producers of org. amendments to classify their products to establish recommendations for their application and help farmers to accomplish management goals. This can be used, e.g., to revise the humus calculation used by the Verband deutscher landwirtschaftlicher Untersuchungs und Forschungsanstalten e.V. (VDLUFA), which aims to determine the humus supply of soils in an easily accessible way in order to ensure high yields and achieve low nutrient surpluses. For this purpose, the humus equivalent (HÄQ) is used. The HÄQ value provides information about the demand of organic matter, which occurs in addition to the crop-specific carbon input through roots and stubble. For crops not yet parameterized, the E_{HUM} value can be used as a reproducible method of parameterization (Gasser et al., 2021a). Furthermore, models which calculate the soil matter fluxes can support the evaluation and effectiveness of different substrates, consider their retention times and nutrient release, and thus help to create a comprehensive analysis of all kinds of org. amendments. By applying the methods developed in this thesis, the analysis of org. amendments is easily scalable to the field site and can help to calculate different scenarios considering management changes or effects of climate change.

The objectives and findings of this thesis can be embedded into an interdisciplinary context between different stakeholders and support those stakeholders in decision making where political agendas, environmental processes and practical implementations must be reconciled (Figure V-2). In the course of climate change, soil management has to be adapted to secure food productivity. Therefore, political stakeholders must constantly adapt regulations and political strategies, whereat strategies to mitigate climate change through increased use of org. amendments can be one measure to increase C-sequestration. Furthermore, the accumulation of SOC with its soil structuring properties, which can improve water storage, reduce erosion risk, and promote nutrient storage and long-term fertilization, must also be included in ways of considering human interactions with soil (Siedt et al., 2021). Here, scenario analysis can be a powerful tool to react to the challenges of climate change and to frame policies where different management strategies are compared in terms of their sustainability and economic benefits as presented by Hawes et al. (2019), where trade-offs between biotic, abiotic, and economic components of agroecosystems get compared to set political incentives. Considering soils as a circular system in which nutrient losses are minimized and nutrient inputs can be accurately determined to meet crop demands may be as important as mitigating climate change to ensure crop production and food security in a changing global climate. As such processes are also highly site-dependent, models can be used to predict the behavior, amounts, species, and location of nutrients. These models can be used to build up a sound understanding of these processes and the field site they are applied to, where a comprehensive database can help to deal with the high variety of org. amendments and their different dynamics. It should not be forgotten that farmers are the group most intensively involved in soil management. In order to accompany the transformation processes towards sustainable agriculture and circular economy, models with relatively low data input, such as the CNP-model, can serve as an advisory tool or indicators derived from the model can be used to support and initiate these processes.

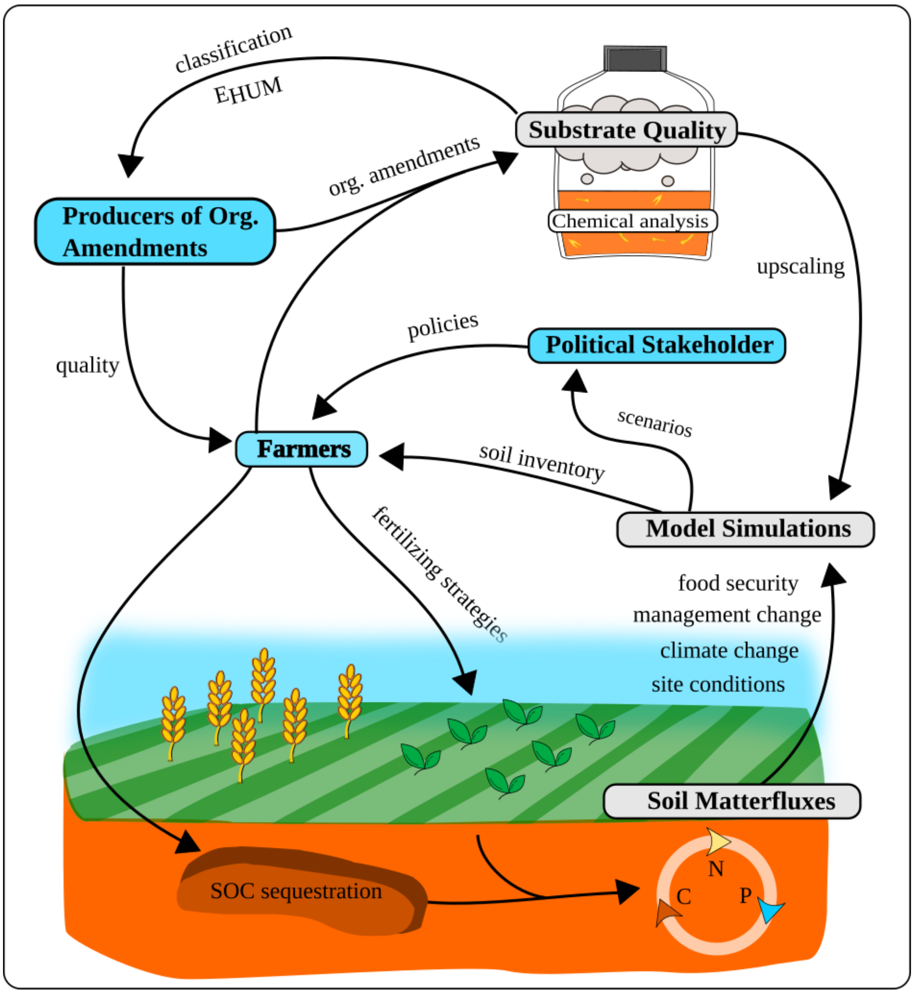

Figure V-2: Scheme of the overarching context of the thesis, with different stakeholders (blue) and how the elaborated methods can support decision-making and be integrated into management practices.

(5): Organic residues are composed of a variety of components which consequently affect the dynamics on arable soils. In order to cope with the multiple demands and uses of different stakeholders, the presented model approaches can help to classify their use and give prognoses about their behavior. This way, political stakeholders can be supported to set incentives, while producers of org. amendments and farmers can be supported in realizing political decisions and adapt their management strategies in order to close nutrient cycles and to react to climate change.

V.4 Conclusion

The thesis proposes a method of model parametrization based on laboratory results which are transferred to the field scale and thus can help to close the gap between laboratory and field scale approaches to determine the dynamics of org. amendments. Furthermore, the thesis closes research gaps between applied experiments from laboratory to field scale and the proposed modelling approaches serve as a multiscale tool, which can help to aggregate those findings into advisory metrics or evaluate the impact of shifts in management practices.

The development of the CCB model into the CNP-model with an integrated P-module can help to accomplish a more holistic evaluation of org. amendments due to the implementation of a further important macro-nutrient for plants. This can contribute to a more targeted use of organic amendments according to their fertilizing effect and help to analyze the nutrient and life cycle of those org. amendments, and thus can help to ensure sustainably high yields and strengthen the soil in its functions.

The thesis can promote the benefits of org. amendments by supporting the classification of the amendments in terms of their best use and optimal application. New methods for the characterization of organic residues must be developed to keep up with the large variety, the constantly developing processes, and the production of org. amendments to return them to nutrient cycles. The approaches presented here can help to understand the complex effects of these amendments and to express them in easily accessible units and metrics. This information can enable stakeholders at different levels to implement and accomplish their respective goals, ultimately paving the way towards more circular nutrient management and sustainable agricultural practices.

V.5 Outlook

The thesis could successfully answer the stated research questions, but extended fields of research emerge from the conducted work. It would be worthwhile to further investigate incubation experiments regarding possibilities of expressing the plant availability of N and P in a similar metric as the E_{HUM} value. This way, org. amendments could be characterized in terms of their fertilizing effect to create taxonomies which classify org. substrates and allow the use of those amendments to better suit the desired management goals.

The P-module was successfully introduced, nevertheless, the complexity of the P cycle comprises further interactions and processes, which are not represented in the first version. This may include the pH-dependence of P sorption, leaching processes, etc., but here the main task will be to keep a low data input to grant the aimed low entry threshold of the CNP-model for the users while still accomplishing good results.

The proposed methods could further be completed by investigating methods to either derive parameters from chemical analysis or to evaluate the substrate quality from those analyzes, especially if no incubation data for org. substrates are available. This way, the gap between laboratory and field conditions could be further closed, less time-and cost-intensive methods could be developed, and missing data compensated.

