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NORWEGIAN UNIVERSITY OF LIFE SCIENCES • UNIVERSITETET FOR MILJØ- OG BIOVITENSKAP
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PHILOSOPHIAE DOCTOR (PHD) THESIS 2011:69

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MODELING ORGANIC MATTER DECOMPOSITION AND NITROGEN DYNAMICS IN AGRICULTURAL SOILS: ENVIRONMENTAL IMPACTS OF PLANT PRODUCTION SYSTEMS

MODELLERING AV NEDBRYTNING AV ORGANISKE MATERIALE OG NITROGENDYNAMIKK I
LANDBRUKSJORD: MILJØINNVIRKNINGER FRA PLANTEPRODUKSJONSSYSTEMER

SIGNE KYNDING BORGEN

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Modellering av nedbrytning av organiske materiale og nitrogendynamikk i
landbruksjord: miljøinnvirkninger fra planteproduksjonssystemer

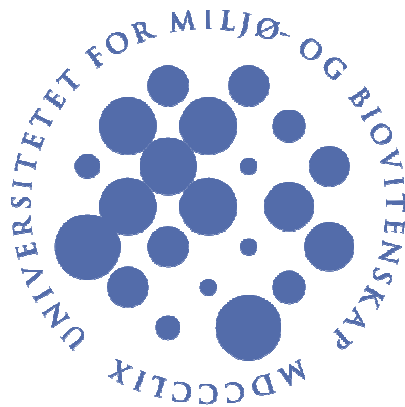
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PREFACE

The work presented in this thesis was carried out from April 2007 to September 2011, primarily at the Norwegian University of Life Science in Ås, Norway, but also during several visits at Colorado State University in Fort Collins, USA. In this time, I have gained professional respect and personal appreciation for my main advisors. Thanks to Marina Bleken for support at a critical time to deliver a challenging first manuscript, to Tor Arvid Breland for continuing a positive collaboration that I have much appreciated, to Keith Paustian for saving and inspiring my interest in soil science, and to Lars Bakken for delivering at crucial moments, trusting me with great freedom, and keeping research in constant motion. Freedom opens doors and these have been entered. Over the years I found wonderful collaborators without whom this work could not have been completed, many thanks to Sander Bruun, Hanne Weichel Lunde, Peter Dörsch, Arne Grønlund, Olof Andréén, Thomas Kätterer, to Lars Molstad for equation support, and to Trygve Fredriksen for professional field and lab assistance as well as vital life support. Many thanks are given to everyone at IPM for providing a cozy working environmental and for being helpful. During this PhD adventure a myriad of sacrifices have been made but luckily opportunities arose equally. I have always wondered what is really going on in soil, and at this point I have a few ideas. I have learned tremendously about soils, organic matter decomposition and modeling, but also about human interactions, work relationship, adapting to change, solitude, companionship, focusing, relaxing, decision-making, persistence, and stress! I owe so much to all my friends, specifically I thank Natasa for providing mental sanity, Karen for talks of soil and life, Anna for showing how to finish, Daniel for sarcasm and thesis edits, Sunetro for calming effects, Kayla for writing tips and positivism during summer lunch breaks by the pond, Rosie for illustrating academic love and commitment, Katrine for ground control when absolutely needed, to my dear friends in Denmark who still have time for me and to everyone in FODOS – it was indeed a pleasure and I wish you all the best. I deeply appreciate the support from my mother, Svend, father, Esther, Martin, Maria, Asger, and Liva; thank you for being there and for understanding the priorities that had to be made during these years. I hope to have you all closer in life at some point soon. Finally, I thank the most important beings in my life: my heart Carlos for love and support, and my little tiger Janis for always meowing with me. You have both suffered from my travels and I look forward to living with both of you. In the end, I need to say that horses and yoga have made a significant contribution to the making of this PhD. Namaste,

Ås, 30 September 2011

Signe Kynding Borgen

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Paper I:

Borgen, S.K., Molstad, L., Bruun, S., Breland, T.A., Bakken, L.R., and Bleken, M.A. (2011).
Estimation of plant litter pools and decomposition-related parameters in a mechanistic model.
Plant and Soil 338: 205-222

Paper II:

Borgen, S.K., Lunde; H.W., Bakken, L.R., Bleken, M.A., and Breland, T.A.
Nitrogen dynamics in stockless organic clover-grass and cereal rotations.
Submitted to Nutrient cycling in Agroecosystems

Paper III:

Borgen, S.K., Grønlund, A., Andrén, O., Kätterer, T., Tveito, O.E., Bakken, L.R., Paustian, K.
CO₂ emissions from cropland soils in Norway estimated by IPCC default and Tier 2 methods.
Submitted to Greenhouse Gas Measurement and Management.

*Modeling organic matter decomposition and nitrogen dynamics in agricultural soils:
environmental impacts of plant production systems*

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ABSTRACT

Agricultural plant production has negative environmental impacts such as nitrate leaching and emissions of greenhouse gasses (N₂O and CO₂). Both phenomena are affected by the decomposition of soil organic matter and plant litter in soil, which is influenced by soil properties, climate, and agricultural management. Modeling is essential to improve the understanding and to predict the effects of management and its dependence on climate and soil properties. This thesis compiles three modeling studies performed with the objective to enhance our understanding of how organic matter decomposition and N dynamics in agricultural soils influence environmental impacts from plant production. Models have been applied at three levels of scale, ranging C and N mineralization of plant residues decomposed under lab conditions, field N dynamics, and a national C balance inventory for cropland.

For optimal utilization of green manure and crop residue amendments, N mineralized during plant residue decomposition should be synchronized with plant N demand to minimize N losses to the environment. To achieve such synchronization, we need good prediction of net N mineralization immobilization kinetics during decomposition of relevant agricultural plant materials. This requires robust estimation of the partitioning of plant litter C and N into rapidly and slowly decomposing pools. This study presents a novel approach to partition plant C and N between two litter pools (rapidly and slowly decomposing), i.e., the simultaneous optimization of plant-specific and global parameters (against observed C and N mineralization kinetics in laboratory incubations). The study demonstrated that for a majority of the 76 plant residues, the model was able to predict C and N mineralization with reasonable precision. However, outliers were detected, which may indicate that the use of a global parameter for the C/N-ratio of the microbial biomass is not valid in all cases (i.e., specific plant materials appear to stimulate the growth of microbes with higher or lower C/N ratios than the ratio for the majority of the residues). Biochemical fractionation (SCD) and NIR-spectra of the plant residues were available and used for regression analyses to predict the optimized partitioning of C and N between the litter pools, thus searching for ways to accurately predict partitioning parameters using NIR and SCD data. Validation against a part of the dataset, which was not used for regression analyses, demonstrated that partitioning parameters obtained by regression models of NIR and SCD data were more appropriate than from chemical fractions directly.

To investigate the environmental and production efficiency of organic stockless grain production, we studied the N dynamics in organic clover-grass and cereal of a stockless organic farm in Southeast Norway for an 8-10 year period using an ecosystem model (SPN). Additionally, scenario simulations of alternative crop rotations and plowing season in the present (1980-2009) and future (2071-2100) climate conditions were performed to explore the potential for improving stockless organic grain production. In an evaluation of efficiency indicators based on production and environment, only marginal improvements were possible by changing management, and this was also the case for the simulations using the future climate. This study clearly indicates that external nutrient resources are necessary to substantially improve the N use efficiency in stockless cereal systems. Consequently, such systems may be discouraged in the future and the reintegration of livestock is recommended.

With the objective to estimate the soil C balance of Norwegian cropland on mineral soils, the IPCC methodologies for default (Tier 1) and Tier 2 were applied to agricultural activity data for the inventory period 1999-2009. National CO₂ emissions were primarily caused by a reduction in manure available. The default Tier 1 method overestimated the decline in soil organic C, particularly for crop rotations without manure applications, compared to the Tier 2 method. National net CO₂ emissions were 313 Gg CO₂ yr⁻¹ for Tier 1 and 139 Gg CO₂ yr⁻¹ for Tier 2. A reduction in livestock numbers during the inventory period appears to be an important reason for the high emissions. Thus, the emissions (as estimated) could be reduced by maintaining a high number of livestock. However, in the total greenhouse gas budget, the accompanying methane emissions from enteric fermentation would more than outweigh the reductions in CO₂ emissions by high livestock numbers. Thus, care should be taken when focusing greenhouse gas mitigating strategies on C sequestration. This study highlights the need for integrated emission budgets for policy development and also for the collection of agricultural activity data regarding manure application practices such as application rates, water content, C content, and import-export dynamics.

This thesis delivers a contribution to the understanding of organic matter decomposition and N dynamics in agricultural soils by modeling studies performed at different scales. The findings herein support the notion that several factors beyond the biological system are crucial to reduce the adverse environmental impacts from agricultural soils, e.g., consumption patterns, market dynamics, and legislation. Also, fundamentally restructuring current production systems by reintegration of livestock and arable farming seems the best option to improve N use efficiency and sustain soil organic matter levels. To optimize the biological capacity to reduce environmental impacts, agroecosystem models that account for plant and livestock interactions are indeed needed and useful tools to characterize sustainable agricultural systems.

Modellering av nedbrytning av organiske materiale og nitrogendynamikk i landbruksjord: miljøinnvirkninger fra planteproduksjonssystemer

SAMMENDRAG

Landbrukets planteproduksjon har negative miljømessige konsekvenser som for eksempel nitratutvasking og utslipp av klimagasser (N₂O og CO₂). Begge fenomener påvirkes av nedbrytning av jordas organiske materiale og planterester i jord, som er påvirket av jordas egenskaper, klima og agronomisk praksis. Modellering er viktig for å bedre forståelsen og forutsi effekten av praksis og dennes avhengighet av klima og jordsmonnsegenskaper. Denne avhandlingen sammenslår tre modellstudier utført med det formål å forbedre vår forståelse av hvordan nedbrytning av organisk materiale og N dynamikk i dyrket jord påvirker miljøet fra planteproduksjon. Modeller ble anvendt på tre nivåer: karbon (C) og nitrogen (N) mineralisering fra planterester nedbrutt under kontrollerte forhold i laboratorium, N dynamikk i felt, og et nasjonalt C budsjett for dyrket mark.

For optimal utnyttelse av grønn gjødsel og planterester tilført jorden og minimere N tap til miljøet, bør N mineralisert fra nedbrytning av planterester være synkronisert med plante N opptaket. For å oppnå en slik synkronisering, trenger vi god prediksjon av netto N mineraliserings- og immobiliseringskinetikk under nedbrytning av plantematerialer. Dette krever robust estimering av fordelingen av plante C og N i raskt- og sakte-nedbrytende puljer. Denne studien presenterer en ny tilnærming til å skille plante C og N mellom to planterestpuljer, dvs. simultan optimalisering av plantespesifikke og globale parametere (mot observerte C- og N-mineralisering kinetikk i laboratorieinkubasjoner). Studien viste at for et flertall av de 76 planterestene, var modellen i stand til å forutsi C- og N-mineralisering med tilstrekkelig presisjon. Men der var *outliers*, hvilket kan tyde på at bruken av en global parameter for C/N-forholdet for den mikrobielle biomasse ikke er gyldig i alle tilfeller (dvs. spesifikke plantematerialer ser ut til å stimulere veksten av mikrober med høyere eller lavere C/N-forhold enn de som vokser på flertallet av planterester). Biokjemiske fraksjonering (SCD) og NIR-spektra av planterester var tilgjengelig og ble brukt for regresjonsanalyser for å forutsi den optimaliserte fraksjonen av C og N mellom plantepuljene, og dermed søke etter måter å nøyaktig forutsi fraksjonsparameterne ved å bruke NIR og SCD data. Validering mot en del av datasettet, som ikke var brukt for regresjonsanalysene viste at fraksjoneringsparameterne ved regresjonsmodeller av NIR og SCD data var mer passende enn fra kjemiske fraksjoner direkte.

For å undersøke miljø- og produksjonseffektivitet av økologisk husdyrløs kornproduksjon, studerte vi N dynamikken i et vekstskifte med kløvergress og korn på en gård i Sørøst-Norge for en 8-10 års periode ved hjelp av en økosystemmodell. I tillegg, ble scenario simuleringer av alternative vekstskifte og pløyesesong under nåværende (1980-2009) og fremtidige (2071-2100) klimaforhold utført for å undersøke potensialet for forbedring av husdyrløs økologisk kornproduksjon. I en evaluering av effektivitetsindikatorer basert på produksjon og miljø var bare marginale forbedringer mulige ved å endre vekstskifte og pløyesesong og dette var også tilfellet for simuleringer med det fremtidige klima. Denne studien indikerer klart at eksterne næringsstoff er nødvendig for å vesentlig forbedre produktivitet og bærekraft i husdyrløse kornsystemer. Derfor bør slike systemer kanskje frarådes i fremtiden og muligens burde husdyr reintegreres.

Med det formål å estimere jord C balansen i norsk dyrket mark på mineraljord ble IPCC standard (Tier 1) og Tier 2 metodene anvendt med landbruksaktivitetsdata for beregningsperioden 1999-2009. Nasjonale CO₂-utslipp var hovedsakelig forårsaket av en reduksjon i husdyrgjødseltilgjengelighet. Standard Tier 1 metode overvurdert nedgangen i jord organisk C, spesielt for vekstskifter uten husdyrgjødsel i forhold til Tier 2 metoden. Det nasjonale netto CO₂-utslipp var 313 Gg CO₂ år⁻¹ for Tier 1 og 139 Gg CO₂ år⁻¹ for Tier 2. En reduksjon i husdyrtallet i løpet av beregningsperioden synes å være en viktig årsak til utslippene. Dermed kan utslippene (som estimert) reduseres ved å opprettholde et høyt antall husdyr. Men totale klimagassutslipp fra landbruket målt i CO₂-ekvivalenter ville dermed øke fordi metanutslipp fra gjæring i vommen fra et større antall dyr veier tyngre enn den oppnådde reduksjonen i CO₂-utslippene fra jorden. Derfor bør man være forsiktig med å fokusere klimagassformildende strategier for C lagring i jord. Denne studien understreker behovet for integrerte utslippsbudsjetter for politikktvikling og også for innsamling av data om driftspraksis vedrørende husdyrgjødsel, så som bruksmengder, vanninnhold, C innhold, og import-eksport dynamikk.

Denne avhandlingen gir et bidrag til forståelsen av nedbrytning av organisk materiale og N dynamikk i landbruksjord ved modellstudier utført på ulike skalaer. Funnene her støtter oppfatningen at flere faktorer utover det biologiske system er avgjørende for å redusere miljølempene fra dyrket mark, for eksempel forbruksmønster, markedsdynamikk og lovgivning. Modelleringsøvelsene støtter også oppfatningen at reintegrering av husdyr og kornproduksjon kan forbedre N effektiviteten i landbruket som helhet, og bidra til å opprettholde jordas innhold av organisk materiale. For å optimalisere den biologiske evnen til å redusere miljøbelastningen, er agroøkosystemmodeller, som inkluderer plante- og husdyrinteraksjonen, et nyttig verktøy for å karakterisere bærekraftige landbrukssystemer.

1 INTRODUCTION

Scientific evidence suggests several negative environmental impacts of agricultural soil management, among those are the emissions of greenhouse gases (GHG) and nitrate leaching (Vitousek *et al.*, 1997). The quantities of emissions and nitrate leaching partly depend on agricultural management practices, but are also determined by climatic conditions and soil properties. In order to minimize the negative effects, we need a detailed understanding of the turnover and decomposition of soil organic matter (SOM) where carbon (C) and nitrogen (N) is mineralized. Predicting environmental consequences of management operations is difficult because of the interactive effects involved (e.g., effects of soil moisture and temperature depend on soil texture). Mechanistic models are necessary for prediction of agrosystem responses to perturbations and to improve process understanding. Thus models are important tools for the development of sustainable agricultural practices with reduced environmental impacts. This chapter provides a background of the environmental effects related to C and N cycling in agricultural soils (i.e., nitrate leaching, emissions of N₂O and CO₂), soil organic matter turnover by decomposition, humification, and mineralization, and how residue and tillage management affect the C and N dynamics in agricultural soils.

Environmental impacts of C and N cycling in agricultural soils

From an agro-environmental point of view, the goals regarding the management of C and N turnover within agrosystems are conflicting. During decomposition of organic matter, C is mineralized and carbon dioxide (CO₂) returns to the atmosphere. Hence, net accumulation of soil organic carbon (SOC) is desirable. But the mineralization of SOM is essential for agrosystems that rely on N recycling for plant productivity because N mineralization is impossible without mineralizing the carbon skeleton to which organic N is covalently bound. The ultimate measure of success in reconciling the two opposing targets (C sequestration and plant N assimilation), is cord></Cite></EndNote>(¶ ¶ HYPERLINK ¶ \l "_ENREF_148" ¶ \o "West, 2002 denitrification, and ammonia emission. Improving the N resource-use efficiency is essential for the development of sustainable and environmentally sound food production (Spiertz, 2010).

Agrosystems that sustain a maximum of SOC without sacrificing the delivery of mineral N to growing crops would provide such production.

Nitrogen losses from agricultural soil affect both the local and the global environment. Nitrate (NO_3^-) pollutes the waterways and emission of nitrous oxide (N_2O) contributes to global warming and the destruction of stratospheric ozone (Ravishankara *et al.*, 2009). Beside N_2O , soil may also be sources of other greenhouses gasses such as methane (CH_4) and CO_2 . Long-wave solar energy reflected from Earth's surface is partly absorbed in the atmosphere and partly irradiated into space. Greenhouse gasses in the atmosphere increase the absorption of the energy that would otherwise have been emitted into space, which leads to global warming. The GHG effect also causes adverse climate changes because the hydrological cycles interact with the biogeochemical cycling of elements. There is no longer uncertainty that climatic changes are caused by human activity and inaction has been deemed inexcusable (Richardson *et al.*, 2009). Therefore, there is a need to control global environmental impacts from agricultural soils.

Nitrate leaching

Elevated NO_3^- levels in run-off water from agricultural fields pose negative environmental consequences such as groundwater pollution and the eutrophication of rivers, lakes, and oceans, which may cause algae blooms and subsequent anoxic conditions in the water element. Nitrate leaching is determined by NO_3^- concentration in the soil and the downward movement of water through the soil profile. Soil texture effects on water (and nitrate) retention in the soil were documented in the laboratory (Gaines and Gaines, 1994) as well as in the field. Larger leaching losses have been measured in fields of course-textured sand than in heavy clay soils (Vinten *et al.*, 1994; Korsath *et al.*, 2003; Munch and Velthof, 2007), which has also been simulated in modeling studies, e.g., with the DAISY model (Pedersen *et al.*, 2009). Soil NO_3^- levels are sustained by mineral fertilizers and SOM mineralization and are diminished by plant N uptake, denitrification losses, and net microbial assimilation of mineral N. These factors are the targets for any attempt to synchronize high soil mineral N concentrations with the demand for growing crops and to minimize off-season concentrations of nitrate in the soil. The most significant mineral N sink in the system is the uptake by growing plants; hence, the leaching potential is

largest when plant growth is interrupted, at harvest or by tillage. The latter does not only terminate the assimilation of mineral N by the plants, but also induces microbial activity by the breakdown of aggregates releasing previously unavailable substrate. This may cause transient bursts of net N mineralization (Thomsen and Sørensen, 2006). The use of cover or catch crops (Thorup-Kristensen *et al.*, 2003), deep rooting crops (Kristensen and Thorup-Kristensen, 2004; Thorup-Kristensen *et al.*, 2009) and appropriate time of plowing are therefore crucial instruments to minimize leaching.

Nitrous oxide emissions

Atmospheric air consists of 78% N₂ (3.87×10^{21} g) and an N₂O concentration of just 311 ppb (Schlesinger, 1997). Nitrous oxide is a potent GHG with a specific global warming potential (per mass) 310 times that of CO₂. Denitrification is the major process producing biological N₂O, in which N₂O is an intermediate in the stepwise reduction of NO₃⁻ to N₂ (NO₃⁻ → NO₂⁻ → NO → N₂O → N₂.) Nitrification also contributes to N₂O emissions but relatively little in agricultural soils (Ludwig *et al.*, 2004; Mørkved *et al.*, 2007). The bacteria responsible for denitrification are mainly facultative anaerobic heterotrophs and the process is directly regulated by the partial pressure of O₂, labile SOC availability, and the NO₃⁻ concentration (Figure 1). In systems depending on organic N sources, the availability of mineral N is determined by decomposition, which is controlled by soil temperature and moisture, the quality of the substrate, and soil properties. Decomposition determines both the rate of nitrate concentration and the availability of labile SOC, which further complicates the process compared to systems driven by artificial fertilization where soil mineral N contents are more easily forecast.

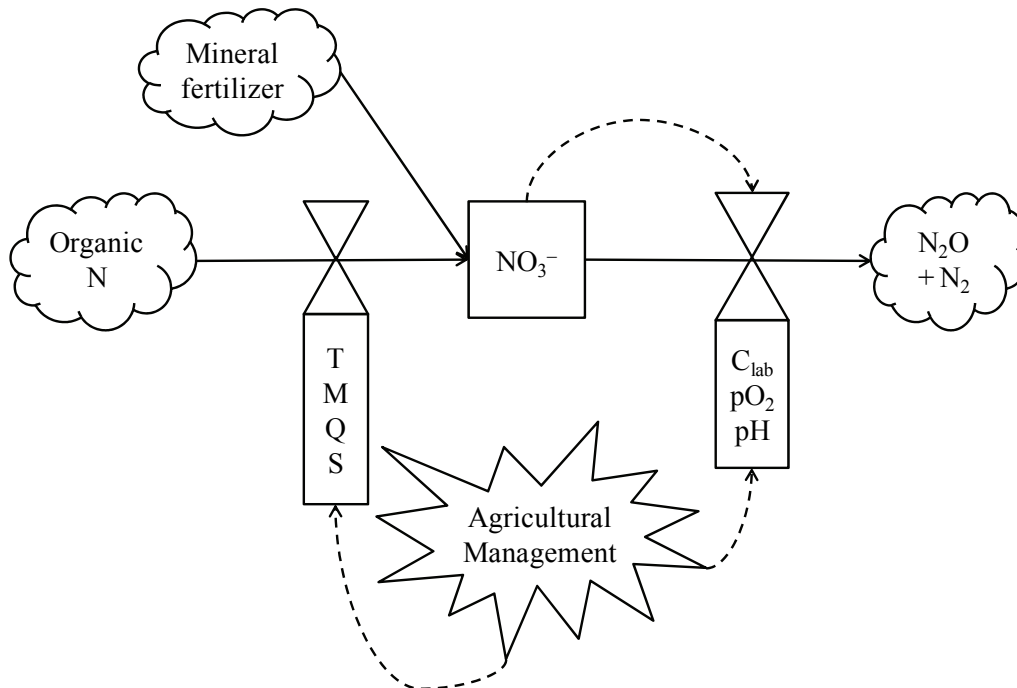


Figure 1 Denitrification controllers in agricultural soils. Nitrogen flows (solid arrows) are controlled by the factors listed in the bow tie boxes. Stippled arrows indicate external influences. T: temperature, M: moisture, Q: quality of substrate, S: soil properties, C_{lab}: labile SOC, pO₂: partial oxygen pressure.

Field measurements of N₂O emission are often correlated with rainfall events and the general assumption has been that most emissions occur during the cropping season at peak microbial activity. However, large emissions have been measured during the off-season; in the late fall, winter (Goossens *et al.*, 2001; Ruser *et al.*, 2001; Pennock *et al.*, 2005) and the spring due to freeze-thaw events (Dörsch *et al.*, 2004). Such off-season emissions measured under snow cover are apparently non fertilizer-driven, i.e., emissions may occur independently of fertilizer level (Ruser *et al.*, 2001). Spring-time emissions (in temperate climates) were found to be diurnally fluctuating and coincide with peak temperature during the day (Skiba *et al.*, 1996). Soil physical properties also influence denitrification primarily by water infiltration and retention characteristics, since water content determines the oxygen distribution in the soil matrix. Denitrification losses measured in the lab for different soil textures under the same water-filled pore space and bulk density were similar (Aulakh *et al.*, 1991). Thus, soil texture and structure

has no direct effect on denitrification when the air-filled porosity is kept the same for all soils, but indirectly through controlling the soil moisture content *in situ*. In the field, management aspects were found to be more important for predicting measured N₂O emissions than soil physical properties (Goossens *et al.*, 2001).

Carbon dioxide emissions

CO₂ is a trace gas in the atmosphere with a volumetric concentration of ~0.039% (390 ppm). The atmospheric CO₂ concentration has increased from a mass of 548 Pg C (10¹⁵ g) since pre-industrial times (before 1860s) to current levels of 750 Pg C (Paul and Clark, 1996; Schlesinger, 1997). Future increases are estimated at a rate of 2 ppmv per year (Richardson *et al.*, 2009). The majority of terrestrial CO₂ emissions originate from fossil fuel combustion and land-use changes (Schlesinger, 1997; Janzen, 2004). Emissions from agricultural soils are, however, particularly interesting because soil can function as a sink and a source of atmospheric CO₂. The C flux linking the atmosphere with land vegetation is one of the largest global fluxes (Schlesinger, 1997) and soil is the largest terrestrial C pool with an estimated size of 2400 Pg C (Brady and Weil, 1999). Agricultural management exerts a large influence on soil CO₂ emissions, especially through organic matter inputs and soil tillage practices (Paustian *et al.*, 2000). Predictions of C fluxes require soil organic matter models that account for cultivation disturbances and the environmental conditions provided by the climate and soil biogeochemical characteristics.

Modeling agricultural systems

As is the case for any problem solving, choosing the proper tool for the job is of paramount importance for a good result. In order to select the appropriate model to elucidate cause-effect relationships within the soil agroecosystem, an understanding of model features is necessary. Mathematical models are attempts to simplify reality by formal expression using equations. Models are characterized by their abstraction level (process representation), dynamism, time step interval, space representation, and randomness (Haefner, 2005). Soil C and N models are often mechanistic (explicit representation of biological processes), dynamic (able to predict changes over time and in the future), continuous in time (any time step may be applied), spatially discrete (consist of compartments), and deterministic (no stochastic or random elements).

Objectives of ecosystem modeling are to enhance our understanding of empirical observations and to improve our ability to predict how a system reacts to change, which may be used to design experiments for rigid hypothesis testing. Understanding how an agricultural system functions as a whole, requires that interactions of individual pieces of the system are taken into account. This is extremely difficult to do without formalization of subsystem behaviors and the interactions between them. However, when subsystems are formalized, the comprehension of the whole system behavior is facilitated, particularly its response to perturbation. If models are very complex (many components, process equations and parameters), it can be as difficult to understand the model output, as it is to understand empirical observations of nature; the model loses transparency. To enhance model transparency, and thereby making it easier to interpret model responses, it is desirable to make models as simple as possible, in terms of the number of processes represented, parameters and input variables selected. Applying this principle of parsimony or Occam's razor improves the chances of understanding the behavior of the model, adequately representing the underlying structure of the modeled phenomenon, and minimizing the risk of overfitting. Individual processes and parameters, therefore, need scrutiny by evaluating the sensitivity of model output to changes made either in parameter values or of implemented functions. Sensitivity tests are crucial for another reason; it is important to distinguish between parameters that require minor calibration efforts and those needing more attention.

Agroecosystem models are often model-complexes composed of submodels or modules. Simplified, the structure of many models used on agricultural systems, e.g., CANDY, DAISY, DAYCENT, DNDC, and NCSOIL can be illustrated by three submodels of crop growth, soil C and N microbial transformation (decomposition and N mineralization), and heat and water transport in the soil (Figure 2). In the SPN model, crop growth may be modeled dynamically based on radiation, sun light, temperature and mineral N availability (Bleken *et al.*, 2009) or as a logistic function based on available mineral N (Vold *et al.*, 1999a; Borgen *et al.*, submitted). Heat and water transport is simulated offline by the COUP model (Jansson and Karlberg, 2001; Jansson and Moon, 2001) as it is not dynamically affected by crop N uptake and microbial transformations. Thus COUP simulations provide input data of soil temperature, moisture and

water transport to the other modules. Soil microbial C and N transformations are modeled by Nitrosim (Vold *et al.*, 1999b; Borgen *et al.*, 2011), which is a modification of the SOILN model (Johnsson *et al.*, 1987). Driven by the heat and water transport module, soil C and N transformations are influenced by the plant N uptake and agricultural management such as residue inputs and tillage operations.

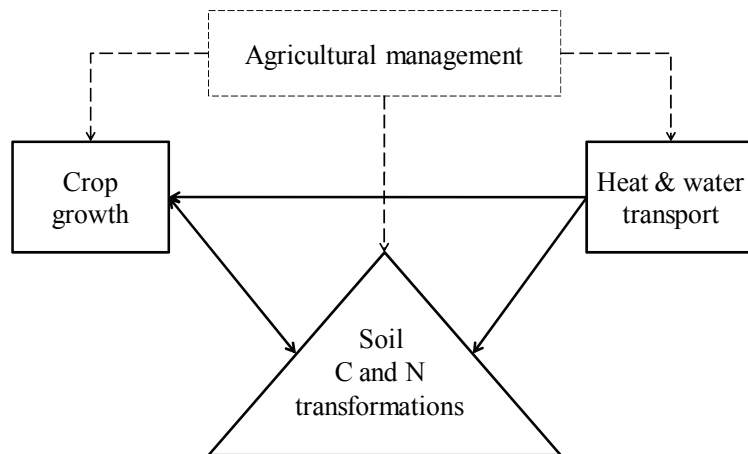


Figure 2 Common structure for ecosystem models consisting of submodels (solid) and external influence (stippled).

Modeling soil organic matter turnover

Soil organic matter (SOM) is essential for soil fertility by contributing to cation exchange and water-holding capacity, nutrient cycling, and aggregate formation. Although SOM is only a small fraction of total soil mass (1-6%), it is crucial for plant growth in the field (Brady and Weil, 1999). The C content of SOM is often set as 58% of organic matter, which gives a conversion factor of 1.78 from C to SOM, but a range between 1.4 and 2.5 has recently been suggested as plausible (Pribyl, 2010). The turnover of SOM includes decomposition of dead organic matter (i.e., plants, soil fauna and microbial residues) where polymers are broken into monomers, humification where organic matter is embedded in the soil matrix as stabilized compounds, and mineralization where the covalently bound elements (H, O, C, N, S, and P) of organic molecules are transformed into inorganic compounds (H_2O , CO_2 , NH_4^+ , H_2S , and PO_4^-). SOM is a heterogeneous mix of partially-decomposed plant residues, soil macro fauna,

microorganisms, by-products of decomposition, and humified substances that consist mainly of lignin and lignin-like aromatic polymeres, lipids (waxes), and proteins (Paul and Clark, 1996). In soil science, there has been a longstanding tradition of separating fulvic and humic acids, and humin using chemical fractionation involving water, alkali and acid solutes. These pools are entirely operational, however, with no clear molecular representation. Although ^{14}C -dating of these pools have shown an increasing age from fulvic acid to humads, they are more or less irrelevant to dynamic modeling of SOM mineralization kinetics.

To simplify the heterogeneity of SOM, biogeochemical C and N models are constructed of discrete pools or compartments of different decomposability (e.g., readily labile, microbial biomass and recalcitrant humic compounds), based on experimentally observed mineralization rates (preferably in long-term experiments). In the SPN model, fresh organic material enters the system partly as Litter 1 (metabolic or rapidly-decomposing) and partly as Litter 2 (structural or recalcitrant) depending on the quality of the litter. A fraction (f_e ; microbial growth efficiency) of the decayed litter material enters the microbial biomass pool (and $1-f_e$ is respired as CO_2) and a fraction (f_h ; humification coefficient) of the decayed biomass material enters the humus pool (Figure 3). A complete non-reactive inert pool may also be envisioned. Newly assimilated biomass is given by the C and N inflows to the biomass pool coming from litter, humus and biomass itself.

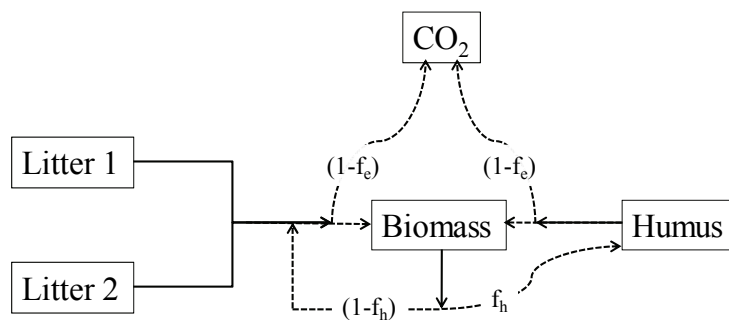


Figure 3 General SOM model structure: microbial respiration ($1-f_e$) occurs from all pools. Solid arrows are the primary (first-order) decay rates of each pool, dashed lines are for split flows, i.e., a fraction of decaying biomass material is humified (f_h), the rest ($1-f_h$) is reincorporated as

microbial biomass, and the substrate consumption by microbes (from litter, humus and biomass) is split between a fraction (f_e) as new biomass and a fraction ($1-f_e$) mineralized.

Perhaps a more realistic conceptualization of SOM is that it consists of a continuum of these pools, which can be modeled by continuous quality distributions (Bruun *et al.*, 2010). The theoretical concept of the non-compartmental cohort model is not new (Bosatta and Ågren, 1985), but few efforts have been made to parameterize them, e.g., by Joffre *et al.* (2001) using near-infrared reflectance spectrometry (NIRS). In contrast, parameterization of compartmental models has received much attention. Two main approaches can be identified, either to ‘model the measurable’ or ‘measure the modelable’ (Elliott *et al.*, 1996). To ‘model the measurable’ implies that easily measurable variables, e.g., mineralization rates, are used as a basis for construction and parameterization of model pools. To ‘measure the modelable’ is to measure the pools of a model (biomass, humus, undecomposed litter etc.). The dominating approach has been to model the measurable. Attempts to measure the modeled pools directly were not done for any of the models reviewed by McGill (1996), but recent advances have been made combining conceptual models with fractionation scheme of soil structure (Six *et al.*, 2002) or pore space distributions (Kuka *et al.*, 2007), suggesting that the trend may be reversing in the future.

Plant litter and SOM decomposition

Decomposition can be defined as the separation of materials into their constituent parts through biodegradation of organic materials (Paul and Clark, 1996). During litter decomposition three main events occur: leaching (of monomers and water soluble polymers), physical fragmentation (disintegration of structures), and catabolism (chemical alteration); (Swift *et al.*, 1979). Leaching of labile compounds, such as carbohydrates and amino acids, is primarily driven by rainfall. Fragmentation of organic material enhances enzymatic attack on polymers by removing the outer more resistant layer of the organic residue and by increasing the surface area of the litter. Several biophysical factors promote fragmentation, e.g., freeze-thaw or wet-dry cycles, soil tillage and macro faunal activity such as earthworms. During catabolism, the key players being fungi, bacteria and soil micro fauna (e.g., nematodes, protozoans, mites, and amoebae) decompose larger molecules to smaller/simpler ones (e.g., fermentation to organic acids) and mineralization

may occur. Although the processes involve numerous different substances, enzymes and organisms in complex food webs, the rate of decomposition and mineralization can be modeled as simple first-order kinetics, where the rate of change is given by $\frac{dC}{dt} = -C \times k$, with C being the size of the pool and k the decay rate. The quantity of the C pool at any time t can be calculated by integrating the differential equation, giving $C_t = C_0 e^{-kt}$, where C_0 is the initial pool size.

Microbial decomposition rates are controlled by environmental conditions and substrate availability. Microbial metabolic activity increases with temperature within a certain range. The nature of the response (exponential) appears to be similar for most organisms, but the temperature range tolerated (max and min) are widely different for different organisms. At the community level such individual characteristics are leveled out by the diversity of the populations. Since the soil temperature normally does not exceed maximums tolerated by components of the community, most biogeochemical models operate with a single temperature response function, thus the decay rate is multiplied with a response factor (r) based on soil temperature for each time step. Two commonly used functions are the Ratkowsky function and the Q_{10} function, both showing similar response to increasing temperature, but Q_{10} is more responsive and also sensitive to changes in the Q_{10} value as illustrated in Figure 4.

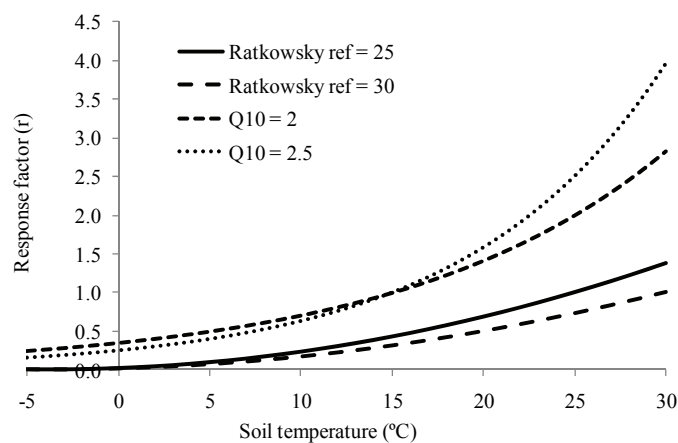


Figure 4 Response factors (r) as a function of temperature represented by Ratkowsky and the Q_{10} functions with two parameter values.

The temperature response function by Ratkowsky (Ratkowsky *et al.*, 1982) is a quadratic function of the absolute minimum (T_{\min}) and the optimum reference (T_{ref}) temperature for microbial activity $r(T) = \frac{(T - T_{\min})^2}{(T_{\text{ref}} - T_{\min})^2}$, where T_{\min} was estimated at -3.8°C (Kätterer *et al.*, 1998) and T_{ref} generally set at 30°C . Reducing T_{ref} to 25°C has a minor effect under dominating Scandinavia soil temperature (Figure 4). The response of the Q_{10} function $r(T) = Q_{10}^{(T - T_{\text{base}})/10}$ with T_{base} (base temperature) of 15°C , is also hardly influenced by changes in the Q_{10} value under the Nordic climate.

The sensitivity of organic matter decomposition to rising temperatures and how this may best be modeled has been debated (Davidson and Janssens, 2006; Kirschbaum, 2006), because it is a relevant topic in relation to global warming and climate change. Certain crucial processes may be performed by microbes with different temperature optima, e.g., net N immobilization was inhibited at lower temperatures where net N mineralization continued during decomposition of plant residues (Andersen and Jensen, 2001; Magid *et al.*, 2004) and also microbial respiration is considered especially sensitive below 5°C (Brady and Weil, 1999). Thus at lower temperatures, the actual microbial response may possibly divert from the response function.

The soil moisture effect on decomposition in most models is represented by a factor between 0-1. For soil moisture contents below the wilting point, Θ_{wp} ($\text{pF} \geq 4.2$), the response factor is zero and within a certain soil moisture interval from Θ_1 to Θ_2 (e.g., $\text{pF} 4.2\text{-}3$) the response can be given by a power function $r = \left(\frac{\Theta_{\text{wp}} - \Theta}{\Theta_1 - \Theta_{\text{wp}}} \right)^m$. Both the linear response, when m equals 1 as illustrated in Figure 5 and the concave response curve obtained when $m > 1$ are being used (Andrén and Paustian, 1987; Johnsson *et al.*, 1987; Bergström *et al.*, 1991; Lomander *et al.*, 1998). At moisture contents larger than Θ_2 the response may stay at 1 or decline to a chosen value (Figure 5).

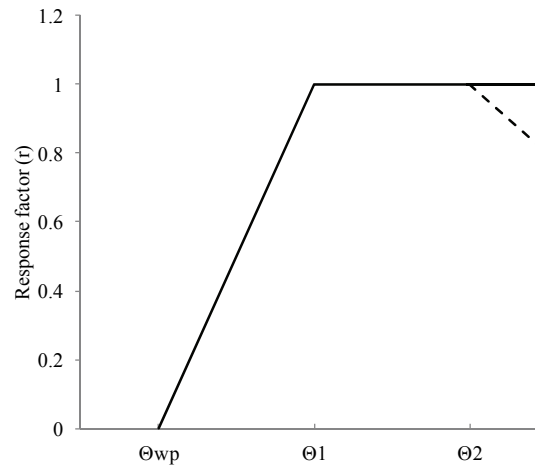


Figure 5 Response function the effect of soil moisture on decomposition here illustrated by a linear response between the water content at wilting point Θ_{wp} and Θ_1 (a chosen parameter value). When the soil water content approaches saturation (Θ_2) the response function may decline (stippled line) or stay constant (solid).

Soil texture exerts a control on decomposition; sandy soils tend to have higher decomposition rates than clay soils (Ladd *et al.*, 1992; Gordillo and Cabrera, 1997). This effect can be modeled differently depending on the mechanistic assumptions. Müller and Höper (2004) modified the decay rates in the DAISY model by a factor of 0.5 for soils with clay contents > 25%. In CENTURY, microbial growth efficiency is modified by a factor (F_T ; the fraction of C lost due to microbial respiration) calculated as $F_T = 0.85 - 0.68 \times T$, where T is the silt plus sand content (Parton *et al.*, 1994). Although both approaches provide the same response, the latter is founded on reasonable assumptions that microbial decay products are less physically protected with increasing sand content and thus the stabilization efficiency (f_e) decreases. ICBM contains a third approach in where the water content at wilting point is a function of the clay content and at field capacity, a function of the SOC content (Andrén *et al.*, 2004; Kätterer *et al.*, 2006). A fourth approach, which is especially relevant for long-term simulations, is to modify the humification efficiency of the soil as detailed in the next section.

Humification of organic material

Humification, i.e., formation of stable humus compounds, has received much attention recently since it affects the long-term storage of C in soil. The composition of humus is not well defined; Piccolo (2001) concluded that humus is composed of supramolecular associations of self-assembling heterogeneous and relatively small molecules. Also, there is a lack of knowledge of the mechanisms controlling the process. Chapin III *et al.* (2002) summarized several relevant steps such as selective preservation of recalcitrant materials, microbial transformation, polyphenol formation, quinone formation, and abiotic condensation. Others focus primarily on the importance of organo-mineral complex formation for long-term stabilization of SOC (Kögel-Knabner *et al.*, 2008).

Soil texture influences humification through the several mechanisms such as physical protection as occluded SOC in aggregates, chemical protection by association with mineral surfaces, and biochemical protections by recalcitrance (Six *et al.*, 2002). Because of these various influences soil texture may control the distribution between the fractions of biochemically and physically associated SOC, although it is not a universal indicator of total C stabilization (Plante *et al.*, 2006). Krull *et al.* (2003) argues that chemical recalcitrance (e.g., formation of black carbon or charcoal) may be the most important mechanism in agricultural active soils, because the influences of soil texture on aggregation and adsorption slow down decomposition but do not hinder it.

Although humification is rarely modeled mechanistically, a few attempts have been made. Hassink and Whitmore (1997) developed a model explicitly considering adsorption-desorption kinetics of protected organic matter and von Lützow (2008) based their conceptual model on stabilization processes. But due to the number of pools and mechanisms involved, the Lützow model could not be used for field simulations (Ludwig *et al.*, 2008). In most compartmental models humification is described by a single factor (i.e., f_h in Figure 3). The humification coefficient can be calibrated by model fitting to observed mineralization kinetics in long-term experiments, while others estimate h_f as a function of the clay content, e.g., in CN-SIM and CENTURY. Petersen *et al.* (2005) used $h_f = 1/(R+1)$ based on the equation fitted by Coleman

and Jenkinson (1996): $R = 1.67 (1.85 + 1.6 \exp(-7.86x))$, where x is the clay content (kg kg^{-1}). Accordingly, the humification coefficient can take a value between 0.15 and 0.24 for zero to 100% clay (Petersen *et al.*, 2005). In CENTURY, the formation of humus is defined as $h_f = 0.003 + 0.032T_c$ where T_c is the clay content (Parton *et al.*, 1994).

How to estimate the initial size of the humus pool is also an issue of debate. Several strategies have been applied, e.g., radio carbon dating (Coleman *et al.*, 1997; Petersen *et al.*, 2005), standard values (Jensen *et al.*, 1997), fixed fractions of measured SOC (Falloon *et al.*, 1998), equilibrium assumptions, pre-simulation periods (Bruun and Jensen, 2002), using NIRS (Michel and Ludwig, 2010), and mineralization incubation experiments (Breland and Eltun, 1999). Field simulations of long-term SOC trajectories are sensitive to humus pool initialization (Puhlmann *et al.*, 2006). For short-term simulations of N dynamics, it is less likely to be a problem due to the relatively low decay rate of the humus pool. For example, in SPN the decay rate of the humus pool (k_h) at optimal soil moisture and temperature (15°C) is $0.000085 \text{ day}^{-1}$, giving a half life of 22 years ($\ln(2)/k_h$). Under Nordic climatic conditions, the average field decomposition rate is approximately 1/4 of decay rate, meaning that in Norwegian fields, the half life of the humus pool is around 90 years.

N mineralization and immobilization

Mineralization and immobilization of N is closely linked with the decomposition of organic matter and C cycling. During microbial decomposition of organic matter, dissolved organic N is released. SOM mineralized by decomposer microbes results either in net N mineralization or immobilization depending on the C/N ratio of the decomposing material, the C/N ratio of the organisms, and their growth efficiency. The primary product of mineralization is ammonium NH_4^+ , which may subsequently be oxidized to nitrate NO_3^- by nitrification. If microbial growth on the substrate is limited by the availability of organic N, net immobilization will occur (if mineral N is available). Both forms of mineral N may be immobilized by microbes (Chapin III *et al.*, 2002), although NH_4^+ is preferred because the enzymes responsible for NO_3^- assimilation in all microorganisms are strictly controlled by the availability of reduced N.

The mineralization rate in a particular soil is influenced by long- and short-term controls (Figure 6) with the long-term effects being particularly evident in natural systems. Long-term controls determine the background or base mineralization potential of a given soil, which are determined by the interactions between plants and soil. These interactions are influenced by soil formation characteristics such as biota, time, parent material, and climate. Immediate controls on net N mineralization are, in addition to climate, litter quality (C/N ratio and C quality), plant N uptake, and the C/N ratio of the prominent microbial community.

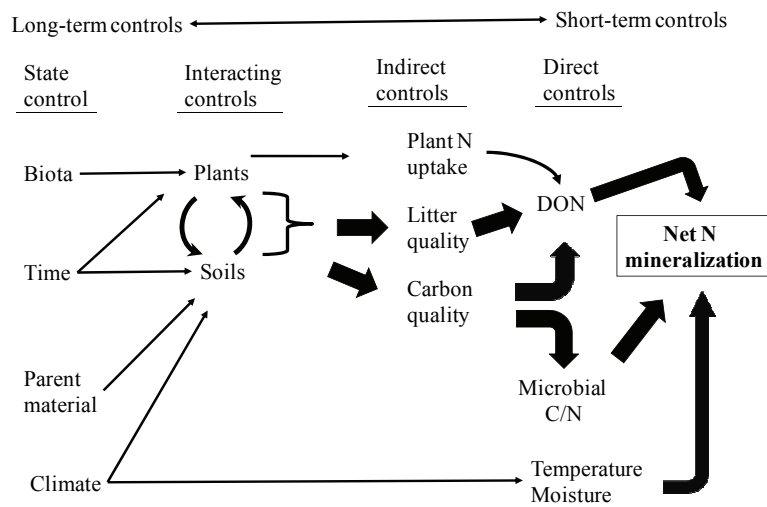


Figure 6 Process controls of net N mineralization, redrawn from Chapin III *et al.* (2002).

Most compartmental SOM models assume a constant C/N ratio of the microbial biomass pool (CN_B). Generally, the net assimilation of mineralized N is determined by the mean N/C ratio of the substrates consumed by the microbes (NC_{SUB}), their growth yield in terms of C (f_e : the fraction of substrate C assimilated as new biomass), and the N/C ratio of the microbial biomass pool ($NC_B = 1/CN_B$). Specifically, the rate of net N mineralization (positive) or immobilization (negative) can be calculated by:

$$\frac{dN_{min}}{dt} = V_C \times NC_{SUB} - V_C \times f_e \times NC_B = V_C \times (NC_{SUB} - f_e \times NC_B),$$

where V_C is the rate of substrate C consumed by the microbes (inflow to biomass pool from litter, humus, and the biomass itself). The model therefore, predicts net mineralization if $NC_{SUB} >$

$f_e \times NC_B$ and net N immobilization if $NC_{SUB} < f_e \times NC_B$. Thus the rate of net N mineralization depends not only on the C/N ratio of the substrate consumed but also on the growth yield and C/N ratio of the microorganisms growing on the substrate.

Simulated net N mineralization/immobilization rates are therefore highly sensitive to the CN_B parameter, but estimating CN_B is not trivial. Fungi generally have higher C/N ratios than bacteria (Berg and McClaugherty, 2008); thus soils dominated by fungal communities should be simulated with higher C/N ratios of the biomass than those dominated by bacteria. But the relative importance of fungal and bacterial metabolism is not a constant characteristic of soils; it depends on the substrates amended. For instance, Bossuyt *et al.* (2001) found that fungal activity dominated over bacterial activity relatively quickly (two weeks) after incorporations of wheat straw (high C/N ratio) compared to the control where no residue were added. It may be necessary to implement a transient alteration of CN_B to accurately simulate the net N mineralization patterns of particular residue types, e.g., increasing CN_B for simulating the decomposition of sunflower and maize straw but reducing the parameters for simulations of oilseed rape stems and elephant grass (Borgen *et al.*, 2011).

Nitrate leaching and denitrification losses

Nitrogen losses through leaching and denitrification are major agricultural pollutants resulting from organic matter decomposition. In ecosystem models, the biological processes affecting the nitrate pool (assimilation by roots and microbes, microbial N mineralization and denitrification) are simulated for separate layers of the soil profile, and the transport of nitrate between layers is calculated by the concentration and vertical water flow (Johnsson *et al.*, 1987; Jansson and Moon, 2001). In some models, the transport calculation includes consideration of bypass-flow in macropores, which may have a lower nitrate concentration than the soil layer (Ragab *et al.*, 1996).

In mechanistic or process-oriented ecosystem models, N_2O emissions are often predicted by a submodel. The NGAS algorithms were developed for the CENTURY-DAYCENT model (Parton *et al.*, 1996; Del Grosso *et al.*, 2000), and have been implemented in CERES (Gabrielle *et al.*, 2006) and SPN (Bleken *et al.*, 2009; Borgen *et al.*, submitted). The functions of NGAS were

developed by curve-fitting (least-square) to empirical data by Weier *et al.* (1993) of soil respiration rates, denitrification (N_2), and N_2O emission measured in a full-factorial laboratory experiment. Different levels of water-filled pore space, respiration (manipulated by adding C substrate), and NO_3^- concentration were used as independent variables for prediction of N_2O and N_2 production. To calculate the N_2O/N_2 -product ratio it is assumed that as O_2 availability decreases, a larger proportion of N_2O is reduced to N_2 . The approach is based on the law of minimum, i.e., denitrification is controlled by the most limiting factor (labile C respiration, NO_3^- concentration or available O_2). Realistic predictions of respiration and N mineralization-immobilization are essential for a successful application of NGAS (Boyer *et al.*, 2006), but also of models using other approaches to estimate N_2O emissions, e.g., EPIC, SWAT and DNDC (David *et al.*, 2009). Representation of biological or physical processes can be more detailed, e.g., microbial growth kinetics controlling individual steps in the denitrification reduction pathway as in DNDC (1998) or oxygen diffusion in soil microaggregates as modeled explicitly by Smith (1990). Weaknesses of current N_2O modeling approaches are that i) most empirical models ignore the physiology and population dynamics of the denitrifying microbial communities (Bakken and Dörsh, 2007) and ii) substantial challenges exist in extrapolating results from process-oriented models (developed on field scale) to larger scale (Chen *et al.*, 2008).