VI. Appendices

VI.1 Appendix A

VI.1.1 Incubated Substrates

Table VI-1 A: Substrate overview with substrate characteristics and composition, ZF = catch crop, GPS = whole plant silage, C/N = carbon-nitrogen ratio

ID	substrate	data set	incubation period [d]	C/N
2	Digestate: cattle slurry 50 %; maize silage 35 %; grass silage 15 %	1	139.7	5.5
3	Digestate solid separation: cattle slurry 30 %; maize silage 30 %; grass silage 30 %; farmyard 10 %	1	139.7	12.6
4	Digestate liquid separation: cattle slurry 30 %; maize silage 30 %; grass silage 30 %, farmyard 10 %	1	139.7	5.2
5	Digestate: maize silage 85 %; rye GPS 15 %	1	139.7	4.8
6	Cattle manure (fresh)	1	139.7	9.6
7	Cattle slurry	1	139.7	8.9
8	Digestate: pig slurry 50 %; maize silage 50 %	1	139.7	5.2
17	Digestate: cattle slurry 50 %; maize silage 35 %; grass silage 15 %	2	251.46	6.2
18	Digestate solid separation: cattle slurry 30 %; maize silage 30 %; grass silage 30 %; farmyard 10 %	2	251.46	14.4
19	Digestate liquid separation: cattle slurry 30 %; maize silage30 %; grass silage 30 %; farmyard 10 %	2	251.46	5.2
20	Digestate: maize silage 85 %; rye GPS 15 %	2	251.46	5.9
21	Cattle manure (< 1 year)	2	251.46	16.0
22	Cattle slurry	2	251.46	12.0
23	Digestate: pig slurry 50 %; maize silage 50 %	2	251.46	5.4

ID	substrate	data set	incubation period [d]	C/N
24	Rotten cattle manure (>1 year)	2	251.46	6.1
25, 35	11 % grass silage; 2 % grain; 87 % pig slurry	3, 4	41	6
26, 36	10 % maize silage; 90 % cattle slurry	3, 4	41	4.7
27, 37	17 % maize silage; 19 % pig slurry; 64 % cattle slurry	3, 4	41	6.1
28, 38	24 % maize silage; 31 % grass silage; 8 % rye silage; 37 % farmyard manure	3, 4	41	6
29, 39	33 % maize silage; 25 % rye silage; 20% pig slurry; 22 % farmyard manure	3, 4	41	8.3
30, 40	35 % maize silage; 11% grass silage; 8% sorghum; 3% grain; 43% pig slurry	3, 4	41	6.8
31, 41	50 % maize silage; 7% grain; 43% cattle slurry	3, 4	41	5.8
32, 42	52 % maize silage; 8 % grass silage; 2 % grain; 35 % pig slurry; 3 % farmyard manure	3, 4	41	5.3
33, 43	61 % maize silage; 5 % grain; 34 % pig slurry	3, 4	41	5.1
34, 44	100 % maize silage	3, 4	41	6
45	Pea (litter)	5	300.9	26
46	Pea (crop residue)	5	300.9	28
47	Oat (litter)	5	300.9	36
48	Oat (crop residue)	5	300.9	63
49	Oat (coarse roots)	5	300.9	51
50	Maize (litter)	5	300.9	27
51	Maize (crop residue)	5	300.9	73
52	Maize (coarse roots)	5	300.9	75
53	Sorghum bicolor (litter)	5	300.9	30
54	Sorghum bicolor (crop residue)	5	300.9	57
55	Sorghum bicolor (coarse roots)	5	300.9	50
56	Sorghum sudanense (litter)	5	300.9	30
57	Sorghum sudanense (crop residue)	5	300.9	59
58	Sorghum sudanense (coarse roots)	5	300.9	47
59	Maize (ZF), (litter)	5	300.9	37

ID	substrate	data set	incubation period [d]	C/N
60	Maize (ZF), (crop residues)	5	300.9	98
61	Maize (ZF), (coarse roots)	5	300.9	85
62	Winter wheat (green cutting, crop residue)	5	300.9	86
63	Winter wheat (green cutting, coarse roots)	5	300.9	86
64	Winter wheat (litter)	5	300.9	28
65	Winter wheat (crop residue)	5	300.9	154
66	Winter wheat (coarse roots)	5	300.9	56
67	Pea (litter)	6	160.7	26
68	Pea (crop residue)	6	160.7	28
69	Pea (coarse roots)	6	160.7	36
70	Pea (fine roots)	6	160.7	19
71	Oat (fine roots)	6	160.7	32
72	Maize (fine roots)	6	160.7	29
73	Sorghum bicolor (fine roots)	6	160.7	35
74	Sorghum sudanense (fine roots)	6	160.7	35
75	Maize (ZF), (fine roots)	6	160.7	30
76	Maize (ZF), (fine roots)	6	160.7	30
77	Sorghum bicolor (ZF), (fine roots)	6	160.7	32
78	Sorghum bicolor (ZF), (fine roots)	6	160.7	32
79	Sorghum sudanense (ZF), (fine roots)	6	160.7	30
80	Sorghum sudanense (ZF), (fine roots)	6	160.7	30
81	Winter wheat (green cutting, fine roots)	6	160.7	29

VI.1.2 Incubation Experiment Dataset 1 & 2

VI.1.2.1 Chemical Analysis

Bulk soil was collected from the upper layer of an arable loamy sand at Berge (Germany, Brandenburg). Before use, the soil was air-dried and sieved < 2 mm.

The C and N contents of the soil were 0.71 % and 0.06 % of dry matter (DM), respectively. The pH value (determined in 0.01 mol $CaCl_2$) was 5.7. Digestates were taken from several agricultural biogas plants in the Brandenburg area. Dry Matter (DM) content was determined gravimetrically after drying the soil at 105 °C and organic dry matter (ODM) content was calculated as the loss of weight between 105 and 550 °C. The concentration of total nitrogen in the fresh material was determined using the Kjeldahl method. The Corg content was measured in lyophilized grounded samples using an elemental analyzer (Elementaranalysator vario C, Elementar Analysensysteme GmbH, Hanau, Germany).

VI.1.2.2 Experimental Design

40 g of soil were mixed with digestate, in a quantity to add 140 mg of Corg. Mixtures of soil and substrate were placed in 100 ml incubation vessels and moisture content was adjusted to 60% maximum water-holding capacity (WHC). The CO_2 production was determined using a respirometer (CarbO2Bot, prw electronics, Germany). Hourly respiration was measured by the change in conductivity as a result of CO_2-absorption in 0.6 M KOH. During incubation, vessels were opened regularly in order to maintain adequate oxygen concentrations. Empty vessels were used as blanks. Vessels filled with soil only served as a control variant. The experiment was conducted for 140 & 252 days at a temperature of 20 ± 1 °C. All variants were replicated six fold, except for glucose and cellulose acid that were carried out in triplicates. Based on the amount of CO_2 C evolved in each substrate, the cumulative amount of total evolved C was calculated for the entire incubation period. In order to calculate the CO_2 C release out of the organic substrates, the CO_2 C values of the control soil were subtracted from the mixed soil sample CO_2 C values.

VI.1.3 Incubation Experiment Dataset 3 &4

The experimental setup for data set 3 and 4 are to be found in the publication of Sänger et al. (2014).

VI.1.4 Incubation Experiment Dataset 5 &6

The description of the experimental setup for data set 5 and 6 was taken from Mewes (2017).

VI.1.4.1 Setup of the Incubation Study

Apparent course of EOC-induced CO_2-release of 40 plant residues was measured in two incubation experiments under controlled laboratory conditions. The second incubation experiment contained pea residues and all fine roots. In both experiments, straw was included as standard residue. This should allow comparing the results obtained by the two separate experiments. The plant residues were homogenously mixed at a rate of 400 mg EOC per 100 g soil. Then the soil was filled into small tubes (soil columns) at a bulk density of 1.1 g cm-3. Soil columns with and without plant residues were prepared with 3 and 5 replications, respectively. Contrary to previous investigations no mineral N was added, taking limited nitrogen availability into account. Incubation temperature was 22 °C. At the start of incubation, soil water content was adjusted to 20.8 ml H_2O per 100 g soil, expressing 50 % of water holding capacity (ISO 16072). After 301 days of incubation, the mineral N concentration in each soil column was determined in an extract by spectrometric measurement (DIN 19746).

VI.1.4.2 Measurement of CO_2 Release During the Incubation Study

The soil columns were placed in closed jars with 100 ml 0.15 M NaOH at the bottom, absorbing the mineralized CO_2, which was released from the soil columns between two measuring dates. The absorbed CO_2 was precipitated as $BaCO_3$ through the addition of 10 ml 1.5 M $BaCl_2$ solution and measured by titration with 0.3 M HCl and phenolphthalein as indicator. Measurement dates were 1, 3, 7, 14, 21, 35, 56, 77, 98, 120, 162, 217, and 301 days after start of incubation. The apparent decomposition of plant residues was calculated as difference between evolved CO_2 from soil columns with and without plant residue. The course of EOC-induced CO_2-release was calculated by summing up the EOC-induced CO_2 release between two subsequent measurement dates.

VI.1.5 Model Concepts

The following section describes the adaptations made to apply the model concepts to the incubation data. Those adaptations are required to use the model concepts with the same algorithm and especially effect the handling of AOM and FOM and its initial distribution into the model pools.

*C-TOOL**

C-TOOL models the topsoil with three pools denoted as *fresh organic matter* (*fom*), *humus* (*hum*), *resistant organic matter* (*rom*), which are connected in series (Taghizadeh-Toosi et al., 2014).

Further, each of these pools delivers a part of the decomposed matter into its pendant in the subsoil. Since there is no subsoil in an incubation vessel, the transport term of C-TOOL was not applied in this approach

Built for simplicity, the model only distinguishes between two AOM types, plant residues and manure, where residues go completely into FOM and manure has an already decomposed part (fhum) that goes into hum. However, in this application, f_{hum} was optimized for every substrate. The texture dependent humification factor h was calculated according to its original formulation, but we additionally optimized the decay rate of *fom* (k_{fom}), which increased the model performance significantly.