Modeling crop residue affects on soil C and N dynamics

Organic matter enters the soil agrosystem in several ways. Although harvestable products are the main targets for plant production, a large fraction (40-50% of total biomass) is not harvested and will return to the soil as litter residues. Additionally, soil receives large inputs of litter from plants that are not harvested, e.g., catch or cover crops and green manures. In some agricultural systems biological N fixation by legumes is used as the main nutrient source, with the objective to avoid the negative impacts of synthetic fertilizer production (i.e., fossil fuel consumption to drive the chemical synthesis plus that for transportation), or because mineral fertilizers are inaccessible. The incorporation of N-rich plant residues as green manure is a potential instrument for synchronizing net N mineralization with the needs of the growing crops over time. Improving the synchrony and nutrient uptake efficiency from organic inputs may be possible in warm and

humid systems (Myers *et al.*, 1997), but in temperate climates with short growing seasons it is challenging.

Predicting N mineralization and immobilization from litter quality

It is well known that N mineralization/immobilization kinetics induced by residue addition depend on litter quality (Swift *et al.*, 1979; Heal *et al.*, 1997). In order to predict the effect of various litter types on the mineralization-immobilization trajectories, we need instruments to parameterize litter quality, which in the context of compartmental models means to determine the relative amounts of rapidly and slowly decomposing fractions of C and N in the residue. Plant materials are heterogeneously composed; the contents of major plant constituents vary substantially as reported by Jensen *et al.* (2005) using stepwise chemical digestion (SCD) on 76 common agricultural crops in Scandinavian (e.g., lignin: 0.3 - 103.8 mg C g⁻¹, cellulose: 31.4 - 265 mg C g⁻¹, and total C/N ratio: 7 - 227). Plant biochemical constituents decompose at different rates. The percent loss after one year for carbohydrates, hemicelluloses, cellulose, lignin, waxes, and phenols was reported as 99, 90, 75, 50, 25, and 10% (Minderman, 1968). Thus it is challenging to find criteria based on measurable plant components to predict decomposition and net N mineralization patterns. Many attempts have been made based on biochemical properties of plant materials using empirical models such as simple- and multiple-linear regressions (Herman *et al.*, 1977; Mtambanengwe and Kirchmann, 1995; Hadas *et al.*, 2004; Bruun *et al.*, 2005) and multivariate principle component regressions (Ruffo and Bollero, 2003; Morvan *et al.*, 2006). Nitrogen content and the C/N ratio of the residue are generally good indicators of the N mineralization (Janssen, 1996; Bruun *et al.*, 2006). Three typical N mineralization patterns were observed when Jensen *et al.* (2005) grouped the 76 residues by their neutral-detergent-soluble N contents as 1) > 30 mg N g⁻¹, 2) 10-30 mg N g⁻¹, and 3) < 10 mg N g⁻¹, which gave patterns of immediate N mineralization, initial immobilization followed mineralization, and sustained N immobilization, respectively (Figure 7).

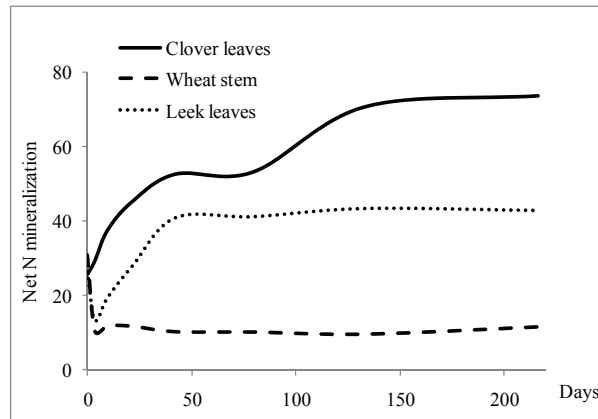


Figure 7 Three typical net N mineralization patterns from agricultural residues exemplified by 1) clover leaves, 2) wheat stem and 3) leek leaves.

Mechanistic models with first-order decay kinetics have described net N mineralization patterns with reasonable success (Pansu *et al.*, 1998; Corbeels *et al.*, 1999; Henriksen and Breland, 1999; Borgen *et al.*, 2011). Most commonly in these models, fresh (added) litter enters the system in two pools of rapidly- and slowly-decomposing material (Pansu *et al.*, 2003). The two-litter pool structure is applied in SPN, where the decomposability of residues is described by the litter pool partitioning parameters P_C and P_N that assign a fraction of total plant C or N to the rapidly decomposing litter pool.

Various methods have been used to estimate the litter pool partitioning parameter (P_C and P_N), however, a single factor for all agricultural and improved grassland residues (disregarding litter quality differences) has also been used (Coleman and Jenkinson, 1996). Biochemical fractions have been used to estimate kinetically-defined litter pools, e.g., acid hydrolysable (Shirato and Yokozawa, 2006), neutral-detergent soluble (Henriksen and Breland, 1999), water-soluble (de Neergaard *et al.*, 2002), cellulose (Müller *et al.*, 2003), and the lignin/N ratio (Parton *et al.*, 1994).

Residue type and SOC stabilization

The effect of litter quality on long-term SOC stabilization in soils is currently debated. Given the potential of soils to mitigate atmospheric CO₂ levels, managing the quality of plant litter to

optimize C sequestration has been suggested. Significantly larger SOC contents were found after 14 years of green manure in a legume rotation compared to a conventional systems where only senescent residues were returned, which led the authors to suggest legume-based systems as an option for C sequestration enhancement (Drinkwater *et al.*, 1998). Corroborating those results, Johnson *et al.* (2007) found significantly different percentages of C remaining after long-term incubation (498 days) of alfalfa and soybean leaves. The theory of selective preservation of recalcitrant compounds is implemented in ecosystems models, e.g., CENTURY and ROTH-C, by directing a fraction of the structural (or slowly decomposing litter) to the humus or passive SOM pool (Paustian *et al.*, 1997).

However, there is evidence suggesting that the content of recalcitrant components in litter hardly affects the long-term stabilization of litter-derived C. Field application of glucose and wheat straw resulted in equivalent amounts of residual C (as SOC) after ten years (Voroney *et al.*, 1989) and in a 3-year tropical field trial where plant litter with different (lignin+polyphenol)/N ratio was incorporated, no difference in the amounts of C remaining in the soil was found (Gentile *et al.*, 2011). These findings support the perception that soil microbial communities are able to degrade residues of any quality (von Lützow *et al.*, 2006; Marschner *et al.*, 2008) and that stabilized material remaining in the soil for long times after litter amendments are products of microbial metabolism rather than recalcitrant components in the residues. Whereas short-term aggregation mechanisms are influenced by litter quality (Martens, 2000), longer-term aggregation is not, but instead depends on the quantity of litter input and its interaction with the soil matrix (Gentile *et al.*, 2011).

Below-ground inputs from roots have been postulated to contribute relatively more to soil C than above-ground residues based on modeling results using long-term field trial data (Kätterer *et al.*, 2011) and literature review (Rasse *et al.*, 2005). Several mechanisms have been held accountable such as physic-chemical protection in deeper horizons, mycorrhiza and root-hair activities providing physical protection, and chemical interactions with metal ions (Rasse *et al.*, 2005). To account for the higher mean residence of root-derived C than shoot-derived C, ecosystem model can have separate litter pool partitioning parameters for the root fraction, e.g., in SPN a larger

fraction of total root C and N is allocated to the slowly-decomposing litter pool (smaller P_C and P_N values), but no direct transfer to the humus pool has been implemented.

Modeling tillage effects on soil C and N dynamics

Tillage operations influence the mineralization of N and the decomposition of organic matter in various ways. Short-term N dynamics are affected by an induced mineralization flush and long-term stabilization of SOC may also be affected depending on other management aspects.

Soil mineral N dynamics

Tillage-induced effects on short-term net N mineralization are primarily caused by the termination of crop growth and incorporation of surface residues into the soil, but may also be caused by the mechanical disturbance of soil structure. When plant growth is terminated by plowing or harrowing in the fall, a period with little (if any) plant N uptake follows, which is likely to result in substantial nitrate leaching losses compared to plowing in the spring (Djurhuus and Olsen, 1997; Stenberg *et al.*, 1999; Askegaard *et al.*, 2011). But fall plowing does not necessarily cause large mineral N contents if a new crop (winter cereal or catch crop) is established soon after plowing (Thorup-Kristensen *et al.*, 2009). The efficiency of catch crops to assimilate soil mineral N in late fall and winter may be variable, however, depending on soil texture, root depth of the catch crop, and precipitation regime, thus several factors determine how plowing time affects the extent of nitrate leaching (Hansen and Djurhuus, 1997; Pedersen *et al.*, 2009). Large amounts of fresh N-rich material are incorporated in the soil during plowing of leys and especially green manure, which may cause significant nitrate leaching (Wallgren and Linden, 1994; Thorup-Kristensen *et al.*, 2003).

To model the response of tillage on N dynamics, ecosystem models need routines that simulate crop harvest and surface residue incorporation. Plant residue incorporation in SPN for example is modeled by a routine that differentiates C and N into plant fractions of roots, harvested material, stubbles and removed residues, but it also simulates the gradual decomposition of surface residues, e.g., senescent plant material and residues from harvested ley that are not plowed. Such surface residues will only gradually come into contact with soil, and thus start to decompose (as they are partly protected against decomposition due to low moisture content before the intimate

contact with soil is established). The residue routine implemented in SPN simulates these aspects in the following manner. At the end of the growth period, above-ground material is distributed by the fractionation constants into harvested plant (*hp*), surface residues (*sr*), and incorporated residue (*inc*), and below-ground material is separated into dead roots (*dr*) and live roots (*lr*). The usual first-order decomposition starts immediately for the incorporated residues and the dead roots by transfer to the litter pools (Figure 8). Material assigned as surface residues and living roots are transferred to the temporary pools LiveRoots and SurfRes, from where the model performs gradual transfers (first-order flow) to the litter pools. Upon tillage, the remaining materials in the temporary pools, which may have accumulated from several harvests, are immediately transferred to the litter pools and the pools are completely emptied. The continuous first-order flows from LiveRoots and SurfRes to the litter pools secures that the temporary pools reach pseudo-steady state levels when simulating several years of ley uninterrupted by tillage.

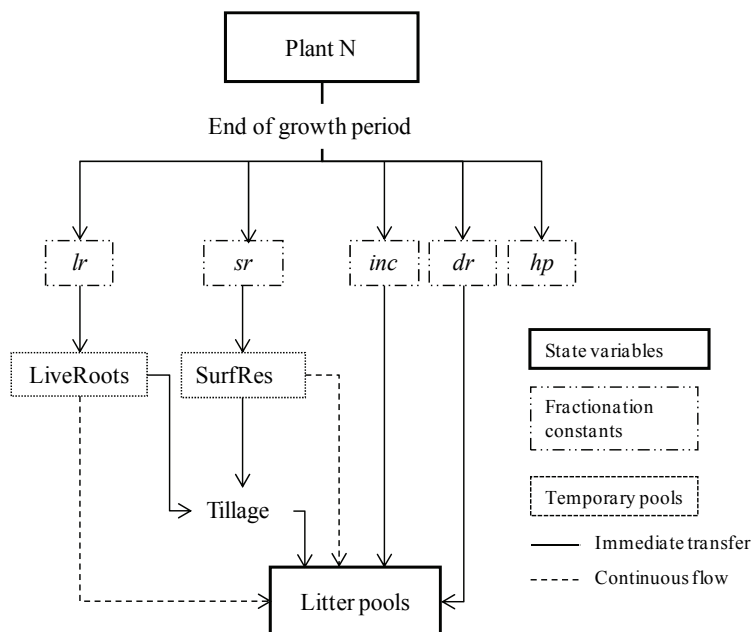


Figure 8 Surface-residue routine in the SPN model. Upon ended growth period the fractionation constants *lr*, *sr*, *inc*, *dr*, and *hp* assign C and N to live roots, surface residue, incorporated residue, dread roots, and harvested plant material, respectively. Temporary pools for surface residues and live roots (LiveRoots and SurfRes) have continuous flows to litter pools and are immediately transferred to the litter pools upon tillage.

The observation that tilling bare soil causes a transient increase in net N mineralization (Powlson, 1980; Calderon *et al.*, 2001; Calderon and Jackson, 2002) is not simulated by the model features described above. The phenomenon is ascribed to the physical disturbance of structure, exposing organic materials to decomposition, which are otherwise protected against enzymatic attack due to their position within the matrix (Beare *et al.*, 1994). Physical disturbance of soil in laboratory experiments (e.g., mixing and/or sieving) are also found to induce transient increases in N mineralization (Hassink, 1992). In SPN, a transient flush of N mineralization after plowing is secured by letting the model transfer a fraction of the microbial biomass to a temporary rapidly-decaying pool, which enhances respiration and N mineralization transiently, i.e., until the pool of rapidly-decaying material is depleted (Bleken *et al.*, 2009). A similar approach was chosen by Henke *et al.* (2008) and Müller *et al.* (2006). Modeling tillage effects in this manner may not adequately represent the mechanisms involved, but it effectively emulates empirical observations of tillage effects.

Tillage has a direct influence on soil porosity and compaction, and thus the ratio of water-filled to air-filled pore space. Plowing may increase aeration above the plow-pan, but may also induce anaerobic microspaces, especially if conducted on wet soil (Bakken *et al.*, 1987). Plowing effects on N₂O emissions may therefore be more challenging to determine and field studies have shown contradicting results. For example termination of a clover-grass sward by plowing enhanced N₂O emissions compared to an unplowed treatment (Estavillo *et al.*, 2002), whereas other studies have shown larger emissions for grassland termination by chemical fallow than full-inversion plowing (King and Ball, 1992; MacDonald *et al.*, 2011). In arable rotations, no-till compared to conventional plowing appear to increase emissions, possibly due to lower air-filled porosity combined with more extensive network of continuous air-filled pore space (for gas transport to the surface) in no-till compared to tilled soils (Ball *et al.*, 2008). In summary, interactions between soil physical parameters (e.g., porosity, bulk density, texture, and aggregate stability) and biological activity need to be considered to determine soil tillage effects.

Carbon sequestration and soil C loss

SOC losses are most drastic (20-30% during the first decades) when native land is cultivated (Schlesinger, 1997). Tillage effects on SOC is implemented in the IPCC guidelines for GHG inventories, where land under reduced tillage (or no-till) have larger SOC stocks than land under annual plowing (IPCC, 2006). For Norway, annual sequestration rates for reduced tillage (versus annual plowing) was estimated to be $140 \text{ g C m}^{-2} \text{ yr}^{-1}$ (Singh and Lal, 2005), which is more than twice the size of the global estimate of $57 \text{ g C m}^{-2} \text{ yr}^{-1}$ by West and Post (2002). Such effects of reduced tillage on SOC are questionable, however. The positive effect on soil C storage from reduced tillage or no-till seems to disappear when measurements of SOC in deeper layers of the soil profile are included. Positive effects on top soil C content of reduced tillage has been reported, but effects tend to reverse in the subsoil, thus no net C accumulation occurs in the top 50 cm profile (Needelman *et al.*, 1999; Dolan *et al.*, 2006; Chivenge *et al.*, 2007). Soil erosion is another confounding factor when evaluating tillage effects on C sequestration. Intensely tilled soils tend to lose more surface soil material by erosion than no-till or reduced tillage regimes (Lundekvam and Skoien, 1998). Since the surface soil has higher SOC content than deeper layers, high erosion would lower total SOC content of the soil profile. The reduction is a physical transport of SOC (to streams/lakes or other areas), however, and should not be interpreted as a net emission of CO_2 .

In Scandinavia, changing tillage practices to no-till for increasing soil C sequestration may not be a viable options because it can result in declining yields (Rasmussen, 1999). Furthermore, the vast majority of arable land has been under cultivation for centuries, thus the SOC levels are probably close to a steady state.

A tillage factor is often implied in models to modify decomposition rates according to tillage intensity and frequency. Estimating the tillage factor based on empirical data is not a simple matter due to the confounding factors of crop residue input and erosion. For prediction of the C sequestration potential of a large-scale adoption of reduced tillage in the Netherlands using ICBM, Vellinga *et al.* (2004) considered the decomposition rate for arable systems to be about three times faster than for grassland rotations. Using the same model, Kätterer *et al.* (2008)

assumed only a 10% reduced decomposition rate for perennial leys compared to the annual cropping rotation. This example emphasizes the scope for deeper studies of tillage effects on decomposition and SOC stabilization for various management systems; thus more robust estimation of the tillage factor is needed.

2 RATIONAL AND OBJECTIVES

Research motivation

The adoption of the term ‘multifunctional agriculture’ as a guideline for developing national agricultural politics (Parra-Lopez *et al.*, 2008) reflects the recognition that agriculture contribute to nation and global welfare in various ways. Food security is one of the most obvious agricultural contributions to national welfare, which is also considered to provide peace between and within nations. In the long term, food security demands environmental sustainability, meaning that agricultural practice does not deteriorate soil fertility of cultivated land. Sustainability is also extended to the quality of natural ecosystems, since these are affected by agricultural production. However, there seems to be a large discrepancy between public opinion about the space given to agriculture cultural production and the goods expected to be retrieved. Thus, it is far from trivial to combine short-term goals (for food security or productivity requirements imposed by market forces) with long-term sustainability and minimal damage to the external environment. However, efforts have been placed within research and development of agricultural production systems that are environmentally friendly.

The modern recognition of environmental problems connected with agriculture can be dated back to Rachel Carson’s book “Silent spring” (1962), which emphasized the toxic effects of agrochemicals, both on humans and the fauna in natural habitats. The book helped to launch a strong environmental movement that effectively demanded a reduction in agrochemical usage. Somewhat later, the loss of excess plant nutrients was recognized as another important negative side effect of agricultural production, and nitrogen was much focused due to its effects on the marine ecosystems, and is still a hot issue. In Scandinavia, this resulted in political intervention regarding fertilizer restrictions as manifested in the North Sea Treaty of 1987. The current loads of reactive N lost from agroecosystems are so large that substantial regional impacts on both terrestrial and aquatic habitats can be detected (Vitousek *et al.*, 1997). But the environmental side effects of agriculture extend to a global scale as well, due to the significant emissions of greenhouse gases such as methane from ruminants and N₂O from cultivated soils (as well as the indirect N₂O emissions from N-enriched natural habitats). Food production is also causing

emissions of CO₂, primarily due to energy demanding machinery and fertilizer production, but also by a net decline in soil organic C (particularly in continuous arable cropping systems). Thus, the atmospheric footprints of agrosystems have implications for global warming, against which we must take action (Richardson *et al.*, 2009), in concurrence with public opinion that we should develop production systems with minimal emissions of GHG.

Environmental movements have tended to adopt organic farming as a remedy to all these malaises. It is more sustainable than conventional farming because less fossil fuel is needed (no chemical fertilizers are used). The absence of agrochemicals is likely to sustain a higher biodiversity of the agroecosystem itself, and in the surroundings, compared to conventional farms. Organic farming is also expected to sustain higher soil organic carbon contents than conventional farming because crop rotations are used (thus avoiding continuous grain cropping). It has also been assumed that organic farms loose less N, because the inputs are lower. For the same reason, it is often expected that the emissions of N₂O were lower in organic than in conventional production systems. Organic farming is most likely superior to conventional farming regarding biodiversity both within and around the agroecosystem. But its performance regarding soil organic C losses, nitrate leaching, and emissions of N₂O needs to be critically evaluated. Not primarily for deciding whether organic farming is better or worse than conventional systems. That discussion is futile; because neither of them is one or the other and neither is static. Conventional farming has changed substantially in response to public demand for more environmentally-friendly production, and is quite variable in terms of intensity and various management regimes. Organic farming has changed and specialized as well, partly driven by societal demands and socioeconomic frameworks. Thus it appears more interesting to search for management options that can reduce N losses and GHG emissions while sustaining soil fertility within the framework of organic farming.

This thesis contains various modeling studies with the common topic being how management practices affect the sustainability and environmental impacts of conventional and organic farming systems. The first paper (I) deals with net N mineralization as influenced by plant litter quality. Incorporating different types of plant litter (at an appropriate time) can be a potential instrument (through management of green manure and crop residues) for improving the

synchronization of net mineralization with crop demand, and thus minimize N losses. For the second paper (II) a case study of an organic farm was selected to investigate the environmental and production efficiencies of organic stockless cereal production in SE Norway and to explore how alternative management practices could improve such systems, currently and in the future given expected climatic changes. Finally in the third paper (III), I considered CO₂ emissions on a national scale by calculating the soil C balance for cropland on mineral soil in Norway using the IPCC framework.

Objectives

The overall objective was to contribute to the understanding of organic matter decomposition and management influences on the environmental impacts from plant production. More specifically, the following research questions were answered:

- 1) How can we determine adequate parameter values for plant residues of various litter quality in order to accurately simulate C and N mineralization?
- 2) What is the potential for improving productivity and minimize environmental effects of organic stockless grain systems?
- 3) What is the national CO₂ emissions budget for cropland on mineral soils in Norway and what causes these emissions?

3 EXTENDED SUMMARY

The three papers included demonstrate application of models on three different scales related to environmental effects of C and N cycling in agricultural ecosystems. The topics include the determination of rapidly- and slowly-decomposing fractions of plant residues for prediction of short-term C and N mineralization (Paper I); nitrate leaching and denitrified N losses as influenced by plowing season and green manure inputs in stockless organic farming systems (Paper II); CO₂ emission from mineral soils affected by changes in cropland management in Norway (Paper III). In the first study, a mechanistic SOM submodel was applied to C and N mineralization patterns measured during incubation, in order to determine the rapidly-decomposing plant litter pools and other decomposition-related parameters (i.e., litter pool decay rates, microbial growth yield and biomass C/N ratio). In the second paper, an ecosystem model was used to simulate field N dynamics of organic clover-grass and cereal crop rotations in a stockless production system, and alternative scenario simulations of management and future climate (global warming) were made. Paper III takes a national point of view, using a C balance model to estimate CO₂ emissions from mineral soils on croplands in Norway. After the individual summaries, this chapter provides concluding remarks and suggestions for future work.

Estimation of plant litter pools and decomposition-related parameters in a mechanistic model (Paper I)

In theory, synchronization of net N mineralization with plant N demand can be improved by the choice of crops, timing of residue incorporation, and soil tillage. This is important for the environmental performance of conventional farming systems, but for low-input and organic farming systems, it is essential to secure productivity. Dynamic modeling of C and N mineralization in soil can be an instrument to design optimal management regimes, but it is strongly dependent on adequate estimation of the parameters that control the mineral N kinetics. One essential aspect of this parameterization is to accurately predict how the net rate N-mineralization-immobilization is affected by incorporation of various types of crop residues.

The objectives of this study were to assess the performance of a mechanistic SOM model to accurately simulate C and N mineralization kinetics during decomposition of various plant litter

types in soil, depending on the methods used to estimate the fraction of rapidly decomposing C and N in each plant residue, i.e., the litter pool partitioning parameters (LPP). The LPP are termed P_C and P_N and are equal to the fraction of C and N assigned to the rapidly-decomposing pool (Litter 1 in Nitrosim), thus $1-P_C$ and $1-P_N$ are allocated to the slowly decomposing litter pool. Also, potential improvements in model simulations were investigated by simultaneously optimizing plant-specific LPP and the global parameters that govern decomposition, which are the litter pools decay rates (k_{L1} and k_{L2}), microbial growth yield efficiency (f_e) and the C/N ratio of the microbial biomass pool (CN_B).

C and N mineralization data from 76 plant materials incubated for 217 days in the lab were simulated by the Nitrosim module for microbial C and N transformations. Nitrosim is a two-litter pool model with a microbial biomass, and an active humus pool, where all pools decay according to first-order kinetics. The biochemical composition of the plant residues were determined by stepwise chemical digestion (SCD) and near infrared reflectance spectra (NIRS) were recorded. We explored the possibility to use SCD and NIRS data to predict optimized LPP values. In summary, three steps were carried out: 1) optimization of plant litter pools against C and N mineralization data of a calibration set, 2) construction of regression models for prediction of the optimized LPP, 3) evaluation of Nitrosim performance when initialized by LPP obtained by measured biochemical fractions and the regression model estimates.

Specifically, the optimized LPP parameters were obtained by least-squares curve fitting against measured C and N mineralization data by the Levenberg-Marquardt optimization algorithm programmed in MATLAB. The regression models were constructed to estimate the optimized P_C and P_N values (dependent variables) based on the SCD and NIRS data (independent variables). The best regressions models were selected and used to estimate P_C and P_N , which were used to initialize the Nitrosim simulations of the mineralization data. The simulations were evaluated by mean absolute error, modeling efficiency and an information criterion (AIC) using an independent dataset ($n = 15$) that had not been used for the calibration and regression analyses. Moreover, the optimization tool and a relatively large dataset allowed a robust estimation the global-scope parameters (k_{L1} , k_{L2} , f_e , and CN_B) when optimized simultaneously with LPP. After optimization, nine plant materials were identified as clear outliers (large deviations between

modeled and measured C and N mineralization patterns) and for these exploratory optimizations were performed to identify potential causes for model failure.

Neutral detergent soluble (NDS) C and N fractions have previously been used as a direct measure of the rapidly decomposing litter pool fraction (LPP) for modeling C and N mineralization (Henriksen and Breland, 1999). The NDS-based LPP deviated substantially from the LPP estimated by model optimization. On average, the optimized LPP were 30% larger for C and 46 % smaller for N compared to the NDS-based LPPs. This suggests that the material extracted by NDS is far from identical to the easily decomposable fraction of the plant litter. Not only is the total amount of C too low but the C/N ratio is also much too high. LPP values predicted by regression models of optimized LPP values based on biochemical fractions, as well as NIR, resulted in equally good Nitrosim simulations. This was illustrated by reduced mean absolute errors of 13% and 29% for C and N mineralization, respectively when simulations were initialized by regression model estimates compared to initialization using NDS-C and NDS-N directly.

Estimation of the global decomposition-related parameters (k_{L1} , k_{L2} , f_e , and CN_B) by simultaneous optimization with the litter-specific parameters reduced Nitrosim model errors by more than 50% compared to the simulation where only the global parameters were optimized. Exploratory optimizations for individual outlier plant materials showed that parameter adjustment of the C/N ratio of the microbial biomass (CN_B) alleviated model errors. This indicated that the C and N stoichiometry of microbial transformations differ between plant materials of different litter quality. The outlier residues were much better simulated with higher or lower CN_B than that for the rest of the residues, possibly due to a selective stimulation of fungal or bacterial growth, respectively. The study provides a global parameter set that can be applied in comparable SOM models, estimates of the rapidly-decomposing C and N fractions in 76 common Nordic agricultural plant materials, and regression models based on SCD-measured biochemical fractions or NIRS, which may be used for parameter estimation in the future.

Nitrogen dynamics in stockless organic clover-grass and cereal rotations (Paper II)

Organic farming emerged as an environmentally-friendly alternative to conventional farming and thus aims to be so. However, studies have shown that it is not always the case for variables such as nitrate leaching and N₂O emissions, especially if these variables are expressed per unit of produce. Concerns have been uttered that stockless organic farms relying solely on green manure as N fertilizer are hazardous to the environment in the cool temperate regions, where a short growing season and wet springs and autumns facilitate nitrate leaching. Minimizing N losses can be challenging because of the complex cause-effect relationship of climate, soil and agricultural management. In this context, models are useful to explore the combined effects of these factors in realistic model scenarios. Thus models can simulate numerous management and climatic conditions, which would be practically impossible to cover with field trials. Furthermore, the application of models to case studies provides an opportunity to investigate actual practices. The objective of this study was to investigate the N dynamics on stockless organic farming in SE Norway and to explore alternative clover-grass and cereal crop rotations and plowing season in the present and future climates by scenario simulations.

Two fields with different clover-grass ley management were monitored from August 2004 to December 2009 by tri-annual measurements of soil mineral N and collection of recorded yields and crop rotation by the farmer. The ecosystem model SPN (Soil Plant Nitrogen) was applied in two steps. First, we simulated crop N uptake, yields, soil mineral N contents, nitrate leaching and denitrification losses from two different fields that were converted to organic farming in 2000 and 2003, respectively. The simulations were evaluated by comparison with measured yields and soil mineral N contents. Reported grain yields were relatively moderate (between 3.5 Mg ha⁻¹ and 4.5 Mg ha⁻¹) and adequately simulated. The simulated mineral N contents were also in good agreement with measurements. Second, we simulated alternative management scenarios of cereal undersown with a winter clover-grass ley that differed in the frequency and distribution of annual ley years under spring and fall plowing. The scenarios were simulated with historic and future weather data, the latter based on the A2 emission scenario (IPCC) simulated by the HadAM3 model (Hadley Center) and scaled down regionally to a 55 x 55 km² grid. To evaluate their relative environmental impact, indicators of performance were calculated. These were grain

produced per unit of N input (N yield/input), N losses by denitrification and leaching per unit of N input (N loss/input), N losses per unit of grain produced (N loss/yield), and greenhouse gas emissions (CO₂ and N₂O).

The simulated soil mineral N was generally low (1-4 g N m⁻²), except for one year where an extended period of black fallow for mechanical weeding resulted in severe nitrate leaching losses (12.7 g N m⁻² yr⁻¹). Mean annual leaching losses during the organic farming period were somewhat larger than measured under comparable conditions; 4.3 and 4.8 g NO₃⁻-N m⁻² for the two fields. Denitrified losses were between 1.8 g N m⁻² (Field 1) and 2.5 g N m⁻² (Field 2), with N₂O losses constituting 44% (Field 1) and 34% (Field 2) of total emissions.

Simulations of alternative crop rotations showed that increasing the number of years with ley resulted in higher single-year grain yields, but not if two consecutive years with ley were practiced. Averaged over the whole rotation, continuous cereal with clover grass as a winter cover crop showed the largest grain yields. The yields in this rotation were associated with a considerable net reduction (by mineralization) of soil humus. Spring plowing resulted in higher grain yields and lower nitrate losses by leaching than fall plowing, ascribed to a better synchronization of N mineralization with plant N uptake and larger N inputs from N fixation. Cumulated net N mineralization during the summer season was 20% higher for the spring than the fall plowing of the 1-year ley rotation. Annual net N mineralization was hardly affected by plowing time, thus fall plowing resulted in a larger share of total N mineralization off-season. The simulated denitrification and N₂O emissions reflect this effect of plowing time on the seasonal distribution of mineralization in the soil. Annual denitrification, and especially in the growing season, was enhanced by spring plowing, whereas the opposite was the case off-season (higher rates for fall than for spring plowing).

Environmental indicators suggested that only modest improvements can be obtained by changes in plowing time and ley-grain rotation. Overall, the environmental indicators were in favor of the spring plowed continuous grain rotation. Based on N efficiency, the indicators ignore other agronomic aspects such as perennial weeds, phytosanitation, fungal disease and aphid infestations that may be problematic under annual monoculture conditions, and possibly

aggravated by spring plowing. Predicted climate changes (simulations with future weather scenarios) had marginal effects on the environmental indicators, however, nitrate leaching increased substantially because of the warmer winters reducing the period of soil frost. The importance of winter cover crops or catch crops seems to increase in the future. In conclusion, it is a challenge to simultaneously pursue long- and short-term production and environmental goals in a stockless organic cereal production. Alternative measures, aside from the management of crop rotation and plowing season, are needed to improve the nutrient cycling in these systems, e.g., recycling of plant residues by biogas digestion or composting with municipal waste. Improving the environmental legitimacy of stockless organic grain production depends on a more rational utilization of the clover-grass biomass ley than direct incorporation as green manure. Another reasonable option may be to abandon the stockless systems and reintegrate livestock.

CO₂ emissions from cropland soils in Norway estimated by IPCC default and Tier 2 methods (Paper III)

Although the effects of agricultural management on SOC dynamics are well documented, they are often ignored in national inventory reports submitted to the UN Framework on Climate Change. Such inventories are often based on the assumption that SOC levels are in steady state (hence no net CO₂ emissions from cropland), and this is also the case for the Norwegian national inventory. The objective of Paper III was to estimate net CO₂ emissions (or removals) by cropland on mineral soils in Norway. In accordance with the IPCC (Intergovernmental Panel on Climate Change) methodology, we applied the default (Tier 1) method and developed a model-based Tier 2 method for a comparison of the two methods. In the Tier 1 method, the soil C reference stocks and stock change factors are default values derived from the IPCC guidelines, whereas for Tier 2 they were estimated by model simulations using country-specific climate and soil data. Both methods apply the same agricultural activity data and agrozone division and thus only differ in values for soil C reference stocks and stock change factors. The stock change factors are defined as the relative change in SOC stocks between the equilibrium states of a management system compared to a reference condition. By default the reference condition is the native soil (pre cultivation).

Norway was divided into 31 agrozones based on a combination of counties and climate zones, which is utilized by the Norwegian Agricultural Authorities. This facilitated the compilation of agricultural activity data, i.e., areas and yields of the major crops (cereals, leys, and root crops) and livestock numbers. Areal data of major crops and livestock numbers (for estimation of manure availability) were used to define 16 management systems and determine their individual area. The activity data was collected for 1999 and 2009, which was the chosen inventory period. Also, climate data of air temperature, precipitation and estimated potential evapotranspiration were collected for 1980-2009 from 32 000 measurement stations on arable land in Norway. For each agrozone a 30-year climate series of daily means was calculated, which was used for the estimation of the model-based Tier 2 parameters.

For the Tier 2, the Introductory Carbon Balance Model (ICBM) of Andrén and Kätker (1997) was used to estimate the soil C reference stocks and stock change factors. The ICBM assumes soil C transformations through two SOC pools that decay according to first-order kinetics modified by a factor representing the external response on decomposition, which is the product of the temperature, moisture and tillage effects. The climate data was used as input to calculate soil temperature and moisture (including soil texture effects) response factors. A new reference condition was defined as continuous ley with a moderate manure application, for which the reference C stocks were calculated by the steady state solution of the model per agrozone and major soil texture type. Crop yields per agrozone were used to estimate C inputs. Stock change factors were calculated for each management system per agrozone and soil texture type.

The ICBM-estimated soil C reference stocks were similar to the default stocks. The estimated stock change factors, however, differed from the default values, especially for crop rotations without manure application, as they were smaller. Consequently, decomposition rates and SOC losses were larger when estimated by the default method compared to the Tier 2. This resulted in annual net CO₂ emissions that were twice as large when estimated by the default Tier 1 method (313 Gg CO₂ yr⁻¹) compared to the Tier 2 (138 Gg CO₂ yr⁻¹). The major management change over the inventory period (1999-2009) was caused by declining manure applications; national manure availability was estimated to have been reduced by 32 %. Although declining livestock resulted in large CO₂ emissions, the smaller number of cattle reduced methane emissions by 259

Gg CO₂-eq yr⁻¹ from enteric fermentation. Thus had livestock numbers been maintained, the reduction in annual CO₂ emissions would have been counterbalanced by CH₄ emissions in the total greenhouse gas budget. Including calculations of all GHG is crucial before financial incentives for farmers are brought in motion to promote C sequestration management practices. Encouraging reduced organic matter amendments by reducing livestock production would also deteriorate soil fertility, water-holding capacity and nutrient cycling, which may substantially impede the sustainability and N use efficiency of especially organic systems. Finally, it should be noted that for Norway the default and Tier 2 methods are sensitive to assumptions regarding manure application practices (i.e., application rates and crop preferences), and thus illustrate the demand for appropriate activity data to obtain a reliable national CO₂ emissions estimate.

Concluding remarks

The work compiled in this thesis illustrates how models may be applied on different scales depending on the research questions. Scrutinizing mineralization patterns of numerous plant materials measured in the lab combined with a mechanistic model and an optimization routine, quantified rapidly- and slowly-decomposing C and N in plant materials of various litter qualities. Plant-specific calibration of the litter pool partitioning parameters (LPP) was crucial for simulations of mineralization patterns measured in the lab. However, simulations of mineral N for entire field N dynamics were only marginally affected by LPP when varied within a relevant range: differentiating LPP for red and white clover had a minimal effect on the mineral N simulations made for stockless organic grain systems. Thus such refinements at a low scale do not necessarily provide better predictions at larger scales.

Simulations of clover-grass and cereal rotations illustrated the difficulties of improving environmental and production efficiencies of stockless organic grain systems. With careful weed management (avoiding long lasting black fallows), such systems may be acceptable in South East Norway. But to substantially improve the productivity and long-term sustainability of the system, it may be necessary to include external nutrient sources (e.g., animal manure or municipal waste). Clover-grass and cereal rotations where ley biomass is used directly as N fertilizer have low productivity in terms of edible products per hectare. The legitimacy of the

rotations would be increased by exploiting the ley biomass for energy production before returning its N content to the soil. The combination of catch crop (sown with grain) and spring plowing reduce the risk of leaching, which appears to be crucial in the future, but does not improve the sustainability of stockless organic systems when evaluated on efficiency indicators of environment or productivity. Sustainable organic cereal production seems to be obtainable only through alternative green manure biomass utilization or reintegration of livestock.

During the past ten years, Norway has seen a decline in livestock numbers. Consequently, manure applications were reduced, which resulted in the majority of the estimated CO₂ emissions from cropland on mineral soils. Reestablishing animal manure inputs, by reintegrating livestock and arable production, would reduce CO₂ emission, as well as improve N use efficiency in organic systems. However, if livestock numbers are increased methane emission from ruminants, would counterbalance any positive C sequestration effect (or reduced CO₂ emissions) in the total greenhouse gas budget. A reintegration, i.e., moving livestock from the north to the south, would not necessarily increase numbers because of the market regulation on dairy production.

Overall, the conclusions of this thesis provide a small, but important, contribution to understanding how agricultural management practices impact the environment. A holistic evaluation of environmental impacts is necessary. Model applications considering all influential factors are of paramount importance to understand system dynamics and enable stringent analyses of specific process details that need to be connected on a higher hierarchical level. The specific conclusions obtained were:

- Estimation of rapidly-decomposing plant litter pools by regression models for initialization of a mechanistic model improved the simulation performance compared to initialization by biochemical fractions directly.
- The potential for improving N use efficiency of organic stockless cereal production in Norway is marginal through managing crop rotation and plowing season, thus alternative

strategies are necessary, e.g., recycling green manure through biogas digestion or (more drastically) abandoning the stockless system and re-integrate livestock.

- CO₂ emissions for Norwegian cropland on mineral soil were caused by reduced manure availability during the inventory period and were larger when estimated by the default Tier 1 method compared to the Tier 2.

In conclusion, the modeling studies presented in this thesis have provided knowledge about the decomposition of organic matter and N dynamics as influenced by agricultural management in plant production. The understanding gained from modeling would have been difficult to obtain through empirical analysis of data.

Recommendations for future work

This thesis delivered specific analyses of net N mineralization induced by plant litter quality, field N dynamics in stockless organic systems and a soil C budget for cropland in Norway, herein summarized with a practical perspective of environmental challenges in Norwegian agricultural. Many other detailed model studies can be chosen, which will contribute to improving the understanding of environmental effects of C and N cycling in agricultural soils. A major necessity is the integration of knowledge gained from reductionist approaches (e.g., mechanistic process-oriented modeling or empirical lab studies) within larger model frameworks that consider aspects of livestock production, economic profitability and legislative incentive. Such integration demands improved communication between science fields, expanding the boundaries of models by broadening the qualifications of modelers, and increasing the communication between interdisciplinary scientists and specialists.

Reducing environmental impacts of agricultural production will not come from science alone; it also requires public understanding and collaboration. Finding appropriate units of measure that incorporates economic and societal aspects of greenhouse gasses is necessary. Consumer expectations are conflicting in the requirements of increasing food production (especially meat) while simultaneously reducing environmental impacts. Agriculturally production for large

societies cannot exist without disturbing nature. Thus efforts should be place to increase general awareness of the relationships between food consumption, agricultural production and pollution. Educating the public about how current consumer patterns determine the type of agricultural production is decisive in order to overcome the unrealistic expectations imposed by the public upon agriculture. Improving the communication of scientific results to the public is a crucial task in order to achieve a sustainable food production in the future.

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Paper I

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Estimation of plant litter pools and decomposition-related parameters in a mechanistic model

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Abstract Modeling the C and N dynamics during decomposition of plant residues depends on robust estimation of the litter pool partitioning (LPP) of residues, i.e. the fraction of their C and N allocated to rapidly and slowly decomposing pools. We searched for ways to estimate LPP by analyzing data on C and N mineralization during decomposition of 60 widely different plant residues, using a simple model with two litter pools and one microbial pool. LPP and relevant global parameters were estimated by model optimization (Levenberg-Marquardt-least-squares algorithm) in one operation. These kinetically-defined LPP values were used in regression analyses against data from stepwise chemical digestion (SCD) and near-infrared reflectance (NIR) analysis of the plant residues. LPP

predicted by these regression models resulted in better performance than LPP from measured neutral-detergent-soluble (NDS) C and N when validated on independent data ($n=15$ plant residues). The results demonstrated the potential improvement by simultaneous estimation of residue specific LPP and global parameters, and that kinetically-defined LPP can be equally well predicted by NIR as by total N and NDS-C. Model failure for a minority of the plant-residues could partly be removed by altering the microbial C/N ratio (global optimum 7.1) within the range 5–15, possibly reflecting a variable dominance of bacteria or fungi.

Keywords N mineralization/immobilization · Near infrared reflectance spectrometry (NIR) · Neutral detergent soluble (NDS) · Optimization · Soil organic matter model

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Introduction

Plant litter decomposition is an important source of mineral nitrogen (N) for organic, low-input and some conventional agricultural systems (Seneviratne 2000). Nitrogen is frequently the key nutrient limiting agricultural productivity and causes several negative environmental impacts. In low-input systems, a careful synchronization of N mineralization with crop growth (Myers et al. 1997) is a necessity to sustain high production while minimizing environmental impacts such as greenhouse gas emissions and nitrate

leaching. Predicting N immobilization/mineralization during decomposition of crop residues and green manures requires a modeling approach that takes adequate account of plant residue quality in the simplest way possible.

Most soil organic matter (SOM) models are based on the assumption that decomposition can be modeled by conceptual pools that decay according to first-order kinetics with pool-specific rate constants (Minderman 1968; Paustian et al. 1997). Multi-compartmental ecosystem models such as CANDY (Franko et al. 1995), CENTURY (Parton et al. 1987), DAISY (Bruun et al. 2003), DNDC (Li et al. 1994), NCSOIL (Nicolardot and Molina 1994), RothC (Coleman et al. 1997), SOILN (Johnsson et al. 1987), and STICS (Nicolardot et al. 2001) all include SOM sub-models of varying complexity. Although the structure of the soil microbial communities may influence the decomposition rates, most models ignore this component, since the main factor driving decomposition is the chemical and physical nature of the litter compounds (Swift et al. 1979). Most commonly, plant residues are partitioned into a rapidly and a slowly decomposing litter pool (Pansu et al. 2003). While this partitioning is specific for each plant residue type, the decay rates of the two (or more) litter pools and other parameters governing C and N mineralization during decomposition (microbial decay rate, growth yield, and C/N ratio) are usually global (shared), that is, common for all plant residues. Two methodological problems arise in this type of modeling: 1) what is the best approach to partition litter between easily degradable and recalcitrant C and N pools, and 2) how can we find the best set of global parameter values applicable to a broad range of agricultural crop residues?

Direct quantification of the litter pools by chemical analyses is complicated due to the diversity of molecular structures and bonds within the major plant compounds (Paustian et al. 1997) and due to the physical heterogeneity of plant residues (Chesson 1997). Stepwise chemical digestion (SCD) separates organic material into fractions of soluble, cellulose, hemicellulose and lignin-like substances (Mertens et al. 2002; Van Soest et al. 1991). Using SCD data to partition C and N into the litter pools of mechanistic SOM models can improve predictions of C and N mineralization relative to a default constant value (Probert et al. 2005; Quemada and Cabrera 1995), especially if the C/N ratio of each fraction is

determined (Henriksen and Breland 1999a; Henriksen et al. 2007). However, it is not obvious how such data should be analyzed in order to partition residue C and N into rapidly and slowly decomposing litter pools. Water-soluble C and N have been found to underestimate the rapidly decomposing litter pool in the DAISY model (De Neergaard et al. 2002), and the use of SCD data in a mechanistic three-litter-pool model resulted in somewhat overestimated plant residue C and N mineralization (Henriksen et al. 2007). Henriksen et al. (2007) also predicted SCD data from near infrared reflectance spectra (NIR) data, which resulted in similar model performance as using SCD data directly. NIR provides repeatable and accurate measurements with low cost and time consumption and is, therefore, commonly used for prediction of fractions obtained by SCD (Foley et al. 1998; Pasquini 2003). A litter decomposability index (Gillon et al. 1999) and parameters of various C and N mineralization models (Bruun et al. 2005; Joffre et al. 2001) have been predicted from NIR, as well as plant biochemical fractions (Stenberg et al. 2004).

An alternative to chemical analysis (or to using NIR to predict such data) is to estimate litter pool partitioning by model fitting to measured C and N mineralization, as done by Breland and Eltun (1999) for SOM pools. Fitting partitioning parameters in this manner would make them kinetically defined according to the C and N mineralization trajectories observed for each plant residue. However, mineralization experiments are time-consuming and costly; hence, we need alternative predictors. One alternative would be to conduct a regression analysis of kinetically-defined partitioning parameters (dependent variable) against SCD-data. Another alternative is to use NIR spectra as prediction variables (by partial least square regression), thus circumventing a linkage to chemically-extractable plant components. To our knowledge, this approach has not been tested before.

There is an interdependency, however, between the residue-specific partitioning and global (shared) parameters such as decay rates of the litter pools and microbial biomass as well as the parameters governing the C/N stoichiometry of microbial reactions (microbial growth yield and C/N ratio of microbial biomass). By interdependency, we mean that the partitioning of plant residue C and N into litter pools to achieve correctly predicted C and N dynamics is

dependent on the global parameters used. Consequently, an estimation of residue-specific partitioning parameters by model fitting would benefit if the global parameters were adjusted simultaneously. To our knowledge no attempts have previously been made to perform a combined optimization of global and residue-specific parameters. Such a simultaneous optimization applying a large dataset would effectively search the parameter space for a set of global parameter values and individual pool partitioning for each plant residue, improving simulations for a wider range of plant residues, hence, increasing model precision and generality. However, with precision and generality as model objectives, realism is likely to be compromised (Levins 1966).

The use of global parameters for modeling decomposition of all plant residues implicitly assumes that the microbial communities involved in their degradation have identical characteristics (capacity for degrading specific compounds, growth yield, C/N ratio and decay rate) for all plant residues. This is not necessarily the case; plant residues could selectively enhance or inhibit different components of microbial communities, e.g., fungal or microbial growth, resulting in altered decomposition capacity, growth yields, and other biomass C/N ratios than that for the majority of plant compounds. The C and N mineralization patterns of such materials would be poorly predicted by the model, not so much because the litter pool partitioning is wrong but because the global parameter values are inadequate for these particular materials. Investigation of these individual plant materials could test if model performance would improve by changing the litter decay rates, microbial growth yield or biomass C/N ratio, implicitly testing if model inadequacy could be caused by selective stimulations of microbes with a different capacity for degradation and C and N assimilation than those degrading the majority of plant residues.

Our objective was to assess the performance of a two-litter-pool SOM model (Nitrosim) when the initial sizes of the litter pools were determined either as neutral detergent soluble (NDS) or by regression models of kinetically-defined litter pools. The latter implied estimating the litter pool partitioning parameters by model optimization on a comprehensive calibration dataset of C mineralization and N immobilization/mineralization from plant residues ($n=60$) and then selecting and evaluating the predictors based

on either SCD or NIR data. Predictors were either simple-linear, multiple-linear, or PLS (partial least squares) regression models. On an external validation dataset ($n=15$), we tested the hypothesis that the regressions of kinetically-defined litter pools would improve model performance as compared to the direct translation of NDS data to partitioning. We were also interested in finding out if data from NIR were better than SCD as regression model predictor variables.

A closely related objective was to investigate the improvements from simultaneously optimizing the residue-specific litter pool partitioning and the inter-related global parameters (litter pool decay rates and microbial growth yield and C/N ratio). We hypothesized that this approach would identify a set of global parameters that increases the number of crop residues for which Nitrosim can adequately simulate C and N mineralization. We further hypothesized that model inadequacy remaining after such simultaneous optimization could still be serious for certain residues, not due to inadequate litter pool partitioning but because the global parameters are inadequate. Therefore, in a search for potentially explanatory patterns related to microbial community structure, alternative values for the global and residue-specific parameters were investigated in exploratory optimizations using data of single outstanding residues.

Materials and methods

The data

We used published data from controlled experiments of a joint Nordic research project (Jensen et al. 2005). CO₂ evolution and mineral N ($N_{\min} = N-NH_4^+$ and $N-NO_3^-$) from 76 plant materials incubated in a sandy soil at 15°C were measured in triplicate at 14 and 8 occasions ($m=14$ for C and $m=8$ for N), respectively, over 217 days. Factors potentially influencing C and N mineralization, except for plant resource quality, were standardized. Details of the incubation, plant materials, and soil are described by Jensen et al. (2005). SCD was used to quantify C and N in the NDS, hemicellulose, cellulose and lignin fractions, and NIR spectra were recorded (Stenberg et al. 2004). The residues used were from plants commonly cultivated in Scandinavia. They covered a broad spectrum of plant residue qualities (SM Table 1),

implying that N mineralization patterns varied from long-term net immobilization from, e.g., stems of hemp and wheat, to rapid net mineralization, as seen for green leaves of turnip rape and winter rye. Patterns displaying immobilization followed by a mineralization were also represented (SM Figure 1). The plant materials were incubated in five different countries. We used the batch from Iceland as validation data ($n=15$ plant materials), which was, therefore, excluded from the optimization procedures. The remaining four incubation batches are referred to as the calibration dataset.