*CCB**

CCB is also a three pool model with feedbacks between the model pools, *active SOM* (*a-som*), *stabilized SOM* (*s-som*) and *long-term stabilized SOM* (*lts-som*) (Franko et al., 2011). For short time spans, the *lts-som* pool can be assumed to be inert. CCB assigns a substrate/AOM specific decay rate (k_{fom}) and a synthesis coefficient (η_{fom}) for each substrate entering the system. To solve the ordinary differential equation describing the distinct flow rates, the flow was calculated from *fom* to CO_2 (k10) as k_{fom} * (1-η_{fom}) and the flow from *fom* to *a-som* (k12) was computed as k_{fom} * η_{fom}

The environmental impact on SOM turnover in CCB is usually described with a meta-model that works with yearly values of mean temperature and total precipitation. It is derived from the CANDY model (Franko, 1997). Therefore, in contrast to the other models where the respective temperature functions were all applicable, the temperature function was used as described in the CANDY model:

$$rT = 2.1 \cdot \exp(\frac{T-35}{10})$$

*CENTURY**

Century has evolved into a highly complex model that considers several environmental processes such as soil turnover, crop growth and others. The focus of this approach is solely on the SOM turnover sub model. As for the application to laboratory conditions, concepts like leaching and surface litter pools are negligible, the model was reduced to the soil pools *METABOLIC* (m), *STRUCTURAL* (*str*), *ACTIVE* (a), *SLOW* (s) and *PASSIVE* (p). Where m only feeds in a, *str* in a and s, while a, s and p have several feedbacks. This corresponds to an earlier version of Century, but for the parametrization, the more recent model description of with corresponding decomposition values and temperature function was used.

CENTURY splits AOM between m and *str* by a function of the lignin-to-N_{tot}-ration (F_m). A second AOM adaption is the influence of the total fraction of lignin in *str* on its decay rate (k_{str}). In this approach k_{str} and (for numerical reasons) f_{lig} that is $(1/F_m) + 1$ were fitted without considering the actual lignin content of AOM.

*ICBM**

ICBM was introduced by Andrén and Kätterer (1997) as a two-pool serial model with *young SOM* (y) and *old SOM* (o), where all AOM enters y with no further differentiation. In later publications (Bolinder et al., 2007; Poeplau et al., 2015), y was replaced by two or three distinct categories of y (i.e. root, straw and manure).

The concept of multiple y pools was therefore expanded and the flow rates from y to CO_2 (k10) and y to o (k12) were fitted for each substrate individually. For the temperature response, the "Ratkowsky"-function was used, as described in Kätterer et al. (1998).

*RothC**

RothC comprises four active pools, *Decomposable Plant Material* (*dpm*), *Resistant Plant Material* (*rpm*), *Microbial Biomass* (*bio*), *Humified OM* (*hum*) and a central texture-dependent factor x hat splits all decomposed matter between CO_2 production and *bio*+*hum* build up (Coleman & Jenkinson, 1999).

Other than in the original model description, effective flow rates were used, as the partial recycling of *bio* and *hum* apparently reduces the formal decay rate of these pools. The quality of added organic material can be expressed by only one parameter (f_{hum}) using the partitioning function proposed by Dechow et al. (2019), to distribute AOM between *dpm* and *rpm* or *rpm* and *hum*.

*Yasso**

Originally, the Yasso model was developed for forest environment but also applied successfully to cropland by Karhu et al. (2012) and Akujärvi et al. (2014). The model has four distinct FOM pools denoted as *acid hydrolysables* (a), *water solubles* (w), *ethanol soluble* (e) and *none of the other* (n) with many feedbacks between them, and one *humus* pool, to which all other pools deliver C. Instead of fitting the distribution of AOM into the four different pools, which gave no reliable solution, AOM is only distributed between w, with the highest decay rate, and e, that would otherwise have no substantial input. This was accomplished using the parameter p_w ($w = p_w$, $e = 1\text{-}p_w$) while a and n were initially set to 0.

For the flow rates the mean values within the described confidence limits given in Tuomi et al. (2011) were used.

VI.2 Appendix B

VI.2.1 Regression Nitrogen Analysis

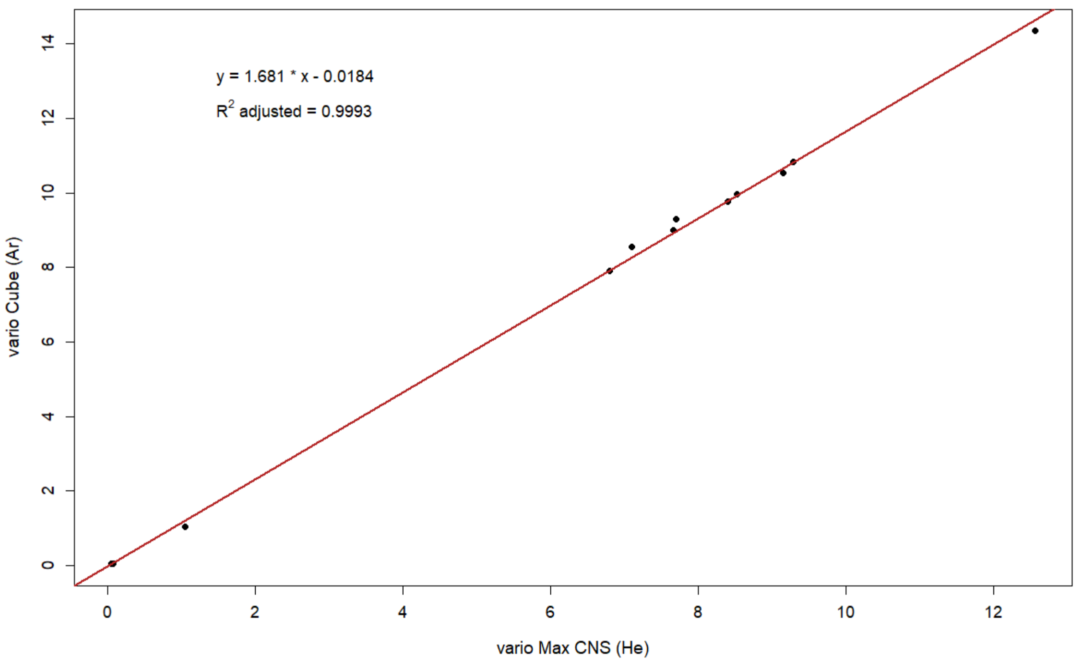

Figure VI-1: regression between the two carrier gases (Helium and Argon) used to analyze the total Nitrogen content

VI.2.2 Experimental Setup for the Organic Fertilisers

VI.2.2.1 Chemical Analysis

Bulk soil was collected from the upper layer of an arable loamy sand at Berge (Germany, Brandenburg). Before use, the soil was air-dried and sieved < 2 mm. The C and N contents of the soil were 0.71 % and 0.06 % of dry matter (DM), respectively. The pH value (determined in 0.01 mol CaCl2) was 5.7. Digestates were taken from several agricultural biogas plants in the Brandenburg area. Dry Matter (DM) content was determined gravimetrically after drying the soil at 105 °C and organic dry matter (ODM) content was calculated as the loss of weight between 105 and 550 °C. The concentration of total nitrogen in the fresh material was determined using the Kjeldahl method. The Corg content was measured in lyophilized grounded samples using an elemental analyzer (Elementaranalysator vario C, Elementar Analysensysteme GmbH, Hanau, Germany).

VI.2.2.2 Experimental Design

40 g of soil were mixed with digestate, in a quantity to add 140 mg of Corg. Mixtures of soil and substrate were placed in 100 ml incubation vessels and moisture content was adjusted to 60% maximum water-holding capacity (WHC). The CO_2 production was determined using a respirometer (CarbO2Bot, prw electronics, Germany). Hourly respiration was measured by the change in conductivity as a result of CO_2-absorption in 0.6 M KOH. During incubation, vessels were opened regularly in order to maintain adequate oxygen concentrations. Empty vessels were used as blanks. Vessels filled with soil only served as a control variant. The experiment was conducted for 140 & 252 days at a temperature of 20 ± 1 °C. All variants were replicated six fold. Based on the amount of CO_2 C evolved in each substrate, the cumulative amount of total evolved C was calculated for the entire incubation period. In order to calculate the CO_2 C release out of the organic substrates, the CO_2 C values of the control soil were subtracted from the mixed soil sample CO_2 C values.

VI.2.3 Experimental Setup for the Roots and Stubbles

The description of the experimental setup was taken from Mewes (2017).

VI.2.3.1 Setup of the Incubation Study

Apparent course of EOC-induced CO2-release of 40 plant residues was measured in two incubation experiments under controlled laboratory conditions. The second incubation experiment contained pea residues and all fine roots. In both experiments, straw was included as standard residue. This should allow comparing the results obtained by the two separate experiments. The plant residues were homogenously mixed at a rate of 400 mg EOC per 100 g soil. Then the soil was filled into small tubes (soil columns) at a bulk density of 1.1 g cm-3. Soil columns with and without plant residues were prepared with 3 and 5 replications, respectively. Contrary to previous investigations no mineral N was added, taking limited nitrogen availability into account. Incubation temperature was 22 °C. At the start of incubation, soil water content was adjusted to 20.8 ml H_2O per 100 g soil, expressing 50 % of water holding capacity (ISO 16072). After 301 days of incubation, the mineral N concentration in each soil column was determined in an extract by spectrometric measurement (DIN 19746).

VI.2.3.2 Measurement of CO_2 Release During the Incubation Study

The soil columns were placed in closed jars with 100 ml 0.15 M NaOH at the bottom, absorbing the mineralized CO_2, which was released from the soil columns between two measuring dates. The absorbed CO_2 was precipitated as $BaCO_3$ through the addition of 10 ml 1.5 M $BaCl_2$ solution and measured by titration with 0.3 M HCl and phenolphthalein as indicator. Measurement dates were 1, 3, 7, 14, 21, 35, 56, 77, 98, 120, 162, 217, and 301 days after start of incubation. The apparent decomposition of plant residues was calculated as difference between evolved CO_2 from soil columns with and without plant residue. The course of EOC-induced CO_2-release was calculated by summing up the EOC-induced CO_2 release between two subsequent measurement dates.

VII. References

Ajwa, H., & Tabatabai, M. (1994). Decomposition of different organic materials in soils. *Biology and Fertility of Soils, 18*(3), 175-182. doi:10.1007/BF00647664

Akujärvi, A., Heikkinen, J., Palosuo, T., & Liski, J. (2014). Carbon budget of Finnish croplands — Effects of land use change from natural forest to cropland. *Geoderma Regional, 2-3*, 1-8. doi:10.1016/j.geodrs.2014.09.003

Alewell, C., Ringeval, B., Ballabio, C., Robinson, D. A., Panagos, P., & Borrelli, P. (2020). Global phosphorus shortage will be aggravated by soil erosion. *Nat Commun, 11*(1), 4546. doi:10.1038/s41467-020-18326-7

Andersson, H., Bergström, L., Ulén, B., Djodjic, F., & Kirchmann, H. (2015). The role of subsoil as a source or sink for phosphorus leaching. *Journal of Environmental Quality, 44*(2), 535-544. doi:10.2134/jeq2014.04.0186

Andrén, O., & Kätterer, T. (1997). ICBM: the introductory carbon balance model for exploration of soil carbon balances. *Ecological applications, 7*(4), 1226-1236. doi:10.1890/1051-0761(1997)007[1226:ITICBM]2.0.CO;2

Barduca, L., Wentzel, S., Schmidt, R., Malagoli, M., & Joergensen, R. G. (2020). Mineralisation of distinct biogas digestate qualities directly after application to soil. *Biology and Fertility of Soils*. doi:10.1007/s00374-020-01521-5

Barrow, N. J. (2016). The effects of pH on phosphate uptake from the soil. *Plant and soil, 410*(1-2), 401-410. doi:10.1007/s11104-016-3008-9

Bates, J. M., & Granger, C. W. (1969). The combination of forecasts. *Journal of the Operational Research Society, 20*(4), 451-468. doi:10.1057/jors.1969.103

Baveye, P. C., Berthelin, J., Tessier, D., & Lemaire, G. (2018). The "4 per 1000" initiative: A credibility issue for the soil science community? *Geoderma, 309*, 118-123. doi:10.1016/j.geoderma.2017.05.005

Baveye, P. C., Schnee, L. S., Boivin, P., Laba, M., & Radulovich, R. (2020). Soil Organic Matter Research and Climate Change: Merely Re-storing Carbon Versus Restoring Soil Functions. *Frontiers in Environmental Science, 8*. doi:10.3389/fenvs.2020.579904

Begum, K., Kuhnert, M., Yeluripati, J., Glendining, M., & Smith, P. (2017). Simulating soil carbon sequestration from long term fertilizer and manure additions under continuous wheat using the DailyDayCent model. *Nutrient Cycling in Agroecosystems, 109*(3), 291-302. doi:10.1007/s10705-017-9888-0

Benbi, D. K., & Richter, J. (2002). A critical review of some approaches to modelling nitrogen mineralization. *Biology and Fertility of Soils, 35*(3), 168-183.

Bernal, M., Sanchez-Monedero, M., Paredes, C., & Roig, A. (1998). Carbon mineralization from organic wastes at different composting stages during their incubation with soil. *Agriculture, Ecosystems & Environment, 69*(3), 175-189. doi:10.1016/S0167-8809(98)00106-6

Berti, A., Morari, F., Dal Ferro, N., Simonetti, G., & Polese, R. (2016). Organic input quality is more important than its quantity: C turnover coefficients in different cropping systems. *European Journal of Agronomy, 77*, 138-145. doi:10.1016/j.eja.2016.03.005

Boer, M. A. d., Wolzak, L., & Slootweg, J. C. (2019). Phosphorus: reserves, production, and applications. In *Phosphorus recovery and recycling* (pp. 75-100): Springer.

Bolinder, M. A., Andrén, O., Kätterer, T., de Jong, R., VandenBygaart, A. J., Angers, D. A., Parent, L. E., & Gregorich, E. G. (2007). Soil carbon dynamics in Canadian Agricultural Ecoregions: Quantifying climatic influence on soil biological activity. *Agriculture, Ecosystems & Environment, 122*(4), 461-470. doi:10.1016/j.agee.2007.03.001

Bonanomi, G., De Filippis, F., Zotti, M., Idbella, M., Cesarano, G., Al-Rowaily, S., & Abd-ElGawad, A. (2020). Repeated applications of organic amendments promote beneficial microbiota, improve soil fertility and increase crop yield. *Applied Soil Ecology, 156*. doi:10.1016/j.apsoil.2020.103714

Bradford, M. A., Carey, C. J., Atwood, L., Bossio, D., Fenichel, E. P., Gennet, S., Fargione, J., Fisher, J. R. B., Fuller, E., Kane, D. A., Lehmann, J., Oldfield, E. E., Ordway, E. M., Rudek, J., Sanderman, J., & Wood, S. A. (2019). Soil carbon science for policy and practice. *Nature Sustainability*. doi:10.1038/s41893-019-0431-y

Campbell, E. E., & Paustian, K. (2015). Current developments in soil organic matter modeling and the expansion of model applications: a review. *Environmental Research Letters, 10*(12). doi:10.1088/1748-9326/10/12/123004

Capdevila-Cortada, M. (2019). Electrifying the Haber–Bosch. *Nature Catalysis, 2*(12), 1055-1055. doi:10.1038/s41929-019-0414-4

Cerecetto, V., Smalla, K., Nesme, J., Garaycochea, S., Fresia, P., Sorensen, S. J., Babin, D., & Leoni, C. (2021). Reduced tillage, cover crops and organic amendments affect soil microbiota and improve soil health in Uruguayan vegetable farming systems. *FEMS Microbiol Ecol, 97*(3). doi:10.1093/femsec/fiab023

Chea, L., Meijide, A., Meinen, C., Pawelzik, E., & Naumann, M. (2021). Cultivar-Dependent Responses in Plant Growth, Leaf Physiology, Phosphorus Use Efficiency, and Tuber Quality of Potatoes Under Limited Phosphorus Availability Conditions. *Front Plant Sci, 12*, 723862. doi:10.3389/fpls.2021.723862

Cleveland, C. C., & Liptzin, D. (2007). C:N:P stoichiometry in soil: is there a “Redfield ratio” for the microbial biomass? *Biogeochemistry, 85*(3), 235-252. doi:10.1007/s10533-007-9132-0

Coleman, K., & Jenkinson, D. (1999). RothC-A model for the turnover of carbon in soil. *Model Description and Users Guide (Harpenden).*

Coonan, E. C., Kirkby, C. A., Kirkegaard, J. A., Amidy, M. R., Strong, C. L., & Richardson, A. E. (2020). Microorganisms and nutrient stoichiometry as mediators of soil organic matter dynamics. *Nutrient Cycling in Agroecosystems, 117*(3), 273-298. doi:10.1007/s10705-020-10076-8

Cotrufo, M. F., Wallenstein, M. D., Boot, C. M., Denef, K., & Paul, E. (2013). The Microbial Efficiency-Matrix Stabilization (MEMS) framework integrates plant litter decomposition with soil organic matter stabilization: do labile plant inputs form stable soil organic matter? *Glob Chang Biol, 19*(4), 988-995. doi:10.1111/gcb.12113

Damon, P. M., Bowden, B., Rose, T., & Rengel, Z. (2014). Crop residue contributions to phosphorus pools in agricultural soils: A review. *Soil Biology and Biochemistry, 74*, 127-137. doi:10.1016/j.soilbio.2014.03.003

Das, B., Huth, N., Probert, M., Condron, L., & Schmidt, S. (2019). Soil Phosphorus Modeling for Modern Agriculture Requires Balance of Science and Practicality: A Perspective. *J Environ Qual, 48*(5), 1281-1294. doi:10.2134/jeq2019.05.0201

Dechow, R., Franko, U., Kätterer, T., & Kolbe, H. (2019). Evaluation of the RothC model as a prognostic tool for the prediction of SOC trends in response to management practices on arable land. *Geoderma, 337*, 463-478. doi:10.1016/j.geoderma.2018.10.001