The Nitrosim model

Nitrosim is the soil organic matter decomposition submodel of the SPN (soil–plant–nitrogen) ecosystem model (Bleken et al. 2009), which is a refinement of the SOILN and SOILN_NO models (Johnsson et al. 1987; Vold et al. 1999). The ten variables describing the C and N pools are rapidly decomposing litter (litter 1: C_{L1} and N_{L1}), slowly decomposing litter (litter 2: C_{L2} and N_{L2}), microbial biomass (C_B and N_B), active humus (C_H and N_H), respired CO_2 (CO_2), and net mineralized N (N_{min}) (Fig. 1). The decomposition of the four pairs of C and N pools is defined by first-order decay rate constants: k_{L1} and k_{L2} for litter 1 and 2, k_B for the microbial biomass, and k_H for the active humus pool. It is assumed that the difference in decomposition rates observed for plant materials can be ascribed to a residue-specific partitioning of C and N between the two litter pools. All decay rates, the

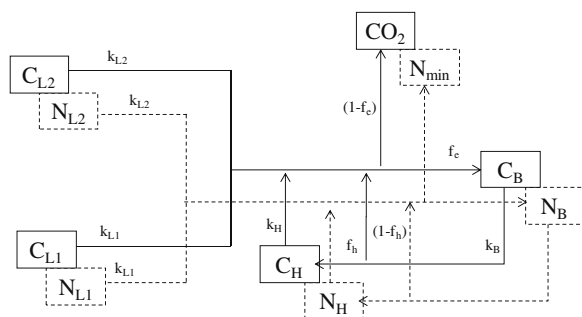


Fig. 1 Schematic presentation of the carbon (C) and nitrogen (N) flows in the Nitrosim model including state variables (*box*), their decay rates (k) and fractionation constants (f). L1 and L2: rapidly and slowly decomposing litter pools, B: microbial biomass, H: humus; CO_2 and N_{min} : mineralized products

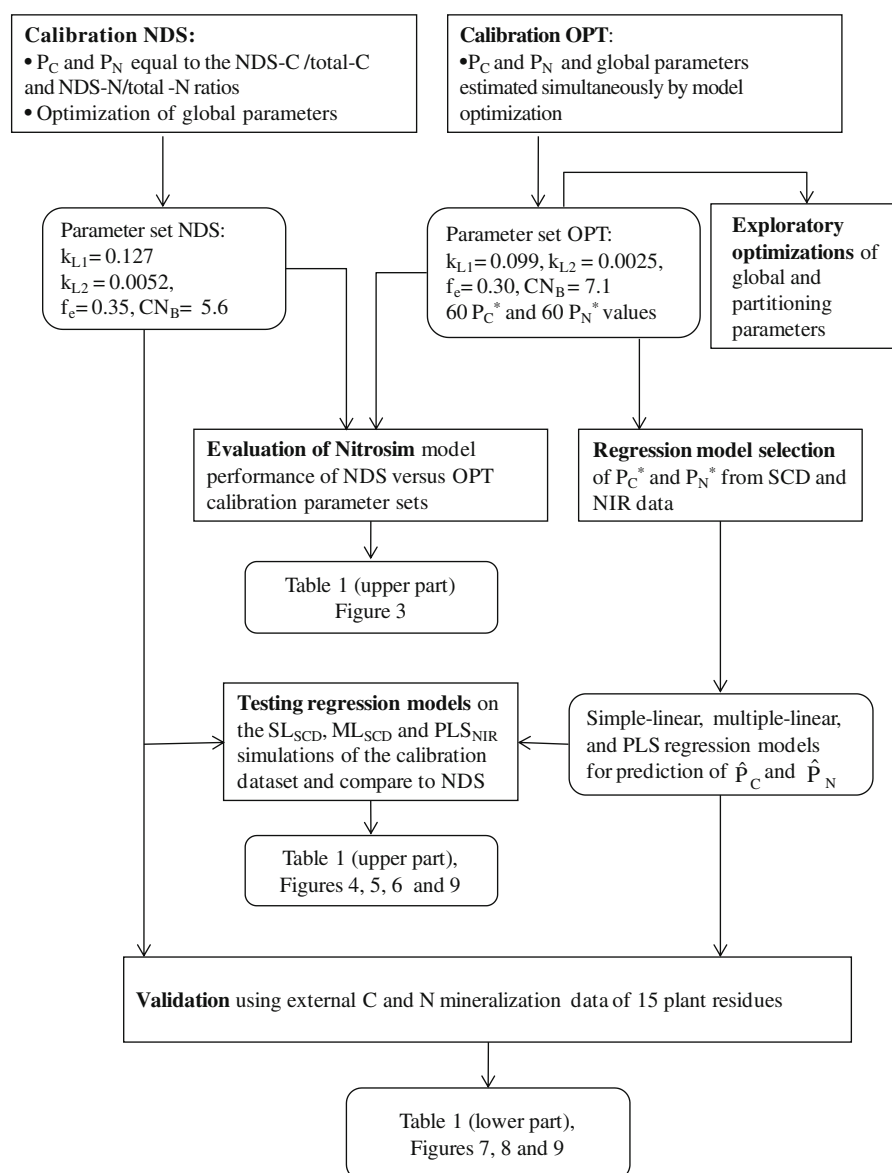
microbial growth yield (f_e , the fraction of decomposed C from litter and humus assimilated into microbial biomass) and the humus yield (f_h , the fraction of microbial biomass decay that is humified) are assumed to be independent of the litter input and are, therefore, referred to as global parameters. The N flows are proportional to the C flows by the C/N ratios of the litter pools and those of the microbial biomass and the humus pools (CN_B and CN_H , both constants). The decomposed N in excess of what is assimilated by microbial growth or humified, determines the net N mineralization. Although being mechanistic by nature, the model can be considered simplistic because it only has two residue-specific parameters, P_C and P_N , which define the fractions of total plant C and N inputs, respectively, assigned to the easily decomposable litter pools.

Calibration by optimization of global and residue-specific parameters

The relevant parameters of the decomposition model (k_{L1} , k_{L2} , f_e and CN_B) were optimized using the observed CO_2 and N_{min} of the calibration dataset ($n=60$; green leaves of lupine was removed due to unrealistic optimization). The default values for the global parameters were $k_{L1}=0.13 \text{ day}^{-1}$, $k_{L2}=0.004 \text{ day}^{-1}$, $k_B=0.002 \text{ day}^{-1}$, $k_H=0.000085 \text{ day}^{-1}$, $f_e=0.3$, $f_h=0.2$, $CN_H=10$, and $CN_B=5.6$. Net respiration and N mineralization caused by the added plant material only were estimated by subtracting the corresponding values from the control soil incubations (soil without plant amendments), thus eliminating the need for estimating the initial size of the microbial and humus pools, which were initialized as zero. For each material the initial N_{min} pool was determined by the mean of the measurements from the first sampling.

Two different Nitrosim calibrations were made depending on the litter pool partitioning method, which resulted in the two global parameter sets of k_{L1} , k_{L2} , f_e , and CN_B , referred to as NDS and OPT (Fig. 2). In the calibration NDS, the litter pool partitioning was based on NDS and the P_C and P_N parameters were equal to the fraction of total litter C and N in the NDS fraction and global parameters were estimated by model optimization giving the NDS parameter set (Calibration NDS, Fig. 2). In the calibration OPT, the P_C and P_N parameters were optimized simultaneously for each

Fig. 2 Illustration of the procedures (boxes) performed and outputs (rounded boxes) obtained from the calibration and optimizations, evaluation, testing and validation of the NDS-based litter pool partitioning, the kinetically-defined (optimized) partitioning, and the prediction of the optimized partitioning. The optimizations were made in two steps: first with respect to CO₂ evolution and then to net N mineralization/immobilization (for further detail, see the text). Global parameter sets consist of litter pool decay rate constants (k_{L1} and k_{L2}), microbial growth yield efficiency (f_c), and C/N ratio of the microbial biomass (CN_B). NDS: neutral detergent soluble, SCD: stepwise chemical digestion, NIR: near-infrared reflectance spectroscopy



plant material ($n=60$), with the global parameters resulting in the OPT global parameter set (Calibration OPT, Fig. 2). The optimized litter pool partitioning parameters are referred to as P_C^* and P_N^* where $*$ indicates that they are kinetically defined. All parameter values were estimated by least squares curve fitting of simulated to observed data (CO₂ and N_{min}) using the Levenberg-Marquardt optimization algorithm in MATLAB with a modified version of *leasqr* (by Shrager, Jutan and Muzic). It was possible to optimize for the global (shared) and the residue-specific parameter values simultaneously because each specific parameter affects only the output related to the data

of that one plant material. This also enabled us to use memoization (Norvig 1992) to speed up the optimization. We found it necessary to perform separate optimization steps against CO₂ and N_{min} . First, parameter values for the litter pool decay rates (k_{L1} and k_{L2}), the microbial growth yield (f_c), and for OPT also P_C were estimated by optimizing the model performance with respect to CO₂ emission. Secondly, the C/N ratio of the microbial pool (CN_B), and for OPT also P_N were estimated with respect to N_{min} data. The estimated values of the two global parameter sets are shown in Fig. 2. The resulting C and N mineralization simulations (NDS and OPT) were

evaluated by statistics of mean absolute errors and modeling efficiency (Evaluation of Nitrosim, Fig. 2)

Exploratory optimizations

In order to investigate the causes of remaining model failure after the simultaneous optimization (OPT), we conducted individual model optimizations for different global parameters (Exploratory optimizations, Fig. 2). We explored the consequences of assigning local (residue-specific) parameter scope to the global parameters (k_{L1} , k_{L2} , f_c , and CN_B) for selected materials as follows: i) litter pool decay rates (k_{L1} and k_{L2}) were assigned local scope for the residues with the largest model errors for C and N mineralization ($n=5$), also allowing P_C and P_N to be re-estimated, ii) microbial growth yield (f_c) was assigned local scope for all residues in the calibration data ($n=60$), while keeping P_C^* and P_N^* fixed, and iii) the C/N ratio of the microbial biomass (CN_B) was assigned local scope together with P_C and P_N for selected residues whose P_N^* was either 1 or 0 ($n=7$). Optimizations for k_{L1} , k_{L2} , and f_c explored the assumption that model failure was not due to an inappropriate litter partitioning, but instead caused by inadequate global parameter values, while optimizations for CN_B additionally sought explanations for unrealistically optimized P_N^* values.

Predictors of the kinetically-defined litter pool partitioning: selection of regression models

To find general predictors of the kinetically-defined litter pool partitioning parameters P_C^* and P_N^* the relationships between them and potential litter quality descriptors, such as C and N in the SCD fractions and NIR data were investigated. We built cross-validated simple-linear, multiple-linear, and PLS regression models and selected the best one for each of the three regression procedures (Regression model selection, Fig. 2).

We observed that the best results were obtained when quantities of C and N in litter (mg C or N g^{-1} plant DM, calculated as $C_{L1}^* = P_C^* \times C_{TOT}$ and $N_{L1}^* = P_N^* \times N_{TOT}$) rather than the actual optimized fractions, were used as the dependent variables in the regression models. The quantity estimated by the three regression models, referred to as \hat{C}_{L1} and \hat{N}_{L1} , together with measured total C and N (C_{TOT} and N_{TOT}) in each residue, were used to calculate the predictions of the

kinetically-defined litter pool partitioning parameters \hat{P}_C and \hat{P}_N . In the process, values outside the range of 0–1 occurred for a few residues, and these were truncated to zero or one.

The performance of the simple-linear, multiple-linear and PLS regression models was tested on the calibration dataset (Testing regression models, Fig. 2) in order to evaluate the loss of information connected to the regression procedures. The Nitrosim simulations using the three regression models for prediction of the kinetically-defined pool partitioning are referred to as SL_{SCD} , ML_{SCD} , and PLS_{NIR} . We applied the same statistics as for the Nitrosim evaluation and the validation procedure (see below).

Simple- and multiple-linear regression models based on SCD fractions

Model combinations were constructed using all available SCD fractions (C and N in NDS, hemicellulose, cellulose and lignin and total). Simple-linear models with one independent variable and multiple-linear models with several independent variables were selected based on the highest coefficient of determination (R^2). Further criteria for selection were $p \leq 0.05$ for all variables included in the model and Mallows' C_p , as computed by Proc Reg with the SAS software (SAS Institute Inc 1989). Because of the collinearity between the variables, we decided to limit the number of independent variables to a maximum of three in the ML models. The best models were fully cross-validated (a leave-one-out approach) using MLR in Unscrambler® software, which gave the final models.

Partial least squares regression models based on NIR

Partial least squares (PLS1) analyses were performed in Unscrambler, to construct regression models for estimation of the kinetically-defined partitioning parameters, P_C^* and P_N^* , from NIR data. To avoid jeopardizing model robustness, we used only the 1100–2500 nm range of the NIR (Bruun et al. 2005). The spectra were transformed from the measured reflectance (R) into absorbance by $A = \log(1/R)$. To smooth the spectra and minimize the effects of nonspecific scatter, we further transformed the data taking the Savitzky-Golay second derivative by fitting the spectra to a second-order polynomial function with four (2nd4) and eight (2nd8) adjacent points on

both sides. Fully cross-validated models with a maximum of ten PLS components were run using the three data formats (un-transformed, 2nd4, and 2nd8). The best models for \hat{C}_{L1} and \hat{N}_{L1} were chosen for the Nitrosim simulation (PLS_{NIR}) by selecting the number of PLS components giving rise to the lowest standard error of prediction (SEP), which is calculated as the standard deviation of the residuals.

External validation of NDS and regression model predictions of kinetically-defined partitioning

To compare NDS-based partitioning with regression models predicting the kinetically-defined pool partitioning, we used a validation dataset ($n=15$) consisting of samples incubated in Iceland (Validation, Fig. 2). The statistics applied were the same as for the evaluation of the simultaneous optimization, the testing regression models, and the external validation. The Nitrosim simulations using regression models to predict the litter pool partitioning are referred to as SL_{SCD}, ML_{SCD}, and PLS_{NIR}.

Evaluation statistics for decomposition model performance of simulated C and N mineralization

Nitrosim performance was evaluated for the five simulation runs (OPT, NDS, SL_{SCD}, ML_{SCD}, and PLS_{NIR}) by calculating the mean absolute error MAE (1.1) and the modeling efficiency EF (1.2) for all plant materials:

$$MAE = \frac{\sum_{i=1}^N |y_i - \hat{y}_i|}{N} \quad (1.1)$$

$$EF = \frac{\sum_{i=1}^N (y_i - \bar{y})^2 - \sum_{i=1}^N (y_i - \hat{y}_i)^2}{\sum_{i=1}^N (y_i - \bar{y})^2} \quad (1.2)$$

Where y_i is the i 'th of the N observations ($N = m \times n$, $n=60$ and 15 plant materials in the calibration and validation datasets, and $m=14$ and 8 sampling occasions of CO₂ and N_{min}, respectively), \hat{y}_i is the corresponding values predicted by the Nitrosim model, and \bar{y} is the average of the observed values. MAE values were also calculated for the individual plant materials ($N = m$).

Frequentist statistics based on hypothesis testing and P values have been criticized for being poor

criteria for selection of ecological models because of the inherent stochasticity, scale-dependency, and nonlinearity of the systems under study (Burnham and Anderson 2002; Hastings et al. 2005). In model evaluation, elements of information theory can be implemented by AIC (an information criterion) to extract and separate information from noise (Akaike 1973). AIC of the j 'th model (or simulation run) was calculated in R software and according to Burnham and Anderson (2002) as

$$AIC_j = N \ln \left(\frac{1}{N} \sum_{i=1}^N (y_i - \hat{y}_i)^2 \right) + 2K,$$

where $K=2$ and is the number of free parameters. The Akaike weights w_j that quantify the probability that simulation model j ($j = 1, 2, \dots, J$) is best among the J models tested, were calculated as

$$w_j = \frac{e^{-\Delta AIC_j/2}}{\sum_{j=1}^J e^{-\Delta AIC_j/2}},$$

with the relative AIC differences (ΔAIC_j) being $\Delta AIC_j = AIC_j - AIC_{\min}$ and AIC_{\min} is the smallest AIC value. Due to its obvious advantage, the OPT model was not included; hence, $J=4$.

Results

Model performance by simultaneous optimization for global and residue-specific parameters

The improvement in model performance from the simultaneous optimization of global and residue-specific parameters was considerable compared to optimization of global parameters only. This is seen in higher EFs and ~50% reduction of MAE both for C and N mineralization (Table 1). The improved performance from OPT was partly due to an effective reduction of a systematic over-estimation of N-mineralization during the early phase and an underestimation during the late phase of the incubations (results not shown). Also, for C mineralization the OPT calibration removed most of the temporal bias by eliminating the initial underestimation. The systematic bias visible in the plot of observed versus predicted values was reduced; the regression lines cohered around the 1:1 line of perfect agreement (OPT, Fig. 3). Especially for N, the regression lines were no longer significantly different from the bisect.

Table 1 Evaluation, testing and validation statistics of Nitrosim simulations of C mineralization and net N mineralization/immobilization applying different litter pool partitioning: measurable neutral detergent soluble C and N (NDS), simple-linear (SL_{SCD}), multiple-linear (ML_{SCD}), or PLS (PLS_{NIR}) regression models, or optimization (OPT). The three regression were based on either stepwise chemical digestion (SL_{SCD} and ML_{SCD}) or near infrared reflectance spectroscopy (PLS_{NIR}) data

for prediction of the kinetically-defined (optimized) pool partitioning. The ‘OPT’ of validation simulation used the global parameter set OPT (see Fig. 2) and optimized pool partitioning. For each model simulation, the relative AIC (Δ AIC), Akaike weights (w), modeling efficiency (EF), and mean absolute errors (MAE mg C or N kg⁻¹ soil) calculated over N ($N = m \times n$, with m sampling times and n plant residues) are reported

Simulation	C mineralization				N mineralization			
	Δ AIC	w	EF	MAE	Δ AIC	w	EF	MAE
Calibration data ($n=60$)								
NDS	9446	1E-39	0.84	478	3581	1E-85	0.66	68
SL _{SCD}	9448	4E-40	0.87	430	3258	2E-15	0.83	45
ML _{SCD}	9267	1E+00	0.89	396	3190	1E+00	0.84	44
PLS _{NIR}	9396	1E-28	0.88	411	3279	4E-20	0.80	49
OPT	§	–	0.96	233	–	–	0.92	29
Validation data ($n=15$)								
NDS	2306	4E-27	0.860	455	877	5E-27	0.40	61
SL _{SCD}	2275	2E-20	0.861	457	785	6E-07	0.71	43
ML _{SCD}	2272	9E-20	0.87	448	756	1E+00	0.64	46
PLS _{NIR}	2184	1E+00	0.90	393	794	5E-09	0.65	50
‘OPT’	–	–	0.98	193	–	–	0.87	26

§ Δ AIC and w are not presented for the optimized model as it is obviously the best

Compared to calibration NDS, calibration OPT resulted in lower decay rates of $k_{L1}=0.099 \text{ day}^{-1}$ and $k_{L2}=0.0025 \text{ day}^{-1}$, and microbial growth yield of $f_c=0.30$, but an increase in the C/N ratio of the microbial biomass to 7.1 (Fig. 2). The kinetically-defined partitioning assigned more C and less N to the rapidly decomposing pool (litter 1) than measured as NDS. Mean values of the optimized fraction parameters ($P_C^*=0.54$ and $P_N^*=0.44$) were 30 % larger for P_C but 46 % smaller for P_N than the measured NDS fractions ($P_C=0.47$ and $P_N=0.82$). The C/N ratios of the optimized litter 1 pool varied much more (20th percentile, median and 80th percentile: 19, 32 and 152) than the NDS-C/NDS-N ratios (same statistics: 10, 18 and 28). Consequently, the optimized slowly decomposing pool (litter 2) had lower C/N ratios (same statistics: 9, 37, 90) than measured by SCD (same statistics: 42, 140, 267). The P_N^* values differed more than P_C^* values, hence, the relative improvement potential in model performance was greater for N than for C mineralization (Table 1), which is also seen from the relative distance between NDS and OPT in the cumulated frequency plots of individual mean absolute errors (Figs. 4 and 5). For six plant materials [barley spikes

(SP), elephant grass, wheat green leaves (GL) 2, wheat stems (ST) 2, 4 and 5] the optimization assigned all N to the slowly decomposing litter pool (i.e., $P_N^*=0$, SM Table 2). Measured NDS-N fractions of these residues were between 0.67 and 0.91 (SM Table 2) indicating that the P_N^* estimates were somewhat unrealistic. However, they all had small N contents (<3 % N except for elephant grass with 13% N). Consequently, large model errors were not observed (SM Table 3).

Exploratory optimizations finding alternative parameter values for outlying plant residues

Although the simultaneous optimization of litter pool partitioning and global parameters (OPT) resulted in good agreement between simulations and measurements for a majority of plant residues, large model errors (MAE>700 mg C kg⁻¹ soil) still occurred for green leaves (GL) of barley and wheat spikes (SP) no 2, which showed a substantially underestimated C mineralization (SM Figure 1 and SM Table 3). Decreasing k_{L1} to 0.03 significantly reduced the errors for both residues (e.g. from 1100 to 350 mg C kg⁻¹ soil for wheat SP 2) and eliminated the pattern of

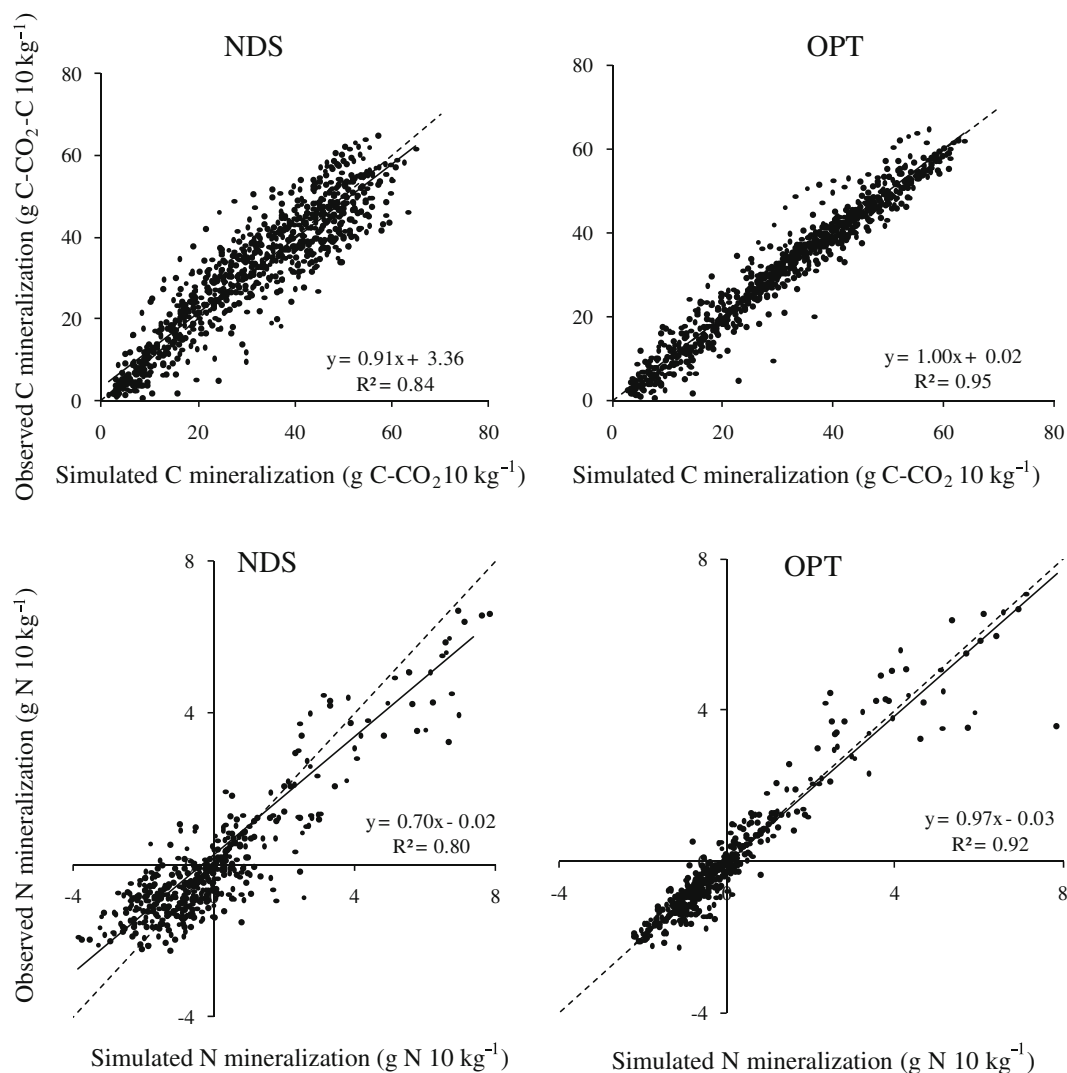


Fig. 3 Observed versus simulated C mineralization (*top*) and net N (*bottom*) mineralization/immobilization (negative values means net N immobilization) illustrating the improvement achieved by simultaneous optimization of global (litter pool

decay constants, microbial biomass C/N ratio and growth yield efficiency) and litter-specific pool partitioning (OPT) compared to optimization of global parameters only and litter pool partitioning from measured NDS neutral detergent soluble C and N (NDS)

initially overestimated CO₂ evolution followed by underestimation for both residues (results not shown). Green leaf materials of rape, turnip rape and winter rye displayed a rapid onset of a substantial net N mineralization, which was not captured by the model (SM Figure 1). The large model errors (MAE > 90 mg N kg⁻¹ soil) could be substantially reduced (by 30, 26 and 33%) by nearly doubling k_{L1} to 0.18 day⁻¹ and reducing k_{L2} to 0.0014 day⁻¹. The partitioning parameters for none of these five residues reached the boundary values of 0 and 1, and the re-estimated partitioning gave equally plausible values.

Using P_C^* and P_N^* and the global parameters OPT except for the microbial growth yield (f_c), we assigned local (residue-specific) parameter scope to f_c and optimized using the whole calibration dataset. No substantial improvement was found in overall model performance when evaluated on CO₂ evolution output, nor did the parameter estimates differ much from the initial values (results not shown).

More realistic P_N values were obtained for the four residues (maize ST 3 and 4, cabbage GL, and sunflower straw) for which P_N^* was one, by increasing CN_B from 7.1 to 15. Especially for the maize stems,

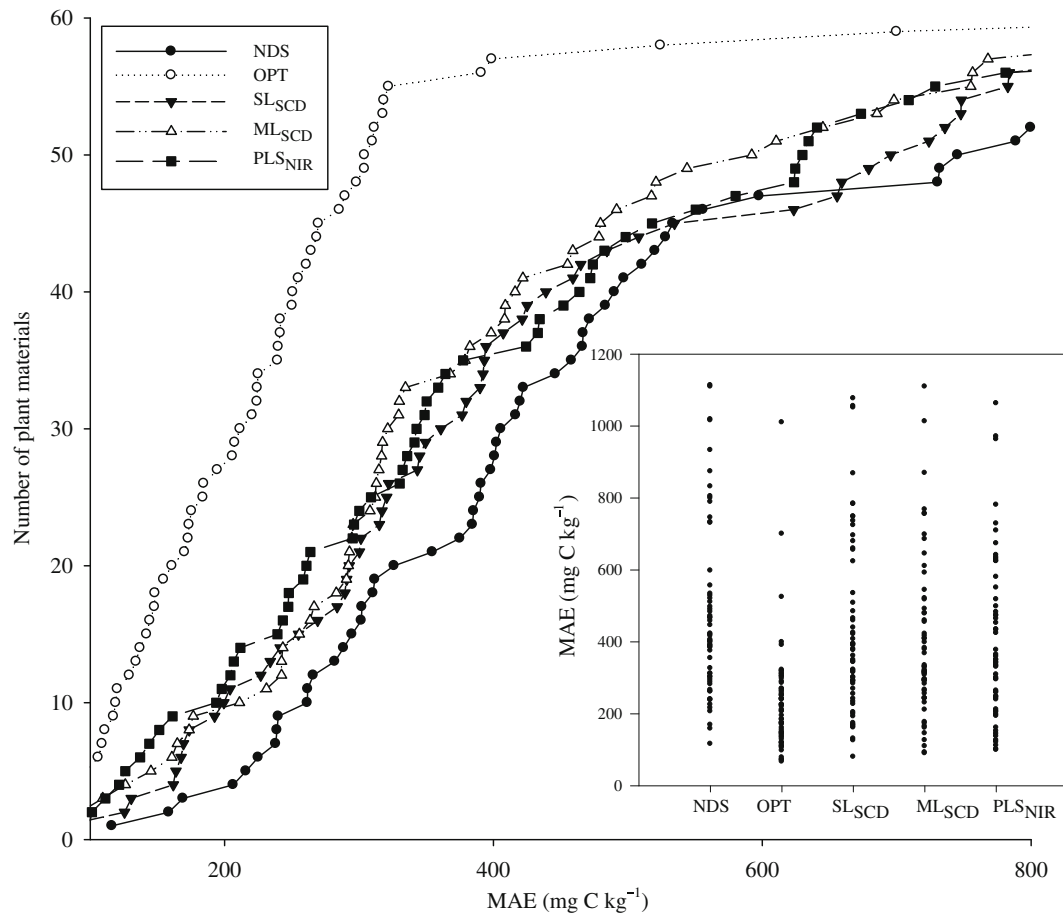


Fig. 4 Cumulative frequency of the mean absolute errors for simulated C mineralization (mg C kg^{-1}) of individual plant materials ($n=60$) for the calibration dataset from simulations OPT, NDS, SL-SCD, ML-SCD, and PLS_{NIR}. Only errors <800 mg

C kg^{-1} are shown: larger errors can be seen in the inserted plot, showing the clusters of mean absolute errors. See Table 1 for explanation of the simulations

model performance was significantly improved ($\sim 60\%$) and the overestimated initial net N immobilization reduced. Cabbage GL and sunflower straw displayed more erratic mineralization patterns; consequently, model improvements were smaller. The unrealistic P_N^* values of zero were corrected to 0.78 (elephant grass), 0.38 (wheat GL 2) and 0.28 (rape ST 2) when reducing CN_B from 7.1 to 5. Model errors increased slightly for elephant grass and rape ST, but for wheat GL MAE was reduced by 44 %.

Selection of the regression models based on SCD or NIR data

The cross-validated regression models for prediction of the kinetically-defined partitioning parameters gave similar correlation coefficients between

predicted and optimized values; for carbon $r=0.81$, 0.87, 0.84 and for nitrogen $r=0.93$, 0.94, 0.89, for the simple-, multiple-linear and PLS models, respectively. No single model was clearly better than others; however, standard error of prediction was smallest for the multiple-linear model (SM Table 4). The cross-validated simple regression models $\hat{C}_{L1} = 0.67C_{NDS} + 99.8$ and $\hat{N}_{L1} = 0.658N_{TOT} - 2.1$ predicted the optimized partitioning parameters well. All units are mg C or N g^{-1} DM. \hat{N}_{L1} could equally well be predicted from NDS-N. The cross-validated multiple regression models were $\hat{C}_{L1} = 0.52C_{NDS} + 1.14N_{NDS} - 0.54C_{TOT} + 358.5$ and $\hat{N}_{L1} = 0.703N_{NDS} - 4.3N_{LIGN} + 0.29$. Red clover was excluded in both \hat{N}_{L1} models because of its high leverage. The best PLS models were for C based on the untransformed NIR spectra and nine PLS components,

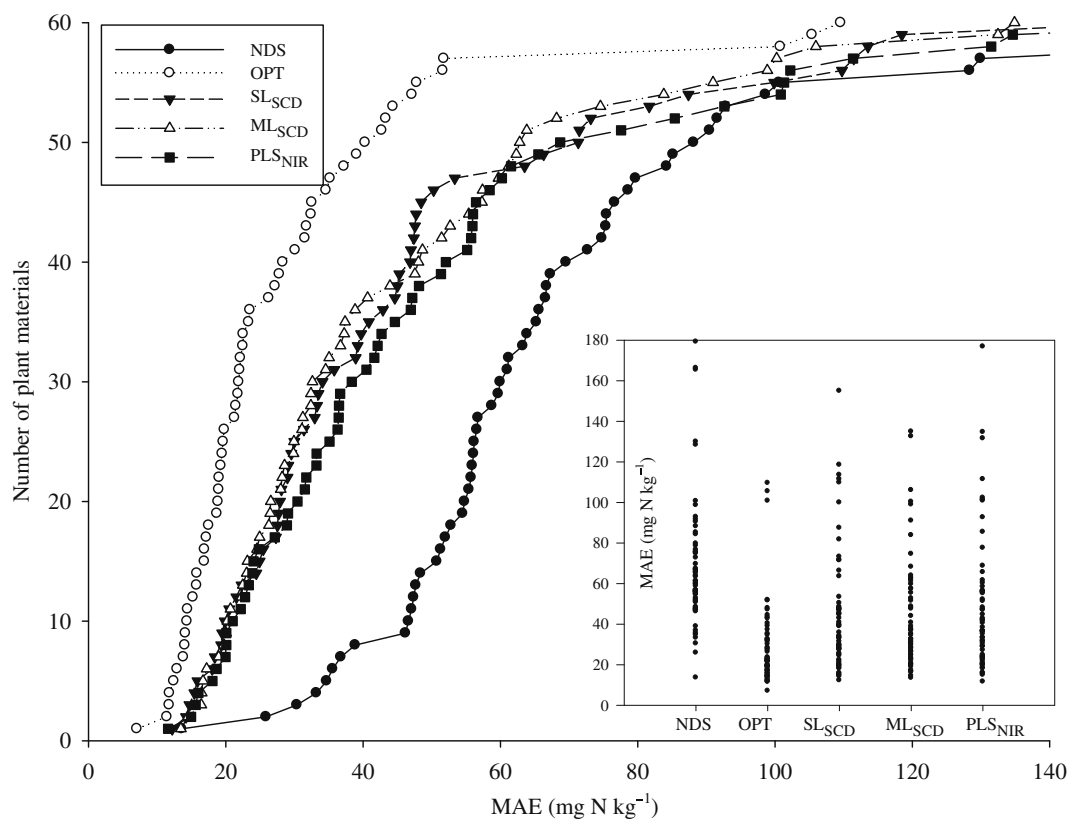


Fig. 5 Cumulative frequency of the mean absolute errors for simulated net N mineralization/immobilization (mg N kg^{-1}) for individual plant materials ($n=60$) in the calibration dataset from simulations OPT, NDS, SL_{SCD} , ML_{SCD} , and PLS_{NIR} . Only

errors $<140 \text{ mg N kg}^{-1}$ are shown: larger errors can be seen in the inserted plot, showing the clusters of mean absolute errors. See Table 1 for explanation of the simulations

and for N on the 2 + 8 transformed NIR spectra and six PLS components. Predictions were of similar accuracy using either spectra transformation (SM Table 4). But the spectral transformation increased the number of negative predictions of \hat{N}_{LI} giving 5, 6, and 7 for the untransformed, 2+4, and 2+8 NIR spectra, respectively (SM Table 4). The best PLS model yielded one $\hat{P}_{\text{C}} > 1$ and seven $\hat{P}_{\text{N}} < 0$ (SM Table 2). The simple- and multiple-linear models gave three and one negative \hat{P}_{N} values, respectively, but not for the same residues. When the predictors were used for the validation dataset, two residues, barley ST 2 and maize ST 5, obtained negative \hat{P}_{N} values by the multiple-linear and PLS models, but not for the simple-linear model.

Testing and comparing the regression models for prediction of kinetically-defined litter pools

The temporal bias seen for the NDS calibration simulation was practically eliminated by the SL_{SCD} ,

ML_{SCD} , and PLS_{NIR} simulations, where the residuals were close to zero after 50 days, especially for N but also for C (Fig. 6). However, there were no marked differences in model errors for individual plant residues between the simulations using the regression models neither for C (Fig. 4) nor net N mineralization (Fig. 5), and the plots of the observed versus predicted values were not statistically different from the bisect for any of the simulations (SM Figures 2 and 3).

Validation of the NDS and kinetically-defined litter pool partitioning methods

When regression models were used to predict the optimized litter pool partitioning, the ability of Nitrosim to simulate C and N mineralization for the validation dataset was improved as compared to simulations using NDS-based partitioning (Table 1; SM Fig. 4).

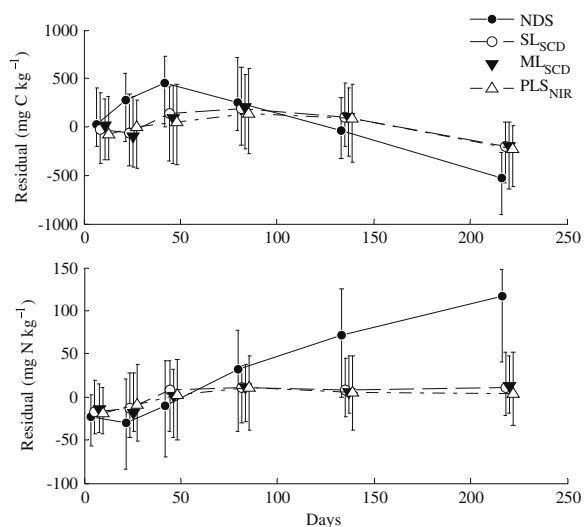


Fig. 6 Distribution of the calibration residual errors ε (C or N kg^{-1} , $\varepsilon = \text{observed} - \text{simulated}$) for C mineralization (top) and net N mineralization/immobilization (bottom) over time from simulations NDS, SL_{SCD} , ML_{SCD} , and PLS_{NIR} . See Table 1 for explanation. Lines join the medians and vertical line join the 20th and 80th percentile. Model simulations have been slightly displaced along the x-axis and the first observation day has been omitted in order to make the figure more legible

Simulated CO_2 evolution

For the NDS validation simulation, the temporal trend of residuals showed an overestimation of early (<50 days) C mineralization followed by an underestimation in the late phase (>150 days; Fig. 7). Among the regression models tested, only the PLS_{NIR} simulations showed an underestimation between 80 and 200 days, which was not seen in the calibration dataset (Fig. 6). To evaluate the overall model performance using different litter pool partitioning methods, we listed various model-performance indicators in Table 1, both for the calibration and the validation datasets. The NDS simulations received the largest validation AIC value but the Akaike weights gave similar probabilities of support to SL_{SCD} and ML_{SCD} compared to NDS (Table 1). The best simulation using regression models was PLS_{NIR} and, compared to NDS, it reduced overall MAE values by 13% and modeling efficiency (EF) was slightly improved from 0.86 to 0.90 (ibid). Further inspection of the cumulated frequency plotted against MAE showed that the advantage of PLS_{NIR} over NDS occurred from reduction in the smaller error values (Fig. 8). For comparative reasons, we included the

simulations ‘OPT’ for which the litter pool partitioning was optimized and the global parameter set OPT was applied (also included in Table 1). Reductions in the number of large errors (>600 mg C kg^{-1} soil) were also reduced from six in NDS to two (ML_{SCD}), three (SL_{SCD}), and four (PLS_{NIR}) for the kinetically-defined pool partitioning (SM Table 3).

Simulated N mineralization

The validation showed a noticeable improvement in simulated net N mineralization by SL_{SCD} , ML_{SCD} and PLS_{NIR} compared to the NDS simulation, as indicated most clearly by the larger EF (range 0.64–0.71 versus 0.40) and smaller mean absolute errors (range 43–50 versus 61 mg N kg^{-1} ; Table 1). The advantage of the kinetically-defined partitioning over the NDS-based one was more pronounced for N than for the C simulations. All Akaike weights for the SL_{SCD} , ML_{SCD} , and PLS_{NIR} simulations were larger than for the NDS simulation (Table 1), lending support to the kinetically-defined partitioning predicted by the regressions models. Mean absolute errors for individual residues using NDS were all larger than 40 mg N kg^{-1} , and the

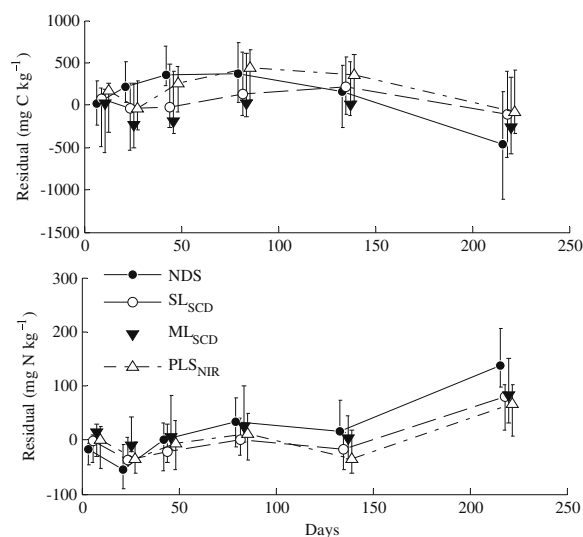


Fig. 7 Distribution of validation residual errors ε (C or N kg^{-1} , $\varepsilon = \text{observed} - \text{simulated}$) for C mineralization (top) and net N mineralization/immobilization (bottom) over time from simulations NDS, SL_{SCD} , ML_{SCD} , and PLS_{NIR} . See Table 1 for explanation. Lines join the medians and vertical line join the 20th and 80th percentile. Model simulations have been slightly displaced along the x-axis and the first observation day has been omitted in order to make the figure more legible

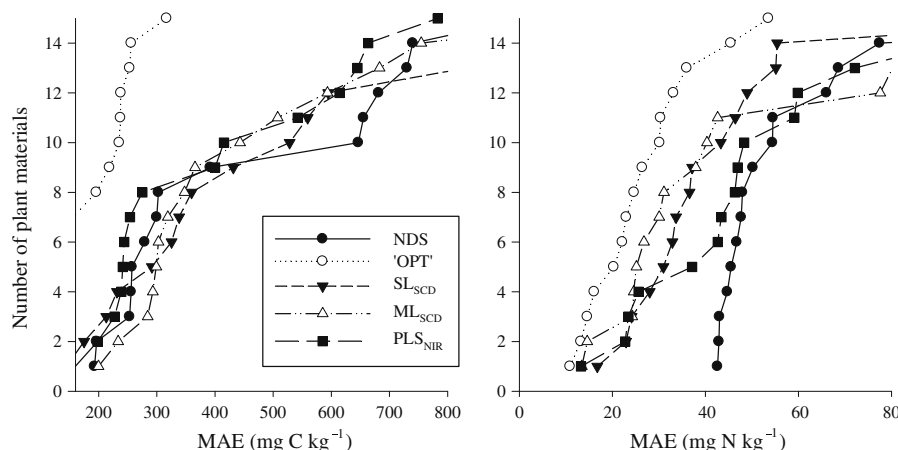


Fig. 8 Cumulative frequency of the mean absolute errors (MAE) for simulated C mineralization (*left*) and net N (*right*) mineralization/immobilization (mg C or N kg^{-1}) of individual plant materials ($n=15$) for the validation dataset from

simulations NDS, 'OPT', SL_{SCD} , ML_{SCD} , and PLS_{NIR} (See Table 1 for explanation). Only errors >160 and $<800 \text{ mg C kg}^{-1}$ or $<80 \text{ mg N kg}^{-1}$ are shown. Symbols in box apply to both figures

smallest MAE values for SL_{SCD} , ML_{SCD} , and PLS_{NIR} were reduced by approximately 50% compared to the errors from the NDS simulation (Fig. 8, SM Table 3). Both the temporal and the systematic biases were reduced by the regression model prediction of the kinetically-defined partitioning compared to the NDS-based partitioning (Figs. 7 and 9).

Discussion

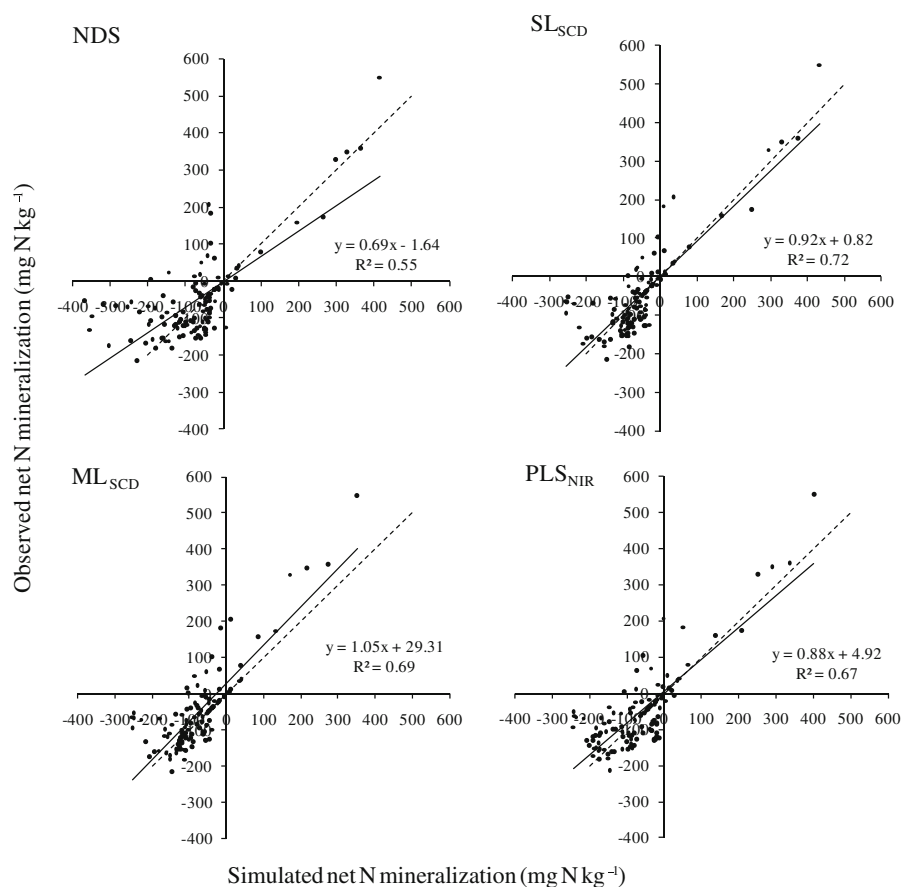
Plant litter pools defined kinetically or measured as NDS

Evaluated on an external validation dataset, our results supported the hypothesis that kinetically-defined partitioning improves the performance of the mechanistic model compared to partitioning according to NDS fractions. Underestimation of initial CO_2 emissions for plant residues with small N contents, which was also seen in CENTURY modeling (Parton et al. 1994), existed in our simulations with using the NDS-based partitioning. This was avoided in the simulations applying the proposed regression models for prediction of the kinetically-defined litter pool partitioning parameters (Fig. 7). Using the kinetically-defined partitioning removed the temporal bias of initial overestimated net N mineralization as seen when using NDS-based partitioning (Fig. 7). This is an important advantage when applying models as a

management tool for improving the N dynamics of agricultural systems. The noise introduced by the regression models almost doubled the model errors as compared to the optimized partitioning parameters (P_C^* and P_N^*), even for the calibration data. Nevertheless, the model performance based on external predictor variables, i.e., SCD and NIR for the litter pool partitioning, was quite satisfactory, possibly due to the major reduction in overall model error by the simultaneous optimization.

In Nitrosim, the estimated partitioning of residue N into the two litter pools was not necessarily proportional to that of residue C; i.e., for each residue, the C/N ratio of the litter pool could be very different from each other. The optimization procedure generally assigned more C (average increase 30%) and remarkably less N (average decrease 46%) to the rapidly decomposing pool than what was measured as NDS. As a result, the C/N ratio of the kinetically-defined litter 1 pool varied much more than the NDS-C/NDS-N ratio. For litter 2, the kinetically-defined C/N ratio was much lower than the NDS-based one. It is likely that the C/N ratios of the kinetically-defined litter pools contributed to the correction of the temporal bias of N mineralization. However, this temporal bias could also reflect a gradual change of the microbial biomass throughout the course of plant residues decomposition, as indicated by Henriksen and Breland (1999a). If so, the estimated C/N ratios are essentially erroneous, and the predictions of N

Fig. 9 Observed versus simulated net N mineralization/immobilization of the validation dataset ($n=15$) using measured NDS-C and NDS-N directly for litter pools partitioning, and simple-linear, multiple-linear, and PLS regression models for prediction of the kinetically-defined litter pool partitioning, respectively, for simulations SL_{SCD} , ML_{SCD} , and PLS_{NIR} . See Table 1 and text for further explanation. NDS: neutral detergent soluble



mineralization kinetics are thus reasonably good for wrong reasons. An alternative could be to diversify the microbial biomass into a litter 1-consuming pool having a low C/N ratio and a litter 2-consuming pool having a higher C/N ratio (Henriksen and Breland 1999b). This would contribute to removing the temporal bias in N mineralization simulated with NDS-based partitioning and would also take account of a possible interaction between residue C/N ratio and biomass C/N ratio (see the discussion of basic model assumptions below). A similar approach was found successful by Petersen (2007) but was abandoned for practical reasons when implementing the module in more comprehensive ecosystem models.

Choice of regression model for prediction of kinetically-defined litter pool partitioning

The simplest statistical models, SL, gave similar reductions in mean absolute errors of N mineraliza-

tion for both the calibration (33%) and validation (30%) data, whereas for C, only a 10% reduction for the calibration dataset was seen (Table 1). For both C and N mineralization, no noticeable advantage was seen by using a multiple- instead of simple-linear regression model. Hence, including NDS-N and total C in addition to NDS-C for prediction of \hat{P}_C did not improve model performance. We found total N to be as good as NDS-N for prediction of \hat{P}_N , which supports the many studies relating net N mineralization primarily to total N concentration or the C/N ratio (Janssen 1996; Kumar and Goh 2003). However, a retarding effect of lignin on N release is well documented and lignin quality, i.e. level of condensation and monomers, has been proposed to explain the difference in decomposition rates (Berg and McClaugherty 2008; Bertrand et al. 2006). In our study, there was no reduction in the errors of the simulated mineralization of the materials high in lignin-N ($>1 \text{ mg g}^{-1}\text{DM}$) when adding the lignin N

variable to the regression model. We conclude that lignin does not need to be considered for estimation of the kinetically-defined N litter pools of common agricultural plant residues. Application of the SL regression model proposed here requires plant residue analysis of NDS-C and total N. Although extraction of NDS-C is less demanding than the extraction of all SCD fractions, it is costly and much less likely to be routinely applied for modeling than NIR analysis.

Generally, NIR analysis produce more precise and repeatable measurement than wet chemistry (Shepherd et al. 2005). Although in the validation, the NIR simulation was slightly better than SL and ML for prediction of C mineralization, improvements were marginal and for N mineralization, NIR performed slightly poorer than the other two regression models. There was no obvious relationship between plant biochemical compositions and large model errors from the NIR simulation. This study confirmed the well-established ability of NIR to predict plant composition and related decomposition model parameters (Bruun et al. 2005; Foley et al. 1998; Shepherd et al. 2005; Stenberg et al. 2004). Considering the time and cost efficiency of NIR analysis, our results advocate the use of NIR as a standard procedure for litter pool partitioning of SOM models.

Validity of basic model concepts and parameter values for modeling soil C and N turnover

There are three implicit assumptions in modeling plant residue mineralization by a two-litter-pool model optimized on global parameters and residue-specific pool partitioning: 1) plant residue decomposability can be expressed by two components each having the same decay rate for all plant materials, 2) microbial growth yield is unaffected by the quality of carbon substrate and process rate, and 3) the C/N ratio of the active microbes is unaffected by substrate quality (unless N assimilation is limited by available mineral N in soil). These assumptions appeared acceptable for a majority of the plant materials, except for a few outlying residues as presented in the exploratory optimizations. For these plant residues, the exploratory optimizations could tentatively identify the cause of model failure as either an altered decay rate for the easily decomposable litter fraction (k_{L1} reduced for wheat SP 2 and barley GL and

increased for green leaves of rape, turnip rape and winter rye), or as an altered C/N ratio of the biomass (CN_B increased from 7 to 15 for maize stems and decreased to 5 for wheat GL 2). These alternative k_{L1} and CN_B values for individual plant residues are within a realistic range, but they should be taken as hypothetical explanations for model failure, which would require further experimental testing. In contrast, the exploratory optimizations did not identify the global microbial growth yield ($f_c=0.3$) as a cause of model failure for any of the plant residues. This indicates that the growth yield was practically unaffected by the residue qualities tested, legitimizing the use of a common growth yield for all substrates. This notion is supported by experimental evidence; a recent study showed that microbial communities sourced from lignified and herbaceous soil habitats, were found to decompose low- and high-quality litter with similar apparent growth yield (Strickland et al. 2009). Moreover, soils with different fungal/bacterial biomass ratio were found to decompose glucose with similar apparent growth yield (Thiet et al. 2006).