Dignac, M.-F., Derrien, D., Barré, P., Barot, S., Cécillon, L., Chenu, C., Chevallier, T., Freschet, G. T., Garnier, P., & Guenet, B. (2017). Increasing soil carbon storage: mechanisms, effects of agricultural practices and proxies. A review. *Agronomy for sustainable development, 37*(2), 14. doi:10.1007/s13593-017-0421-2

Diks, C. G. H., & Vrugt, J. A. (2010). Comparison of point forecast accuracy of model averaging methods in hydrologic applications. *Stochastic Environmental Research and Risk Assessment, 24*(6), 809-820. doi:10.1007/s00477-010-0378-z

Dzombak, R. M., & Sheldon, N. D. (2020). Weathering Intensity and Presence of Vegetation Are Key Controls on Soil Phosphorus Concentrations: Implications for Past and Future Terrestrial Ecosystems. *Soil Systems, 4*(4). doi:10.3390/soilsystems4040073

Edmisten, K. L., Green, J. T., Mueller, J. P., & Burns, J. C. (2008). Winter annual small grain forage potential. II. Quantification of nutritive characteristics of four small grain species at six growth stages. *Communications in Soil Science and Plant Analysis, 29*(7-8), 881-899. doi:10.1080/00103629809369993

Elzhov, T. V., Mullen, K. M., Spiess, A.-N., & Bolker, B. (2016). minpack.lm: R Interface to the Levenberg-Marquardt Nonlinear Least-Squares Algorithm Found in MINPACK, Plus Support for Bounds. Retrieved from https://CRAN.R-project.org/package=minpack.lm

Epelde, L., Jauregi, L., Urra, J., Ibarretxe, L., Romo, J., Goikoetxea, I., & Garbisu, C. (2018). Characterization of Composted Organic Amendments for Agricultural Use. *Frontiers in Sustainable Food Systems, 2*. doi:10.3389/fsufs.2018.00044

Farina, R., Sandor, R., Abdalla, M., Alvaro-Fuentes, J., Bechini, L., Bolinder, M. A., Brilli, L., Chenu, C., Clivot, H., De Antoni Migliorati, M., Di Bene, C., Dorich, C. D., Ehrhardt, F., Ferchaud, F., Fitton, N., Francaviglia, R., Franko, U., Giltrap, D. L., Grant, B. B., Guenet, B., Harrison, M. T., Kirschbaum, M. U. F., Kuka, K., Kulmala, L., Liski, J., McGrath, M. J., Meier, E., Menichetti, L., Moyano, F., Nendel, C., Recous, S., Reibold, N., Shepherd, A., Smith, W. N., Smith, P., Soussana, J. F., Stella, T., Taghizadeh-Toosi, A., Tsutskikh, E., & Bellocchi, G. (2020). Ensemble modelling, uncertainty and robust predictions of organic carbon in long-term bare-fallow soils. *Glob Chang Biol.* doi:10.1111/gcb.15441

Feedipedia - Animal Feed Resources Information System. Retrieved from https://www.feedipedia.org/. Retrieved 01.07.2022, from INRA, CIRAD, AFZ and FAO https://www.feedipedia.org/

Franko, U. (1997). Modellierung des Umsatzes der organischen Bodensubstanz. *Archives of Agronomy and Soil Science, 41*(6), 527-547. doi:10.1080/03650349709366019

Franko, U., Diel, J., & Ruehlmann, J. (2021). Applying CCB to predict management change affected long-term SOM turnover of the Extended Static Fertilization Experiment in Bad Lauchstädt. *European Journal of Soil Science.* doi:10.1111/ejss.13148

Franko, U., Kolbe, H., Thiel, E., & Ließ, E. (2011). Multi-site validation of a soil organic matter model for arable fields based on generally available input data. *Geoderma, 166*(1), 119-134. doi:10.1016/j.geoderma.2011.07.019

Franko, U., & Oelschlägel, B. (1995a). Einfluss von klima und textur auf die biologische aktivität beim umsatz der organischen bodensubstanz. *Archives of Agronomy and Soil Science, 39*(3), 155-163. doi:10.1080/03650349509365898

Franko, U., Oelschlägel, B., & Schenk, S. (1995b). Simulation of temperature-, water-and nitrogen dynamics using the model CANDY. *Ecological Modelling, 81*(1-3), 213-222.

Gami, S. K., Lauren, J. G., & Duxbury, J. M. (2009). Soil organic carbon and nitrogen stocks in Nepal long-term soil fertility experiments. *Soil and Tillage Research, 106*(1), 95-103. doi:10.1016/j.still.2009.10.003

Gasser, A., Nielsen, K., & Franko, U. (2021a). *Inkubationsversuche als Grundlage für die Charakterisierung von organischen Substraten mit mechanistischen Modellen, die Übertragung der gewonnen Parameter auf die Feldskala und die Ableitung von HÄQ Werten für „neue" Fruchtarten.* Paper presented at the 132. VDLUFA Kongress - Optionen für die zukünfitge Landnutzung, Speyer.

Gasser, S. A. A., Diel, J., Nielsen, K., Mewes, P., Engels, C., & Franko, U. (2021b). A model ensemble approach to determine the humus building efficiency of organic amendments in incubation experiments. *Soil Use and Management.* doi:10.1111/sum.12699

Gasser, S. A. A., Nielsen, K., Eichler-Löbermann, B., Armbruster, M., Merbach, I., & Franko, U. (2023). Simulating the soil phosphorus dynamics of four long-term field experiments with a novel phosphorus model. *Soil Use and Management.* doi:10.1111/sum.12881

Gasser, S. A. A., Nielsen, K., & Franko, U. (2022). Transfer of carbon incubation parameters to model the SOC and SON dynamics of a field trial with energy crops applying digestates as organic fertilizers. *Soil Use and Management.* doi:10.1111/sum.12810

Grosse, M., Hierold, W., Ahlborn, M. C., Piepho, H.-P., & Helming, K. (2020). Long-term field experiments in Germany: classification and spatial representation. *Soil, 6*(2), 579-596. doi:10.5194/soil-6-579-2020

Guillaume, T., Bragazza, L., Levasseur, C., Libohova, Z., & Sinaj, S. (2021). Long-term soil organic carbon dynamics in temperate cropland-grassland systems. *Agriculture, Ecosystems & Environment, 305*. doi:10.1016/j.agee.2020.107184

Hagedorn, R., Doblas-Reyes, F. J., & Palmer, T. (2005). The rationale behind the success of multi-model ensembles in seasonal forecasting–I. Basic concept. *Tellus A, 57*(3), 219-233. doi:10.3402/tellusa.v57i3.14657

Hallama, M., Pekrun, C., Mayer-Gruner, P., Uksa, M., Abdullaeva, Y., Pilz, S., Schloter, M., Lambers, H., & Kandeler, E. (2022). The role of microbes in the increase of organic phosphorus availability in the rhizosheath of cover crops. *Plant and soil*. doi:10.1007/s11104-022-05340-5

Harden, J. W., Hugelius, G., Ahlstrom, A., Blankinship, J. C., Bond-Lamberty, B., Lawrence, C. R., Loisel, J., Malhotra, A., Jackson, R. B., Ogle, S., Phillips, C., Ryals, R., Todd-Brown, K., Vargas, R., Vergara, S. E., Cotrufo, M. F., Keiluweit, M., Heckman, K. A., Crow, S. E., Silver, W. L., DeLonge, M., & Nave, L. E. (2018). Networking our science to characterize the state, vulnerabilities, and management opportunities of soil organic matter. *Glob Chang Biol, 24*(2), e705-e718. doi:10.1111/gcb.13896

Hawes, Young, Banks, Begg, Christie, Iannetta, Karley, & Squire. (2019). Whole-Systems Analysis of Environmental and Economic Sustainability in Arable Cropping Systems: A Case Study. *Agronomy, 9*(8). doi:10.3390/agronomy9080438

Haynes, R. J. (1984). Lime and Phosphate in the Soil-Plant System. *Advances in agronomy, Volume 37*, 249-315. doi:10.1016/s0065-2113(08)60456-3

Hess, L. J. T., Hinckley, E.-L. S., Robertson, G. P., & Matson, P. A. (2020). Rainfall intensification increases nitrate leaching from tilled but not no-till cropping systems in the U.S. Midwest. *Agriculture, Ecosystems & Environment, 290*. doi:10.1016/j.agee.2019.106747

Hirte, J., Leifeld, J., Abiven, S., Oberholzer, H.-R., & Mayer, J. (2018). Below ground carbon inputs to soil via root biomass and rhizodeposition of field-grown maize and wheat at harvest are independent of net primary productivity. *Agriculture, Ecosystems & Environment, 265*, 556-566. doi:10.1016/j.agee.2018.07.010

Höcker, S. (2017). *Quantifizierung des Eintrags von pflanzlichem organischem Kohlenstoff in den Boden im Energiepflanzenbau zur Biogasgewinnung.* (Ph.D. dissertation). Humboldt-Universität zu Berlin,