In summary, the exploratory simulations suggested that a few plant residues deviated from the rest by selectively stimulating microbes with either a high C/N ratio (15, presumably dominated by fungi) or a low C/N ratio (5, presumably dominated by bacteria), whereas the effective growth yield (as modeled) was very similar for all plant residues. Our value for microbial growth yield was 0.30, which is lower than the range 0.45–0.60 applied in many other models (Corbeels et al. 1999; Corbeels et al. 2005; De Neergaard et al. 2002; Henriksen et al. 2007; Mueller et al. 1997; Parton et al. 1987). There is no real conflict here; however, since the effect of f_c on the simulated C and N mineralization during residue decomposition depends on the decay rate of the biomass (higher biomass decay rates would demand higher f_c values). The values of the biomass decay rate (k_B) of the cited papers are substantially higher than our relatively low value of 0.002 day^{-1} . We can tentatively identify two alternative calibration regimes here, one operating with low f_c and k_B values and one with high f_c and k_B values. The latter has been chosen by many authors to comply with measured microbial biomass, but this tends to underestimate initial net N mineralization and overestimate late N mineralization during litter decomposition (De Neergaard et al. 2002). A solution to reducing this temporal bias in

simulated biomass and net N mineralization has been to introduce a biomass pool with a lower decay rate (Henriksen and Breland 1999b), or a pool of temporarily protected biomass residues (Mueller et al. 1997). Our lower values for this parameter set (f_c and k_B), appears to achieve reasonable N dynamics for the great majority of plant residues (including those with high C/N ratios) without such complicating elements. The implication of this parameter set is, however, that simulated biomass is much higher than that normally measured by chloroform fumigation or microscopy.

Due to the relatively short incubation period we did not calibrate the humification coefficient ($f_h=0.2$ was used), which regulates the fraction of decaying biomass transferred to the stable humus pool ($k_H=8.5\times 10^{-5}$). We investigated the sensitivity of the model output to changes in this parameter. Adjusting f_h up or down by 50 % had a negligible effect in model errors of approximately 1% of MAE for CO_2 and <1 % for N (result not shown). The fact that model performance was insensitive to changes in f_h is of practical importance because it allows adjustment of this parameter against long-term soil C and N data without deteriorating its ability to predict short term C and N dynamics.

The experiments simulated were planned so as to ensure ample mineral N contents of the soils throughout the incubations. Thus, microbial N assimilation was never limited by mineral N, and phenomena evoked by N limitation of microbial growth were never encountered. Consequently, it would be meaningless in our case to introduce N limitation feedbacks on the decomposition rates as suggested by Manzoni and Porporato (2007) and implemented in the model of Henriksen and Breland (1999b). This is not to say that we deny that such phenomena occur, only that they would not occur in our experiment.

Conclusions

The combined determination of litter pool partitioning and interrelated global parameters effectively identified a set of global parameters by which the C mineralization and N immobilization/mineralization of a large variety of plant materials could be adequately simulated by a simple mechanistic two-litter pool model. As an alternative to this kinetic

determination of plant residue partitioning (which require time-consuming incubation experiments), we found that the partitioning could be estimated with reasonable results by regression models using more easily measurable variables such as near infrared analyses (NIR) or a truncated stepwise chemical digestion scheme (total N and NDS-C). Therefore, we consider the developed regression models, and especially the NIR model due to its convenient, rapid analysis, to improve the ability for robust estimation of kinetically-defined plant litter pools in SOM models. Although certain plant materials posed a challenge to the simplistic model structure, mineralization from the vast majority of the 75 agricultural crop residues were simulated well by Nitrosim.

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Supplementary material tables

SM Table 1: Biochemical composition of the plant materials used in the calibration and validation datasets, measured from stepwise chemical digestion analysis, NDS: neutral detergent soluble, Hemi: hemi-cellulose, Cell: cellulose. GL: green leaves, SP: spikes and pods, and WP: whole aboveground plant.

Common name	Latin name	Carbon (mg C g ⁻¹ DM)				Nitrogen (mg N g ⁻¹ DM)					C/N ratio	
		NDS	Hemi	Cell	Lignin	Total	NDS	Hemi	Cell	Lignin		Total
Alfalfa GL	<i>Medicago sativa</i>	189	47	150	61	447	20	0.3	0.9	0.6	22	20
Barley GL	<i>Hordeum vulgare distichon</i>	106	141	152	15	413	15	2.5	0.3	0.4	18	23
Barley spikes	<i>Hordeum vulgare distichon</i>	307	84	32	2	425	12	1.1	0.1	0.0	13	32
Barley straw	<i>Hordeum vulgare distichon</i>	73	163	194	20	450	3	0.7	0.5	0.3	5	92
Broad bean WP	<i>Vicia faba</i>	157	45	193	56	451	11	1.4	1.1	1.3	15	31
Cabbage GL	<i>Brassica oleraceae</i>	330	21	46	0	397	14	0.2	0.1	0.0	14	27
Carrot GL	<i>Daucus carota</i>	330	23	57	13	423	23	0.9	1.0	0.3	25	17
Cock's foot stem	<i>Dactylis glomerata</i>	147	132	145	11	434	6	1.2	0.2	0.1	8	56
Cock's foot WP	<i>Dactylis glomerata</i>	178	115	134	7	434	18	4.1	0.4	0.3	23	19
Crimson clover flower	<i>Trifolium incarnatum</i>	265	74	102	34	476	32	3.0	0.5	0.5	36	13
Crimson clover GL	<i>Trifolium incarnatum</i>	350	39	58	7	454	35	1.9	0.8	0.2	38	12
Egyptian clover WP	<i>Trifolium alexandrinum</i>	301	42	100	17	460	25	2.1	0.5	0.6	29	16
Elephant grass WP	<i>Miscanthus giganteus</i>	116	122	206	20	463	2	0.1	0.3	0.1	3	173
Flax fibers	<i>Linum usitatissimum</i>	126	54	220	62	462	9	0.1	0.6	0.6	10	46
Flax GL	<i>Linum usitatissimum</i>	315	49	64	36	463	18	2.2	0.6	0.7	21	22
Flax oil	<i>Linum usitatissimum</i>	249	62	138	59	508	14	0.2	0.7	0.7	16	32
Flax stem 1	<i>Linum usitatissimum</i>	175	51	235	83	544	11	0.4	0.5	1.0	13	42
Flax stem 2	<i>Linum usitatissimum</i>	98	71	192	90	452	5	0.3	0.4	0.3	6	74
Flax stem 3	<i>Linum usitatissimum</i>	98	55	203	104	460	3	0.3	0.3	0.4	3	133
Flax WP	<i>Linum usitatissimum</i>	185	63	182	57	487	7	0.8	0.8	0.5	9	53
Hemp GL	<i>Cannabis sativa</i>	358	14	74	20	465	30	0.6	1.2	1.1	33	14
Hemp stem	<i>Cannabis sativa</i>	89	61	265	65	480	3	0.1	0.6	0.7	5	106
Hemp straw	<i>Cannabis sativa</i>	127	50	225	47	449	3	0.3	0.4	0.5	4	107
Leek GL	<i>Allium porri</i>	325	17	69	9	420	35	0.3	0.1	0.2	36	12
Maize GL	<i>Zea mays</i>	188	149	120	3	460	16	7.9	0.4	0.1	25	19
Maize spikes	<i>Zea mays</i>	396	58	31	0	485	16	1.0	0.1	0.0	17	29
Maize stem 1	<i>Zea mays</i>	178	123	139	9	450	9	0.8	0.3	0.1	10	44
Maize stem 2	<i>Zea mays</i>	161	124	144	7	437	12	1.4	0.3	0.1	14	32
Maize stem 3	<i>Zea mays</i>	147	166	142	1	455	6	1.4	0.2	0.0	8	57
Maize WP	<i>Zea mays</i>	142	165	147	4	458	5	1.6	0.8	0.2	7	62
Oil radish GL	<i>Raphanus sativus</i>	277	9	99	4	389	35	1.7	1.3	0.1	38	10
Onion GL	<i>Allium cepa</i>	332	28	90	17	467	16	2.7	0.5	0.6	20	23
Pea WP 1	<i>Pisum sativum</i>	115	81	206	54	457	6	0.1	1.0	0.8	8	56
Pea WP 2	<i>Pisum sativum</i>	126	93	214	51	484	5	0.6	0.9	0.6	7	72
Persian clover WP	<i>Trifolium resupinatum</i>	239	43	117	50	449	17	1.0	0.7	0.5	19	24
Phacelia GL	<i>Phacelia tenacetifolia</i>	310	39	61	11	420	28	2.2	1.4	0.3	32	13
Rape GL	<i>Brassica napus oleifera</i>	329	19	57	0	405	48	0.7	0.4	0.0	50	8
Rape spikes	<i>Brassica napus oleifera</i>	271	51	163	50	534	5	0.3	0.5	0.5	7	80
Rape stem 1	<i>Brassica napus oleifera</i>	107	76	222	52	458	2	0.6	0.3	0.4	4	128
Rape WP	<i>Brassica napus oleifera</i>	348	25	76	7	457	49	1.1	0.4	0.2	50	9

Common name	Latin name	NDS Hemi Cell Lignin				Total	NDS Hemi Cell Lignin				Total	C/N ratio
Red clover GL	<i>Trifolium pratense</i>	325	42	70	12	449	33	5.7	1.4	0.8	41	11
Red clover stem	<i>Trifolium pratense</i>	203	45	159	34	442	13	0.5	0.8	0.7	15	30
Ribbed melilot WP	<i>Melilotus officinalis</i>	247	20	147	36	449	16	0.3	0.4	0.5	17	26
Sugar beet GL 1	<i>Beta vulgaris</i>	294	51	47	6	398	21	3.5	0.4	0.2	25	16
Sunflower straw	<i>Helianthus annuus</i>	100	40	243	63	446	4	0.5	0.9	0.7	6	76
Turnip rape GL	<i>Brassica rapa oleifera</i>	326	38	40	4	408	53	4.6	0.8	0.2	59	7
Turnip rape straw	<i>Brassica rapa oleifera</i>	89	75	214	75	454	8	0.2	1.1	0.9	11	43
WW ryegrass WP 1	<i>Lolium multiflorum</i>	173	113	143	14	444	9	0.9	0.3	0.2	10	44
Wheat GL 1	<i>Triticum aestivum</i>	137	137	166	13	454	7	1.4	1	0.3	10	135
Wheat GL 2	<i>Triticum aestivum</i>	43	205	161	15	423	2	0.6	0	0.3	3	123
Wheat spikes 1	<i>Triticum aestivum</i>	266	96	78	8	449	12	1.2	0	0.2	14	32
Wheat spikes 2	<i>Triticum aestivum</i>	316	73	52	5	446	12	1.1	0	0.1	14	33
Wheat stem 1	<i>Triticum aestivum</i>	190	111	131	20	452	5	1.6	0	0.2	8	59
Wheat stem 2	<i>Triticum aestivum</i>	112	161	182	40	495	1	0.2	0	0.2	2	227
Wheat stem 3	<i>Triticum aestivum</i>	176	128	133	34	472	7	0.5	0	0.2	8	60
Wheat stem 4	<i>Triticum aestivum</i>	215	102	124	12	453	2	0.2	0	0.1	3	165
Wheat stem 5	<i>Triticum aestivum</i>	77	148	216	25	467	3	0.2	0	0.3	3	135
White clover WP 1	<i>Trifolium repens</i>	334	24	68	25	450	35	5.0	4.7	0.5	45	10
Winter rye GL	<i>Secale cereale</i>	240	84	98	11	433	46	5.7	1.5	0.6	54	8
Yellow lupine GL	<i>Lupinus luteus</i>	281	60	90	14	445	35.5	1.7	1.1	0.6	39	11
Yellow mustard straw	<i>Sinapis alba</i>	116	101	185	66	467	4	0.1	0.6	0.5	6	84
Validation data		NDS Hemi Cell Lignin				Total	NDS Hemi Cell Lignin				Total	C/N ratio
Barley stem 1	<i>Hordeum vulgare distichon</i>	126	124	160	21	430	4.6	0.9	0.2	0.2	6	73
Barley stem 2	<i>Hordeum vulgare distichon</i>	75	155	208	35	473	1.9	0.3	0.3	0.4	3	161
Maize stem 4	<i>Zea mays</i>	184	113	142	8	447	2.9	0.4	0.2	0.1	4	128
Meadow foxtail WP	<i>Alopecurus pratensis</i>	126	142	144	11	423	6.1	1.7	0.3	0.3	8	51
Nootka lupine GL	<i>Lupinus nootkatensis</i>	243	47	134	30	454	16.2	1.1	1.3	1.1	20	23
Oats WP	<i>Avena sativa</i>	210	106	123	10	449	5.7	0.5	0.1	0.1	6	71
Rape stem 2	<i>Brassica napus oleifera</i>	123	76	220	48	467	8.2	0.1	0.8	0.8	10	48
Red clover WP	<i>Trifolium pratense</i>	264	31	122	30	447	15.6	0.4	0.9	0.6	18	25
Red fescue straw	<i>Festuca rubra</i>	107	145	158	23	432	8.5	1.2	0.3	0.3	10	42
S. meadow grass straw	<i>Poa pratensis</i>	133	144	137	12	426	9.6	1.7	0.2	0.2	12	36
Sugar beet GL 2	<i>Beta vulgaris</i>	276	47	53	3	378	15.5	1.5	0.2	0.1	17	22
Swede WP	<i>Brassica napus</i>	148	61	189	44	442	10.2	0.0	0.8	0.6	12	38
WW ryegrass WP 2	<i>Lolium multiflorum</i>	192	99	120	9	420	11.9	1.5	0.1	0.1	14	31
White clover WP 2	<i>Trifolium repens</i>	334	24	68	25	450	34.6	5.0	4.7	0.5	45	10
Yellow lupine stem	<i>Lupinus luteus</i>	186	38	179	39	442	11.8	0.4	0.9	0.6	14	32

SM Table 2 C and N litter pool partitioning parameters P_C and P_N , i.e. the fraction of total C and N in the rapidly decomposing pool estimated by: measured as neutral detergent soluble C or N (NDS), kinetically-defined or optimized against mineralization data (OPT), or simple-linear (SL_{SCD}), multiple-linear (ML_{SCD}) and PLS regression (PLS_{NIR}) models predicting the kinetically-defined litter pool partitioning. The regression models were based upon stepwise chemical digestion (SCD) or near infrared reflectance spectroscopy (NIR) data. For validation ‘OPT’ see main Table 1.

No	Common name	Carbon litter pool partitioning (P_C)					Nitrogen litter pool partitioning (P_N)				
		NDS	OPT	SL_{SCD}	ML_{SCD}	PLS_{NIR}	NDS	OPT	SL_{SCD}	ML_{SCD}	PLS_{NIR}
1	Alfalfa GL	0.42	0.44	0.51	0.53	0.57	0.92	0.58	0.56	0.55	0.78
2	Barley GL	0.26	0.52	0.41	0.50	0.44	0.82	0.48	0.54	0.49	0.47
3	Barley spikes	0.72	0.47	0.72	0.71	0.72	0.91	0.00	0.50	0.65	0.92
4	Barley straw	0.16	0.34	0.33	0.35	0.43	0.71	0.07	0.23	0.31	0.22
5	Broad bean WP	0.35	0.40	0.46	0.46	0.38	0.74	0.38	0.51	0.15	0.46
6	Cabbage GL	0.83	1.00	0.81	0.84	1.00	0.98	1.00	0.51	0.71	0.77
7	Carrot GL	0.78	0.84	0.76	0.77	0.80	0.91	0.64	0.57	0.60	0.57
8	Cock's foot stem	0.34	0.50	0.46	0.48	0.47	0.81	0.33	0.39	0.57	0.77
9	Cock's foot WP	0.41	0.52	0.51	0.55	0.53	0.79	0.45	0.57	0.52	0.70
10	Crimson clover flower	0.56	0.62	0.59	0.58	0.53	0.89	0.59	0.60	0.57	0.36
11	Crimson clover GL	0.77	0.81	0.74	0.74	0.76	0.92	0.74	0.60	0.64	0.53
12	Egyptian clover WP	0.65	0.51	0.66	0.64	0.61	0.89	0.28	0.58	0.55	0.67
13	Elephant grass WP	0.25	0.24	0.38	0.37	0.27	0.80	0.00	0.00	0.43	0.00
14	Flax fibers	0.27	0.31	0.40	0.40	0.36	0.87	0.28	0.45	0.40	0.41
15	Flax GL	0.68	0.53	0.67	0.63	0.74	0.84	0.13	0.56	0.47	0.33
16	Flax oil	0.49	0.49	0.53	0.45	0.43	0.90	0.47	0.52	0.47	0.23
17	Flax stem 1	0.32	0.31	0.40	0.31	0.31	0.85	0.07	0.49	0.28	0.38
18	Flax stem 2	0.22	0.36	0.37	0.38	0.43	0.83	0.05	0.31	0.38	0.26
19	Flax stem 3	0.21	0.33	0.36	0.36	0.32	0.73	0.07	0.05	0.16	0.00
20	Flax WP	0.38	0.47	0.46	0.41	0.40	0.77	0.41	0.43	0.34	0.00
21	Hemp GL	0.77	0.72	0.73	0.71	0.76	0.91	0.32	0.59	0.50	0.46
22	Hemp stem	0.19	0.32	0.33	0.31	0.31	0.70	0.27	0.19	0.00	0.62
23	Hemp straw	0.28	0.40	0.41	0.41	0.41	0.74	0.59	0.15	0.10	0.85
24	Leek GL	0.77	1.00	0.76	0.81	0.79	0.98	0.49	0.60	0.67	0.59
25	Maize GL	0.41	0.55	0.49	0.49	0.50	0.66	0.67	0.57	0.46	0.72
26	Maize spikes	0.82	0.62	0.76	0.66	0.63	0.93	0.61	0.53	0.67	0.59
27	Maize stem 1	0.40	0.34	0.49	0.49	0.44	0.88	0.27	0.45	0.60	0.16
28	Maize stem 2	0.37	0.32	0.48	0.50	0.48	0.87	0.41	0.50	0.61	0.37
29	Maize stem 3	0.32	0.61	0.44	0.43	0.46	0.79	1.00	0.39	0.59	0.25
30	Maize WP	0.31	0.37	0.43	0.42	0.51	0.64	0.57	0.37	0.35	0.24
31	Oil radish GL	0.71	0.79	0.74	0.85	0.81	0.92	0.58	0.60	0.64	0.58
32	Onion GL	0.71	0.65	0.69	0.64	0.62	0.81	0.16	0.55	0.45	0.10
33	Pea WP 1	0.25	0.31	0.39	0.39	0.27	0.77	0.37	0.40	0.17	0.00
34	Pea WP 2	0.26	0.31	0.38	0.35	0.38	0.68	0.73	0.34	0.13	0.16
35	Persian clover WP	0.53	0.63	0.58	0.58	0.48	0.88	0.69	0.55	0.52	0.39

No	Common name	NDS	OPT	SL _{SCD}	ML _{SCD}	PLS _{NIR}	NDS	OPT	SL _{SCD}	ML _{SCD}	PLS _{NIR}
36	Phacelia GL	0.74	0.73	0.73	0.77	0.77	0.88	0.51	0.59	0.59	0.41
37	Rape GL	0.81	0.99	0.79	0.91	0.86	0.98	0.75	0.62	0.69	0.54
38	Rape spikes	0.51	0.39	0.53	0.41	0.50	0.81	0.20	0.34	0.29	0.44
39	Rape stem 1	0.23	0.36	0.38	0.37	0.39	0.65	0.56	0.07	0.03	0.59
40	Rape WP	0.76	0.76	0.73	0.76	0.77	0.97	0.72	0.62	0.67	0.59
41	Red clover GL	0.72	0.55	0.71	0.72	0.62	0.81	0.22	0.61	0.49	0.61
42	Red clover stem	0.46	0.48	0.54	0.54	0.54	0.87	0.51	0.51	0.43	0.68
43	Ribbed melilot WP	0.55	0.66	0.59	0.58	0.66	0.93	0.93	0.53	0.54	0.74
44	Sugar beet GL 1	0.74	0.70	0.75	0.80	0.90	0.83	0.52	0.57	0.56	0.84
45	Sunflower straw	0.22	0.43	0.37	0.39	0.39	0.65	1.00	0.30	0.02	0.41
46	Turnip rape GL	0.80	0.88	0.78	0.90	0.91	0.90	0.67	0.62	0.63	0.63
47	Turnip rape straw	0.20	0.44	0.35	0.37	0.34	0.79	0.36	0.46	0.23	0.58
48	WW ryegrass WP 1	0.39	0.57	0.49	0.49	0.55	0.87	0.74	0.45	0.55	0.66
49	Wheat GL 1	0.30	0.50	0.42	0.43	0.42	0.76	0.24	0.44	0.42	0.34
50	Wheat GL 2	0.10	0.43	0.30	0.37	0.53	0.67	0.00	0.04	0.24	0.00
51	Wheat spikes 1	0.59	0.71	0.62	0.60	0.57	0.89	0.83	0.51	0.60	0.67
52	Wheat spikes 2	0.71	0.75	0.70	0.66	0.59	0.90	0.86	0.50	0.63	0.50
53	Wheat stem 1	0.42	0.60	0.50	0.49	0.57	0.71	0.57	0.38	0.43	0.93
54	Wheat stem 2	0.23	0.29	0.35	0.31	0.27	0.66	0.00	0.00	0.27	0.00
55	Wheat stem 3	0.37	0.55	0.46	0.43	0.44	0.88	0.37	0.39	0.55	0.51
56	Wheat stem 4	0.47	0.48	0.54	0.50	0.56	0.85	0.00	0.00	0.52	0.00
57	Wheat stem 5	0.17	0.37	0.33	0.32	0.27	0.73	0.00	0.05	0.25	0.23
58	White clover WP 1	0.74	0.82	0.72	0.73	0.73	0.77	0.70	0.61	0.51	0.60
59	Winter rye GL	0.55	0.66	0.60	0.70	0.70	0.86	0.53	0.62	0.56	0.53
60	Yellow mustard straw	0.47	0.42	0.38	0.37	0.38	0.82	0.16	0.28	0.17	0.54
Validation data		NDS	'OPT'	SL _{SCD}	ML _{SCD}	PLS _{NIR}	NDS	'OPT'	SL _{SCD}	ML _{SCD}	PLS _{NIR}
1	Barley stem 1	0.29	0.38	0.43	0.46	0.38	0.78	0.02	0.30	0.15	0.40
2	Barley stem 2	0.16	0.25	0.32	0.30	0.23	0.65	0.35	0.00	0.00	0.00
3	Maize stem 4	0.41	0.30	0.50	0.48	0.43	0.83	1.00	0.05	0.00	0.00
4	Meadow foxtail WP	0.30	0.21	0.44	0.48	0.40	0.73	0.09	0.40	0.23	0.05
5	Nootka lupine GL	0.53	0.62	0.58	0.57	0.55	0.82	0.82	0.55	0.43	0.36
6	Oats WP	0.47	0.68	0.54	0.52	0.52	0.89	0.43	0.33	0.25	0.56
7	Rape stem 2	0.26	0.33	0.39	0.39	0.31	0.84	0.00	0.44	0.33	0.48
8	Red clover WP	0.59	0.56	0.62	0.61	0.56	0.89	0.50	0.54	0.46	0.59
9	Red fescue straw	0.25	0.36	0.40	0.44	0.36	0.83	0.15	0.45	0.34	0.21
10	S. meadow grass straw	0.31	0.43	0.44	0.49	0.46	0.82	0.25	0.48	0.36	0.24
11	Sugar beet GL 2	0.73	0.99	0.76	0.84	0.83	0.90	0.96	0.54	0.47	0.80
12	Swede WP	0.33	0.58	0.45	0.47	0.48	0.87	0.53	0.48	0.39	0.67
13	WW ryegrass WP 2	0.46	0.55	0.55	0.58	0.56	0.87	0.24	0.50	0.42	0.60
14	White clover WP 2	0.74	0.81	0.72	0.74	0.67	0.77	0.65	0.61	0.46	0.53
15	Yellow lupine stem	0.42	0.64	0.51	0.52	0.55	0.86	0.58	0.50	0.41	0.65

SM Table 3 Mean absolute errors (MAE, mg C or N kg⁻¹ soil) of simulated C and N mineralization of five simulations with the plant litter pool partitioned estimated as: chemically measured neutral detergent soluble C or N (NDS), kinetically-defined or optimized against mineralization data (OPT), or by simple-linear (SL_{SCD}), multiple-linear (ML_{SCD}) or PLS (PLS_{NIR}) regression models predicting the kinetically-defined litter pool partitioning based on stepwise chemical digestion (SCD) or near infrared reflectance spectroscopy (NIR) data. (N_{min} = NO₃⁻ + NH₄⁺).