Iizumi, T., & Wagai, R. (2019). Leveraging drought risk reduction for sustainable food, soil and climate via soil organic carbon sequestration. *Sci Rep, 9*(1), 19744. doi:10.1038/s41598-019-55835-y

Jha, P., De, A., Lakaria, B. L., Biswas, A., Singh, M., Reddy, K., & Rao, A. (2012). Soil carbon pools, mineralization and fluxes associated with land use change in Vertisols of Central India. *National Academy Science Letters, 35*(6), 475-483. doi:10.1007/s40009-012-0082-2

Kallenbach, C. M., Grandy, A. S., Frey, S. D., & Diefendorf, A. F. (2015). Microbial physiology and necromass regulate agricultural soil carbon accumulation. *Soil Biology and Biochemistry, 91*, 279-290. doi:10.1016/j.soilbio.2015.09.005

Karhu, K., Gärdenäs, A. I., Heikkinen, J., Vanhala, P., Tuomi, M., & Liski, J. (2012). Impacts of organic amendments on carbon stocks of an agricultural soil — Comparison of model-simulations to measurements. *Geoderma, 189-190*, 606-616. doi:10.1016/j.geoderma.2012.06.007

Kätterer, T., Bolinder, M. A., Andrén, O., Kirchmann, H., & Menichetti, L. (2011). Roots contribute more to refractory soil organic matter than above-ground crop residues, as revealed by a long-term field experiment. *Agriculture, Ecosystems & Environment, 141*(1-2), 184-192. doi:10.1016/j.agee.2011.02.029

Kätterer, T., Reichstein, M., Andrén, O., & Lomander, A. (1998). Temperature dependence of organic matter decomposition: a critical review using literature data analyzed with different models. *Biology and Fertility of Soils, 27*(3), 258-262.

Khan, K. S., Ali, M. M., Naveed, M., Rehmani, M. I. A., Shafique, M. W., Ali, H. M., Abdelsalam, N. R., Ghareeb, R. Y., & Feng, G. (2022). Co-application of organic amendments and inorganic P increase maize growth and soil carbon, phosphorus availability in calcareous soil. *Frontiers in Environmental Science, 10.* doi:10.3389/fenvs.2022.949371

Klavins, M., Sire, J., Purmalis, O., & Melecis, V. (2008). Approaches to estimating humification indicators for peat. *Mires & Peat, 3.*

Kopittke, P. M., Menzies, N. W., Wang, P., McKenna, B. A., & Lombi, E. (2019). Soil and the intensification of agriculture for global food security. *Environ Int, 132*, 105078. doi:10.1016/j.envint.2019.105078

Körschens, M. (2000). IOSDV Internationale organische Stickstoffdauerdüngungsversuche. *Bericht der Internationalen Arbeitsgemeinschaft Bodenfruchtbarkeit in der Internationalen Bodenkundlichen Union (IUSS), UFZ-Bericht, 15*, 2000.

Lamb, J. A., Fernandez, F. G., & Kaiser, D. E. (2014). Understanding nitrogen in soils. *University of Minnesota Extension,(Revised)*, 1-5.

Lambers, H. (2022). Phosphorus Acquisition and Utilization in Plants. *Annu Rev Plant Biol, 73*, 17-42. doi:10.1146/annurev-arplant-102720-125738

Larney, F. J., & Angers, D. A. (2012). The role of organic amendments in soil reclamation: a review. *Canadian Journal of Soil Science, 92*(1), 19-38. doi:10.4141/cjss2010-064

Lashermes, G., Nicolardot, B., Parnaudeau, V., Thuriès, L., Chaussod, R., Guillotin, M. L., Linères, M., Mary, B., Metzger, L., Morvan, T., Tricaud, A., Villette, C., & Houot, S. (2009). Indicator of potential residual carbon in soils after exogenous organic matter application. *European Journal of Soil Science, 60*(2), 297-310. doi:10.1111/j.1365-2389.2008.01110.x

Levavasseur, F., Mary, B., Christensen, B. T., Duparque, A., Ferchaud, F., Kätterer, T., Lagrange, H., Montenach, D., Resseguier, C., & Houot, S. (2020). The simple AMG model accurately simulates organic carbon storage in soils after repeated application of exogenous organic matter. *Nutrient Cycling in Agroecosystems.* doi:10.1007/s10705-020-10065-x

Li, W., Duan, Q., Miao, C., Ye, A., Gong, W., & Di, Z. (2017). A review on statistical postprocessing methods for hydrometeorological ensemble forecasting. *Wiley Interdisciplinary Reviews: Water, 4*(6). doi:10.1002/wat2.1246

Liang, C., Schimel, J. P., & Jastrow, J. D. (2017). The importance of anabolism in microbial control over soil carbon storage. *Nat Microbiol, 2*, 17105. doi:10.1038/nmicrobiol.2017.105

Maltas, A., Kebli, H., Oberholzer, H. R., Weisskopf, P., & Sinaj, S. (2018). The effects of organic and mineral fertilizers on carbon sequestration, soil properties, and crop yields from a long-term field experiment under a Swiss conventional farming system. *Land Degradation & Development, 29*(4), 926-938. doi:10.1002/ldr.2913

Mann, T., Heckelmann, A., Uckele , H., Jilg, T., Elsäßer, M., Messner, J., Zacharias, B., Roth, U., Vollmer, K.-H., Rather, K., Riedel, M., & Rupp, D. (2021). *Stammdatensammlung*. Retrieved from: www.ltz-augustenberg.de

Martre, P., Wallach, D., Asseng, S., Ewert, F., Jones, J. W., Rotter, R. P., Boote, K. J., Ruane, A. C., Thorburn, P. J., Cammarano, D., Hatfield, J. L., Rosenzweig, C., Aggarwal, P. K., Angulo, C., Basso, B., Bertuzzi, P., Biernath, C., Brisson, N., Challinor, A. J., Doltra, J., Gayler, S., Goldberg, R., Grant, R. F., Heng, L., Hooker, J., Hunt, L. A., Ingwersen, J., Izaurralde, R. C., Kersebaum, K. C., Muller, C., Kumar, S. N., Nendel, C., O'Leary, G., Olesen, J. E., Osborne, T. M., Palosuo, T., Priesack, E., Ripoche, D., Semenov, M. A., Shcherbak, I., Steduto, P., Stockle, C. O., Stratonovitch, P., Streck, T., Supit, I., Tao, F., Travasso, M., Waha, K., White, J. W., & Wolf, J. (2015). Multimodel ensembles of wheat growth: many models are better than one. *Glob Chang Biol, 21*(2), 911-925. doi:10.1111/gcb.12768

Max, P., Martin, A., & Franz, W. (2022). *Verbundvorhaben: Bewertung der Humus- und Nährstoffwirkung von organischen Reststoffen; Teilvorhaben 2: Chemische Charakterisierung der Reststoffe und Ermittlung von deren N- und P-Dynamik in Inkubationsversuchen.* Retrieved from https://www.fnr.de/index.php?id=11150&fkz=22410918

McConnell, C. A., Kaye, J. P., & Kemanian, A. R. (2020). Reviews and syntheses: Ironing out wrinkles in the soil phosphorus cycling paradigm. *Biogeosciences, 17*(21), 5309-5333. doi:10.5194/bg-17-5309-2020

McLaughlin, M. J., McBeath, T. M., Smernik, R., Stacey, S. P., Ajiboye, B., & Guppy, C. (2011). The chemical nature of P accumulation in agricultural soils—implications for fertiliser management and design: an Australian perspective. *Plant and soil, 349*(1-2), 69-87. doi:10.1007/s11104-011-0907-7

Mewes, P. (2017). *Persistence of exogenous organic matter in soil as a cultivation property.* (Ph. D Dissertation). Humboldt-University of Berlin,

Minasny, B., Malone, B. P., McBratney, A. B., Angers, D. A., Arrouays, D., Chambers, A., Chaplot, V., Chen, Z.-S., Cheng, K., & Das, B. S. (2017). Soil carbon 4 per mille. *Geoderma, 292*, 59-86. doi:10.1016/j.geoderma.2017.01.002

Mogollón, J. M., Beusen, A. H. W., van Grinsven, H. J. M., Westhoek, H., & Bouwman, A. F. (2018). Future agricultural phosphorus demand according to the shared socioeconomic pathways. *Global Environmental Change, 50*, 149-163. doi:10.1016/j.gloenvcha.2018.03.007

Morvan, T., Nicolardot, B., & Péan, L. (2005). Biochemical composition and kinetics of C and N mineralization of animal wastes: a typological approach. *Biology and Fertility of Soils, 42*(6), 513-522. doi:10.1007/s00374-005-0045-6

Nielsen, K., Roß, C.-L., Hoffmann, M., Muskolus, A., Ellmer, F., & Kautz, T. (2020). The Chemical Composition of Biogas Digestates Determines Their Effect on Soil Microbial Activity. *Agriculture, 10*(6). doi:10.3390/agriculture10060244

Nobile, C. M., Bravin, M. N., Becquer, T., & Paillat, J. M. (2020). Phosphorus sorption and availability in an andosol after a decade of organic or mineral fertilizer applications: Importance of pH and organic carbon modifications in soil as compared to phosphorus accumulation. *Chemosphere, 239*, 124709. doi:10.1016/j.chemosphere.2019.124709

O'Rourke, S. M., Angers, D. A., Holden, N. M., & McBratney, A. B. (2015). Soil organic carbon across scales. *Glob Chang Biol, 21*(10), 3561-3574. doi:10.1111/gcb.12959

Parton, W., Schimel, D. S., Cole, C., & Ojima, D. (1987). Analysis of factors controlling soil organic matter levels in Great Plains Grasslands 1. *Soil Science Society of America Journal, 51*(5), 1173-1179. doi:10.2136/sssaj1987.03615995005100050015x

Parton, W. J., Ojima, D. S., Cole, C. V., & Schimel, D. S. (1994). A general model for soil organic matter dynamics: sensitivity to litter chemistry, texture and management. *Quantitative modeling of soil forming processes*(quantitativemod), 147-167. doi:10.2136/sssaspecpub39.c9

Paustian, K., Lehmann, J., Ogle, S., Reay, D., Robertson, G. P., & Smith, P. (2016). Climate-smart soils. *Nature, 532*(7597), 49-57. doi:10.1038/nature17174

Poeplau, C., Kätterer, T., Bolinder, M. A., Börjesson, G., Berti, A., & Lugato, E. (2015). Low stabilization of aboveground crop residue carbon in sandy soils of Swedish long-term experiments. *Geoderma, 237-238*, 246-255. doi:10.1016/j.geoderma.2014.09.010

Pothuluri, J., Kissel, D., Whitney, D., & Thien, S. (1986). Phosphorus uptake from soil layers having different soil test phosphorus levels 1. *Agronomy Journal, 78*(6), 991-994. doi:10.2134/agronj1986.00021962007800060012x

Prays, N., Dominik, P., Sanger, A., & Franko, U. (2018). Biogas residue parameterization for soil organic matter modeling. *PLoS One, 13*(10), e0204121. doi:10.1371/journal.pone.0204121

R Core Team. (2019). R: A language and environment for statistical computing. Vienna, Austria: R Foundation for Statistical Computing. Retrieved from https://www.R-project.org/

Ragossnig, A. M., & Schneider, D. R. (2019). Circular economy, recycling and end-of-waste. *Waste Manag Res, 37*(2), 109-111. doi:10.1177/0734242X19826776

Rasse, D. P., Rumpel, C., & Dignac, M.-F. (2005). Is soil carbon mostly root carbon? Mechanisms for a specific stabilisation. *Plant and soil, 269*(1-2), 341-356. doi:10.1007/s11104-004-0907-y

Raymond, N., Kopittke, P. M., Wang, E., Lester, D., & Bell, M. J. (2021). Does the APSIM model capture soil phosphorus dynamics? A case study with Vertisols. *Field Crops Research, 273*, 108302.

Reid, K., Schneider, K., & McConkey, B. (2018). Components of Phosphorus Loss From Agricultural Landscapes, and How to Incorporate Them Into Risk Assessment Tools. *Frontiers in Earth Science, 6*. doi:10.3389/feart.2018.00135

Riggers, C., Poeplau, C., Don, A., Bamminger, C., Höper, H., & Dechow, R. (2019). Multi-model ensemble improved the prediction of trends in soil organic carbon stocks in German croplands. *Geoderma, 345*, 17-30. doi:10.1016/j.geoderma.2019.03.014

Rillig, M. C., Ryo, M., Lehmann, A., Aguilar-Trigueros, C. A., Buchert, S., Wulf, A., Iwasaki, A., Roy, J., & Yang, G. (2019). The role of multiple global change factors in driving soil functions and microbial biodiversity. *Science, 366*(6467), 886-890.

Rowe, H., Withers, P. J. A., Baas, P., Chan, N. I., Doody, D., Holiman, J., Jacobs, B., Li, H., MacDonald, G. K., McDowell, R., Sharpley, A. N., Shen, J., Taheri, W., Wallenstein, M., & Weintraub, M. N. (2015). Integrating legacy soil phosphorus into sustainable nutrient management strategies for future food, bioenergy and water security. *Nutrient Cycling in Agroecosystems, 104*(3), 393-412. doi:10.1007/s10705-015-9726-1

Roy, S., & Kashem, M. A. (2014). Effects of Organic Manures in Changes of Some Soil Properties at Different Incubation Periods. *Open Journal of Soil Science, 04*(03), 81-86. doi:10.4236/ojss.2014.43011

Sänger, A., Geisseler, D., & Ludwig, B. (2014). C and N dynamics of a range of biogas slurries as a function of application rate and soil texture: a laboratory experiment. *Archives of Agronomy and Soil Science, 60*(12), 1779-1794. doi:10.1080/03650340.2014.907491

Sattari, S. Z., Bouwman, A. F., Giller, K. E., & van Ittersum, M. K. (2012). Residual soil phosphorus as the missing piece in the global phosphorus crisis puzzle. *Proceedings of the National Academy of Sciences, 109*(16), 6348-6353. doi:10.1073/pnas.1113675109

Sayara, T., Basheer-Salimia, R., Hawamde, F., & Sánchez, A. (2020). Recycling of Organic Wastes through Composting: Process Performance and Compost Application in Agriculture. *Agronomy, 10*(11). doi:10.3390/agronomy10111838

Shen, J., Yuan, L., Zhang, J., Li, H., Bai, Z., Chen, X., Zhang, W., & Zhang, F. (2011). Phosphorus dynamics: from soil to plant. *Plant physiology, 156*(3), 997-1005.

Siebers, N., Wang, L., Funk, T., von Tucher, S., Merbach, I., Schweitzer, K., & Kruse, J. (2021). Subsoils—a sink for excess fertilizer P but a minor contribution to P plant nutrition: evidence from long-term fertilization trials. *Environmental Sciences Europe, 33*(1). doi:10.1186/s12302-021-00496-w

Siedt, M., Schaffer, A., Smith, K. E. C., Nabel, M., Ross-Nickoll, M., & van Dongen, J. T. (2021). Comparing straw, compost, and biochar regarding their suitability as agricultural soil amendments to affect soil structure, nutrient leaching, microbial communities, and the fate of pesticides. *Sci Total Environ, 751*, 141607. doi:10.1016/j.scitotenv.2020.141607

Sierra, C. A., Müller, M., & Trumbore, S. E. (2012). Models of soil organic matter decomposition: the SoilR package, version 1.0. *Geoscientific Model Development, 5*(4), 1045-1060. doi:10.5194/gmd-5-1045-2012

Sleutel, S., De Neve, S., Prat Roibas, M. R., & Hofman, G. (2005). The influence of model type and incubation time on the estimation of stable organic carbon in organic materials. *European Journal of Soil Science, 56*(4), 505-514. doi:10.1111/j.1365-2389.2004.00685.x

Smith, P., Martino, D., Cai, Z., Gwary, D., Janzen, H., Kumar, P., McCarl, B., Ogle, S., O'Mara, F., Rice, C., Scholes, B., Sirotenko, O., Howden, M., McAllister, T., Pan, G., Romanenkov, V., Schneider, U., Towprayoon, S., Wattenbach, M., & Smith, J. (2008). Greenhouse gas mitigation in agriculture. *Philos Trans R Soc Lond B Biol Sci, 363*(1492), 789-813. doi:10.1098/rstb.2007.2184

Soetaert, K. E., Petzoldt, T., & Setzer, R. W. (2010). Solving differential equations in R: package deSolve. *Journal of statistical software, 33*.

Stockmann, U., Adams, M. A., Crawford, J. W., Field, D. J., Henakaarchchi, N., Jenkins, M., Minasny, B., McBratney, A. B., Courcelles, V. d. R. d., Singh, K., Wheeler, I., Abbott, L., Angers, D. A., Baldock, J., Bird, M., Brookes, P. C., Chenu, C., Jastrow, J. D., Lal, R., Lehmann, J., O'Donnell, A. G., Parton, W. J., Whitehead, D., & Zimmermann, M. (2013). The knowns, known unknowns and unknowns of sequestration of soil organic carbon. *Agriculture, Ecosystems & Environment, 164*, 80-99. doi:10.1016/j.agee.2012.10.001

Sulieman, S., & Mühling, K. H. (2021). Utilization of soil organic phosphorus as a strategic approach for sustainable agriculture. *Journal of Plant Nutrition and Soil Science, 184*(3), 311-319. doi:10.1002/jpln.202100057

Sulman, B. N., Moore, J. A. M., Abramoff, R., Averill, C., Kivlin, S., Georgiou, K., Sridhar, B., Hartman, M. D., Wang, G., Wieder, W. R., Bradford, M. A., Luo, Y., Mayes, M. A., Morrison, E., Riley, W. J., Salazar, A., Schimel, J. P., Tang, J., & Classen, A. T. (2018). Multiple models and experiments underscore large uncertainty in soil carbon dynamics. *Biogeochemistry, 141*(2), 109-123. doi:10.1007/s10533-018-0509-z

Taghizadeh-Toosi, A., Christensen, B. T., Hutchings, N. J., Vejlin, J., Kätterer, T., Glendining, M., & Olesen, J. E. (2014). C-TOOL: A simple model for simulating whole-profile carbon storage in temperate agricultural soils. *Ecological Modelling, 292*, 11-25. doi:10.1016/j.ecolmodel.2014.08.016

Tang, J., & Riley, W. J. (2020). Linear two-pool models are insufficient to infer soil organic matter decomposition temperature sensitivity from incubations. *Biogeochemistry, 149*(3), 251-261. doi:10.1007/s10533-020-00678-3

Tebaldi, C., & Knutti, R. (2007). The use of the multi-model ensemble in probabilistic climate projections. *Philosophical transactions of the royal society A: mathematical, physical and engineering sciences, 365*(1857), 2053-2075.

Tuomi, M., Rasinmäki, J., Repo, A., Vanhala, P., & Liski, J. (2011). Soil carbon model Yasso07 graphical user interface. *Environmental modelling & software, 26*(11), 1358-1362. doi:10.1016/j.envsoft.2011.05.009

Ulén, B., Bechmann, M., Fölster, J., Jarvie, H., & Tunney, H. (2007). Agriculture as a phosphorus source for eutrophication in the north-west European countries, Norway, Sweden, United Kingdom and Ireland: a review. *Soil Use and Management, 23*, 5-15. doi:10.1111/j.1475-2743.2007.00115.x

Urra, Alkorta, & Garbisu. (2019). Potential Benefits and Risks for Soil Health Derived From the Use of Organic Amendments in Agriculture. *Agronomy, 9*(9). doi:10.3390/agronomy9090542

Vaccari, D. A. (2009). Phosphorus: a looming crisis. *Scientific American, 300*(6), 54-59.

Vadas, P. A., Joern, B. C., & Moore, P. A. (2012). Simulating soil phosphorus dynamics for a phosphorus loss quantification tool. *J Environ Qual, 41*(6), 1750-1757. doi:10.2134/jeq2012.0003

Van Kauwenbergh, S. J. (2010). *World phosphate rock reserves and resources*: Ifdc Muscle Shoals.

van Laak, M., Klingenberg, U., Peiter, E., Reitz, T., Zimmer, D., & Buczko, U. (2018). The equivalence of the Calcium-Acetate-Lactate and Double-Lactate extraction methods to assess soil phosphorus fertility. *Journal of Plant Nutrition and Soil Science, 181*(5), 795-801. doi:10.1002/jpln.201700366

Vet, R., Artz, R. S., Carou, S., Shaw, M., Ro, C.-U., Aas, W., Baker, A., Bowersox, V. C., Dentener, F., Galy-Lacaux, C., Hou, A., Pienaar, J. J., Gillett, R., Forti, M. C., Gromov, S., Hara, H., Khodzher, T., Mahowald, N. M., Nickovic, S., Rao, P. S. P., & Reid, N. W. (2014). A global assessment of precipitation chemistry and deposition of sulfur, nitrogen, sea salt, base cations, organic acids, acidity and pH, and phosphorus. *Atmospheric Environment, 93*, 3-100. doi:10.1016/j.atmosenv.2013.10.060

Walworth, J. (2013). Nitrogen in the Soil and the Environment. In: College of Agriculture and Life Sciences, University of Arizona (Tucson, AZ).

Wang, Y., Bauke, S. L., von Sperber, C., Tamburini, F., Guigue, J., Winkler, P., Kaiser, K., Honermeier, B., & Amelung, W. (2021). Soil phosphorus cycling is modified by carbon and nitrogen fertilization in a long-term field experiment. *Journal of Plant Nutrition and Soil Science, 184*(2), 282-293. doi:10.1002/jpln.202000261

Wiesmeier, M., Urbanski, L., Hobley, E., Lang, B., von Lützow, M., Marin-Spiotta, E., van Wesemael, B., Rabot, E., Ließ, M., Garcia-Franco, N., Wollschläger, U., Vogel, H.-J., & Kögel-Knabner, I. (2019). Soil organic carbon storage as a key function of soils - A review of drivers and indicators at various scales. *Geoderma, 333*, 149-162. doi:10.1016/j.geoderma.2018.07.026

Wu, H., & Levinson, D. (2021). The ensemble approach to forecasting: a review and synthesis. *Transportation Research Part C: Emerging Technologies, 132*, 103357.

Wuenscher, R., Unterfrauner, H., Peticzka, R., & Zehetner, F. (2016). A comparison of 14 soil phosphorus extraction methods applied to 50 agricultural soils from Central Europe. *Plant, Soil and Environment, 61*(No. 2), 86-96. doi:10.17221/932/2014-pse

Yan, X., Li, G., Zhang, W., Muneer, M. A., Yu, W., Ma, C., & Wu, L. (2022). Spatio-Temporal Variation of Soil Phosphorus and Its Implications for Future Pomelo Orcharding System Management: A Model Prediction From Southeast China From 1985–2100. *Frontiers in Environmental Science, 10*. doi:10.3389/fenvs.2022.858816

Yeluripati, J. B., del Prado, A., Sanz-Cobeña, A., Rees, R. M., Li, C., Chadwick, D., Tilston, E., Topp, C. F. E., Cardenas, L. M., Ingraham, P., Gilhespy, S., Anthony, S., Vetter, S. H., Misselbrook, T., Salas, W., & Smith, P. (2015). Global Research Alliance Modelling Platform (GRAMP): An open web platform for modelling greenhouse gas emissions from agro-ecosystems. *Computers and Electronics in Agriculture, 111*, 112-120. doi:10.1016/j.compag.2014.11.016

Yu, W., Li, G., Hartmann, T. E., Xu, M., Yang, X., Li, H., Zhang, J., & Shen, J. (2021). Development of a Novel Model of Soil Legacy P Assessment for Calcareous and Acidic Soils. *Frontiers in Environmental Science, 8*. doi:10.3389/fenvs.2020.621833

Zhang, J., Beusen, A. H., Van Apeldoorn, D. F., Mogollón, J. M., Yu, C., & Bouwman, A. F. (2017). Spatiotemporal dynamics of soil phosphorus and crop uptake in global cropland during the 20th century. *Biogeosciences, 14*(8), 2055-2068. doi:10.5194/bg-14-2055-2017

Zhang, W., Liu, K., Wang, J., Shao, X., Xu, M., Li, J., Wang, X., & Murphy, D. V. (2015). Relative contribution of maize and external manure amendment to soil carbon sequestration in a long-term intensive maize cropping system. *Sci Rep, 5*, 10791. doi:10.1038/srep10791

Zicker, T., von Tucher, S., Kavka, M., & Eichler-Löbermann, B. (2018). Soil test phosphorus as affected by phosphorus budgets in two long-term field experiments in Germany. *Field Crops Research, 218*, 158-170. doi:10.1016/j.fcr.2018.01.008

Zirkler, D., Peters, A., & Kaupenjohann, M. (2014). Elemental composition of biogas residues: Variability and alteration during anaerobic digestion. *Biomass and Bioenergy, 67*, 89-98. doi:10.1016/j.biombioe.2014.04.021

VIII. 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.

――――――――――	――――――――――――――――――――――――――――
Datum / Date	Unterschrift des Antragstellers/*Signature of the applicant*

IX. Akademischer Werdegang

Stefan Anton Albert Gasser

E-Mail: antonigasser@gmx.de

Ausbildung

03.2019	Aufnahme des Promotionsstudiums an der Martin-Luther-Universität Halle
2015 / 2018	Masterstudium der Umweltwissenschaften an der Albert-Ludwig-Universität Freiburg
2012 / 2015	Bachelorstudium der Umweltnaturwissenschaften an der Albert-Ludwig-Universität Freiburg
10.2011 / 02.2012	Studium des Umweltingenieurwesens an der TU München

05.2011 | Allgemeine Hochschulreife am Gymnasium Schuldorf Bergstraße

Tätigkeit

06.2023 | Wissenschaftlicher Mitarbeiter am Leibniz-Institut für Gemüse- und Zierpflanzenbau

11.2020 | Übernahme der Projektleitung: Bewertung der Humus- und Nährstoffwirkung von organischen Reststoffen; Teilvorhaben 3: Charakterisierung der Humus, N- und P- Düngewirkung durch Modellierung

03.2019 / 12.2022 | Doktorandenstelle am Helmholtz-Zentrum für Umweltforschung Halle zum Thema C-N-P Modellierung

Publikationen:

01.2023 | Gasser, S. A. A., Nielsen, K., Eichler-Löbermann, B., Armbruster, M., Merbach, I., & Franko, U. (2023). Simulating the soil phosphorus dynamics of four long-term field experiments with a novel phosphorus model. *Soil Use and Management*. doi:10.1111/sum.1288

04.2022	Gasser, S. A. A., Nielsen, K., & Franko, U. (2022). Transfer of carbon incubation parameters to model the SOC and SO dynamics of a field trial with energy crops applying digestates as organic fertilizers. *Soil Use and Management*. doi:10.1111/sum.12810
01.2021	Gasser, S. A. A., Diel, J., Nielsen, K., Mewes, P., Engels, C., & Franko, U. (2021). A model ensemble approach to determine the humus building efficiency of organic amendments in incubation experiments. *Soil Use and Management*. doi:10.1111/sum.12699

Anton Gasser

Leipzig, den 02.10.2023 ______________________________

Unterschrift