No	Plant material	MAE (mg C-CO ₂ kg ⁻¹ soil)					MAE (mg N _{min} kg ⁻¹ soil)				
		NDS	OPT	SL _{SCD}	ML _{SCD}	PLS _{NIR}	NDS	OPT	SL _{SCD}	ML _{SCD}	PLS _{NIR}
1	Alfalfa GL	420	304	407	479	580	33	21	24	29	36
2	Barley GL	731	700	748	698	729	75	33	47	32	33
3	Barley spikes	1109	240	1051	1013	1063	14	22	39	63	101
4	Barley straw	406	161	168	161	433	56	14	16	16	15
5	Broad bean WP	225	144	289	321	144	36	7	15	51	20
6	Cabbage GL	745	137	784	685	137	90	48	73	55	66
7	Carrot GL	262	206	345	291	198	67	52	53	53	55
8	Cock's foot stem	385	78	162	92	111	47	16	21	30	48
9	Cock's foot WP	326	109	131	145	101	48	12	36	15	69
10	Crimson clover flower	238	134	169	177	364	85	43	48	44	85
11	Crimson clover GL	262	322	394	398	309	59	43	47	39	78
12	Egyptian clover WP	732	311	696	645	551	80	22	71	61	111
13	Elephant grass WP	483	174	656	592	207	53	19	30	23	20
14	Flax fibers	402	208	421	422	239	51	32	31	31	32
15	Flax GL	800	98	679	492	963	47	28	82	68	32
16	Flax oil	384	255	300	308	349	67	47	47	48	56
17	Flax stem 1	556	241	535	242	243	48	11	45	35	51
18	Flax stem 2	282	72	80	109	341	52	12	20	22	12
19	Flax stem 3	302	111	193	174	126	65	27	27	26	27
20	Flax WP	295	184	199	317	359	55	24	25	27	30
21	Hemp GL	401	285	284	295	300	128	39	114	84	56
22	Hemp stem	310	117	126	126	121	56	14	15	17	23
23	Hemp straw	158	142	164	165	151	63	17	30	31	19
24	Leek GL	1019	310	1077	869	971	179	52	111	132	101
25	Maize GL	422	120	269	267	247	56	26	28	57	38
26	Maize spikes	1015	524	748	521	518	101	20	45	19	22
27	Maize stem 1	533	148	623	610	424	47	17	18	16	36
28	Maize stem 2	520	129	659	768	673	37	14	22	13	41
29	Maize stem 3	874	195	736	756	634	75	30	45	33	60
30	Maize WP	116	106	255	211	630	66	14	28	28	56
31	Oil radish GL	289	155	227	296	194	93	16	25	23	16
32	Onion GL	355	71	204	90	161	39	23	87	75	25
33	Pea WP 1	239	173	393	409	204	35	17	19	37	29
34	Pea WP 2	266	185	392	242	377	84	12	48	57	62
35	Persian clover WP	466	318	377	382	709	56	35	34	37	43
36	Phacelia GL	169	175	174	256	248	61	32	40	35	52

No	Plant material	NDS	OPT	SL _{SCD}	ML _{SCD}	PLS _{NIR}	NDS	OPT	SL _{SCD}	ML _{SCD}	PLS _{NIR}
37	Rape GL	804	391	868	459	624	88	105	110	106	135
38	Rape spikes	933	251	783	264	624	99	22	33	22	24
39	Rape stem 1	302	225	234	231	264	61	14	29	30	16
40	Rape WP	216	319	293	330	343	73	44	71	49	93
41	Red clover GL	789	250	724	755	434	165	35	155	99	177
42	Red clover stem	240	170	291	312	295	30	13	12	26	20
43	Ribbed melilot WP	398	211	349	379	212	77	32	66	64	42
44	Sugar beet GL 1	206	119	241	416	781	26	19	19	20	58
45	Sunflower straw	446	270	317	293	296	70	19	41	62	37
46	Turnip rape GL	375	269	439	313	330	130	110	118	135	131
47	Turnip rape straw	598	304	459	408	498	64	19	33	20	47
48	WW ryegrass WP 1	471	67	315	292	99	57	23	28	25	23
49	Wheat GL 1	510	221	321	315	336	60	22	43	41	33
50	Wheat GL 2	832	148	484	283	472	75	37	64	60	18
51	Wheat spikes 1	497	224	465	544	641	67	22	39	28	24
52	Wheat spikes 2	1113	1010	1055	1109	1216	92	18	48	25	29
53	Wheat stem 1	458	261	380	455	258	51	15	14	17	45
54	Wheat stem 2	312	239	361	243	261	60	19	18	20	21
55	Wheat stem 3	490	224	390	518	464	55	21	29	48	42
56	Wheat stem 4	391	298	425	330	483	79	28	34	32	36
57	Wheat stem 5	528	264	322	334	452	57	19	28	37	47
58	White clover WP 1	417	399	508	480	474	46	40	50	91	56
59	Winter rye GL	390	241	301	318	332	166	101	100	100	102
60	Yellow mustard straw	467	290	343	368	350	55	20	22	21	35
No	Validation data	NDS	'OPT'	SL _{SCD}	ML _{SCD}	PLS _{NIR}	NDS	'OPT'	SL _{SCD}	ML _{SCD}	PLS _{NIR}
1	Barley stem 1	392	196	213	293	198	46	26	31	24	43
2	Barley stem 2	256	219	360	299	227	69	23	33	30	23
3	Maize stem 4	740	129	832	755	542	179	54	134	132	122
4	Meadow foxtail WP	730	125	940	1101	783	43	15	17	40	43
5	Nootka lupine GL	196	118	175	199	275	77	36	55	80	93
6	Oats WP	647	317	595	683	663	43	30	43	43	59
7	Rape stem 2	257	235	338	319	244	54	20	49	38	72
8	Red clover WP	300	238	325	303	239	45	22	23	27	23
9	Red fescue straw	193	253	292	366	254	47	11	28	13	13
10	S. meadow grass straw	253	237	232	284	241	50	25	37	25	26
11	Sugar beet GL 2	936	150	887	593	614	66	45	55	78	46
12	Swede WP	681	256	528	443	415	48	13	24	15	37
13	WW ryegrass WP 2	279	144	144	233	160	48	16	46	25	60
14	White clover WP 2	303	155	431	348	645	43	33	34	91	47
15	Yellow lupine stem	655	101	559	508	400	55	30	37	31	48

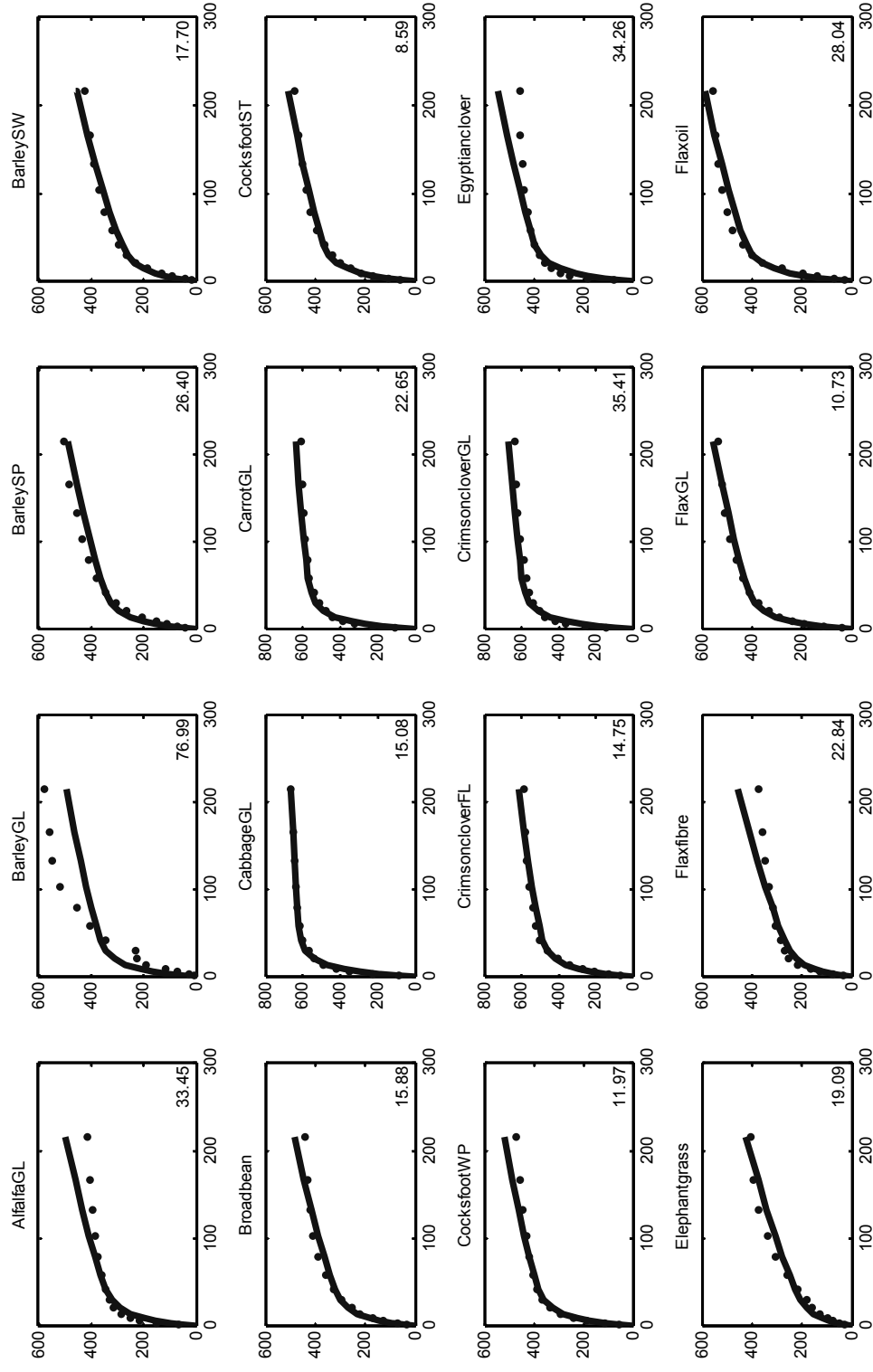
SM Table 4 Prediction statistics for the cross-validated simple-linear (SL), multiple-linear (ML) and PLS regression models for estimation of rapidly decomposing C (C_{L1}) and N (N_{L1}) litter pools (mg C or N g^{-1} DM); standard error of prediction (SEP), correlation coefficient (r), and number of PLS components (PC). The NIR data was in three formats: untransformed spectra (PLS_NIR UT), transformed by 2nd derivate and 2 side point (PLS_NIR 2nd4), and by 2nd derivative and 8 side points (PLS_NIR 2nd8). The selected NIR models used for the Nitrosim simulations are marked *.

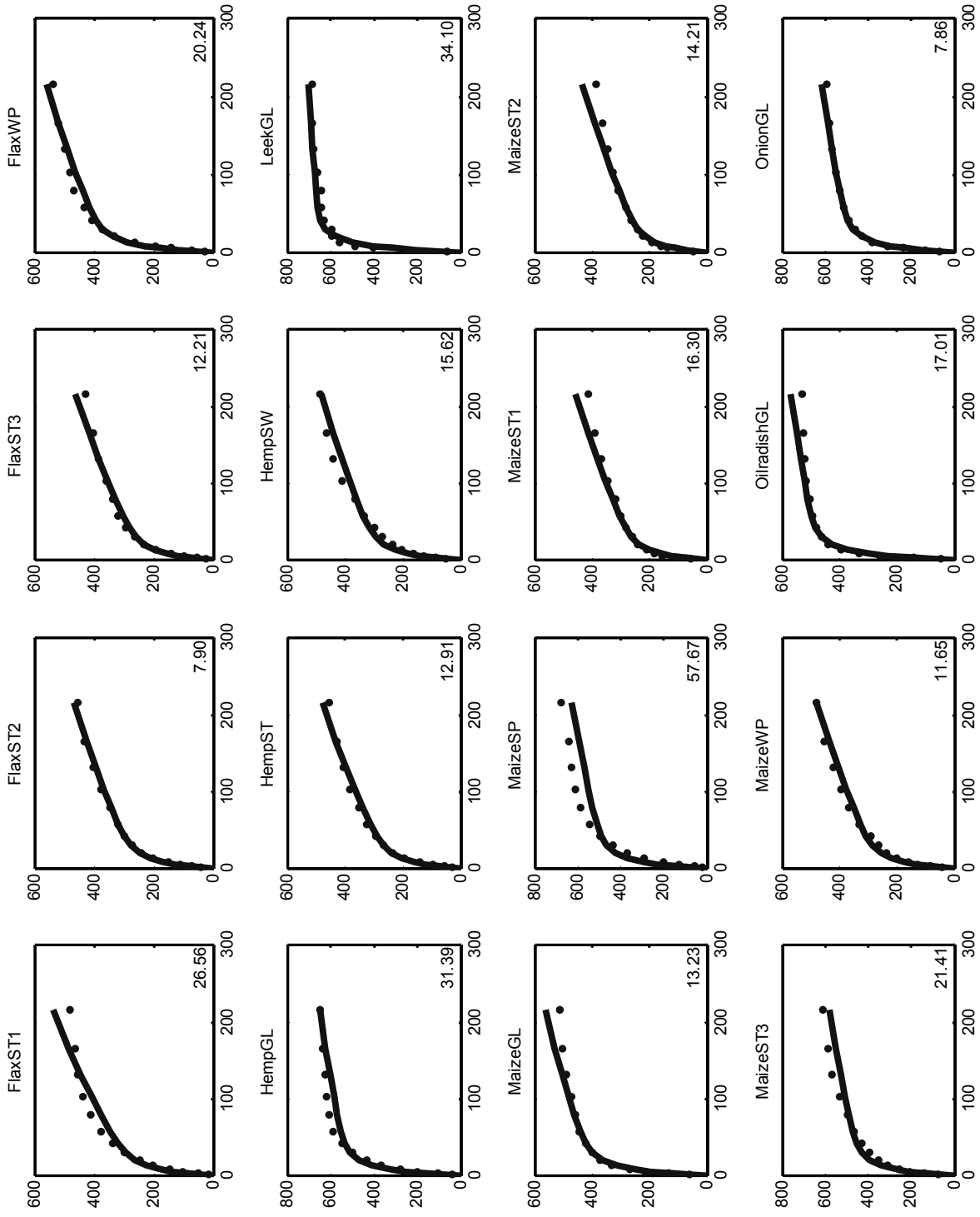
Models	Prediction of C_{L1}			Prediction of N_{L1}		
	SEP	r	PC	SEP	r	PC
SL	45.9	0.805	-	3.7	0.929	-
ML	38.6	0.867	-	3.4	0.943	-
PLS_NIR UT	42.2	0.844	9*	5.0	0.871	6
PLS_NIR 2 nd 4	44.3	0.821	3	4.6	0.892	7
PLS_NIR 2 nd 8	44.8	0.817	2	4.7	0.886	6*

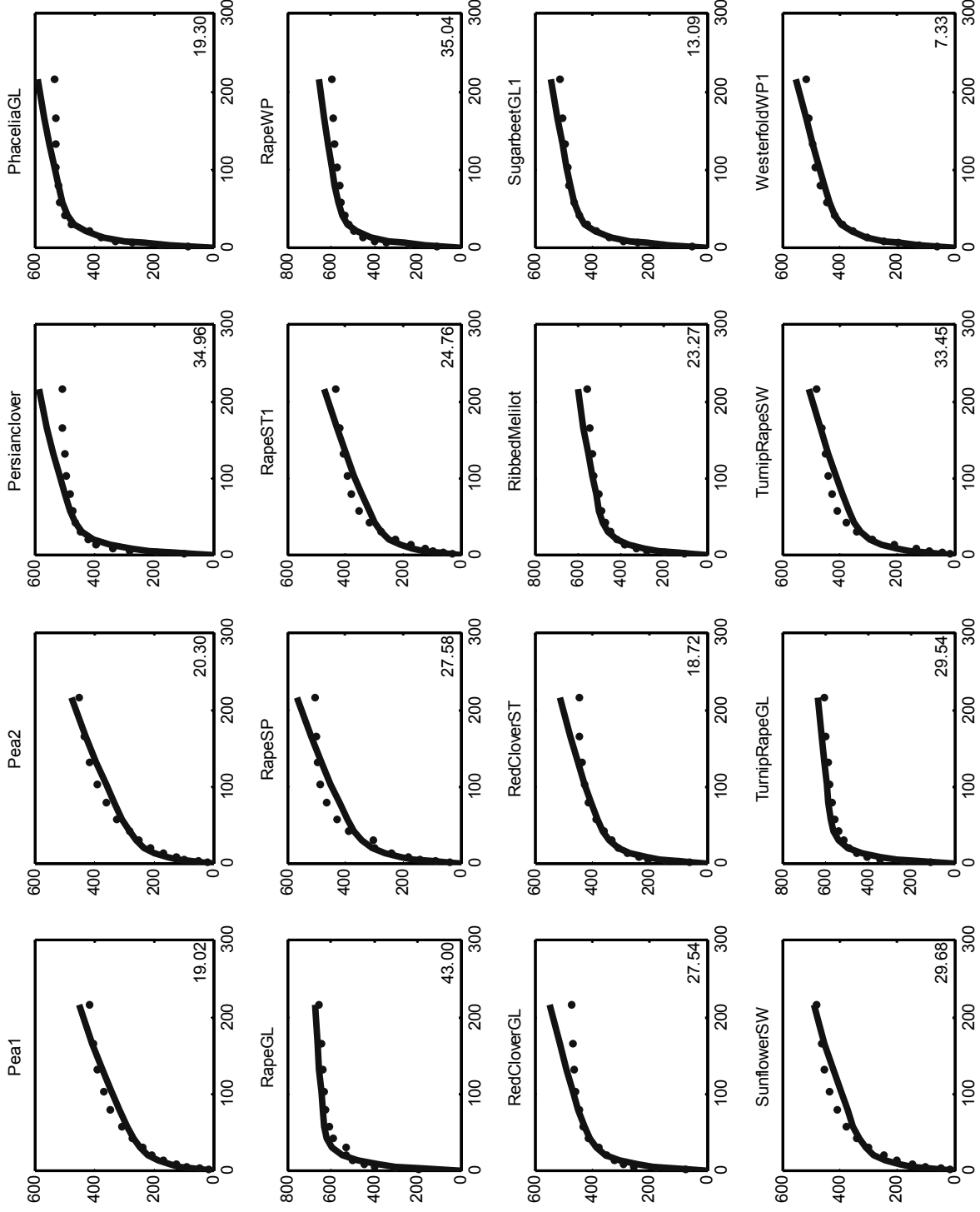
Supplementary material figures

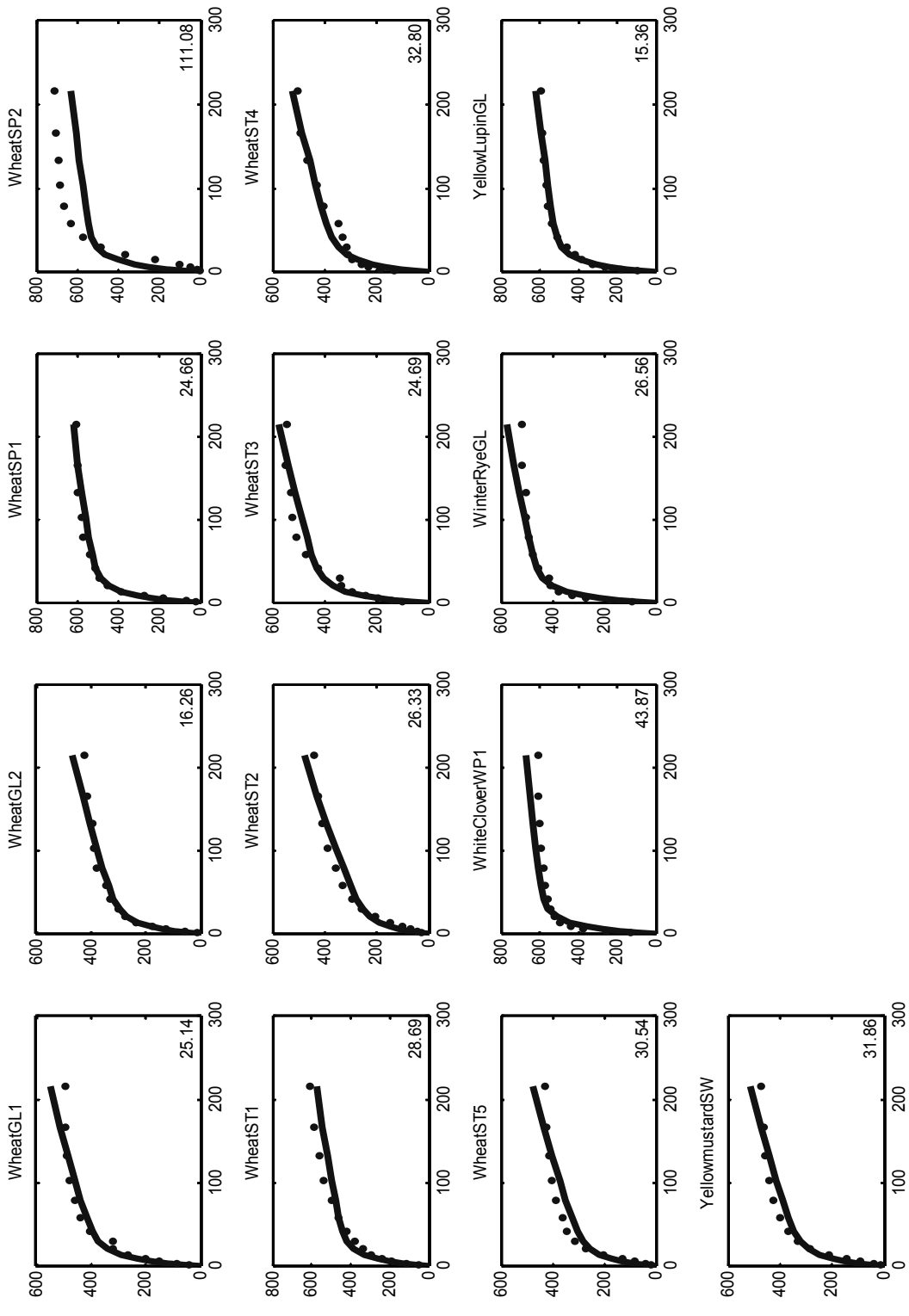
SM Figure 1. Time plots in days of measured (dots) and simulated (line) CO₂ emission (a) and net N mineralization/immobilization (b) of the calibration data set using optimized global parameters and litter pool partitioning (OPT). Mean absolute errors (g C-CO₂ or N_{min} m⁻²) displayed in the bottom right corner.

a) Simulated C mineralization (g C-CO₂ m⁻²)

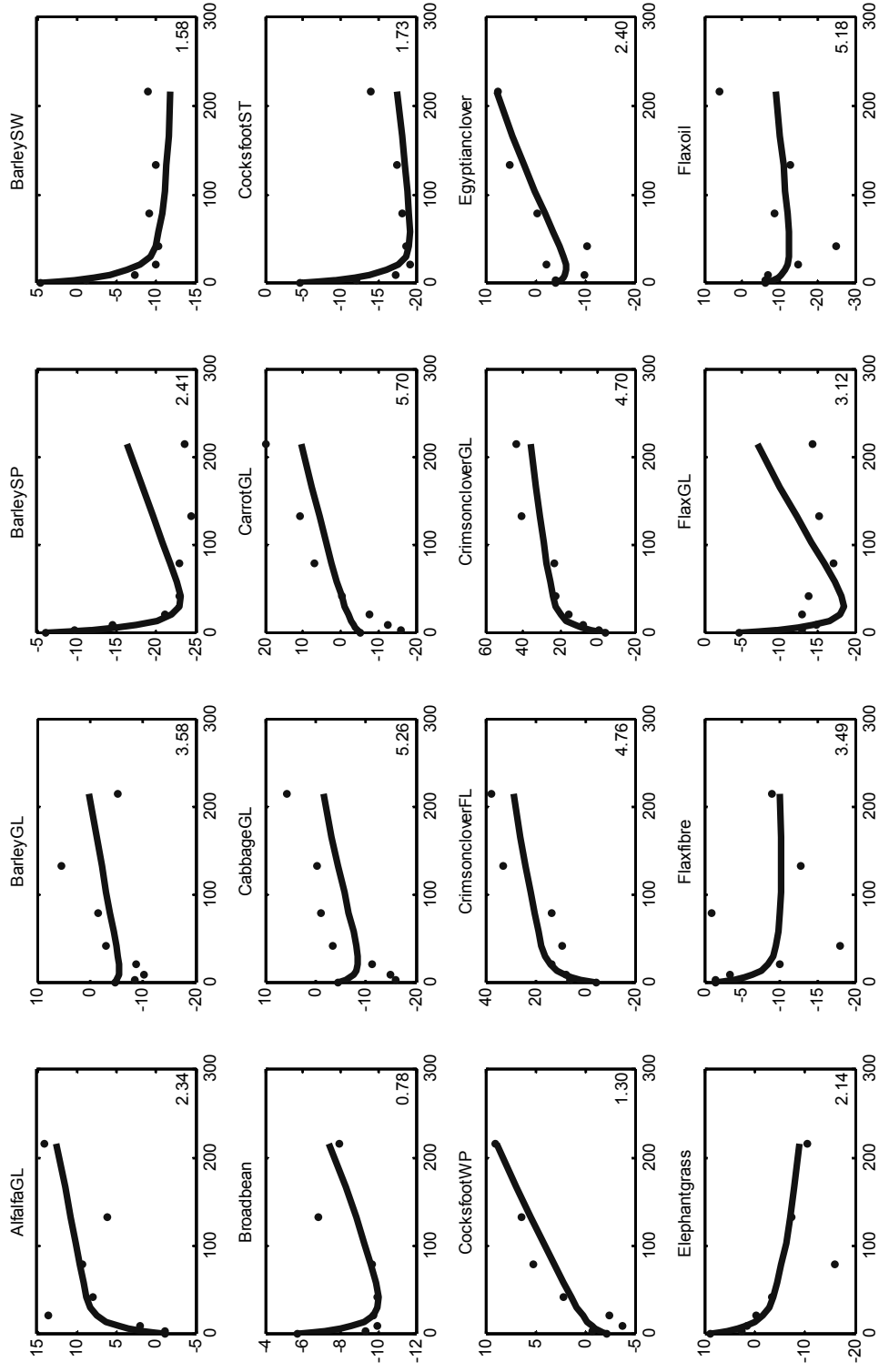


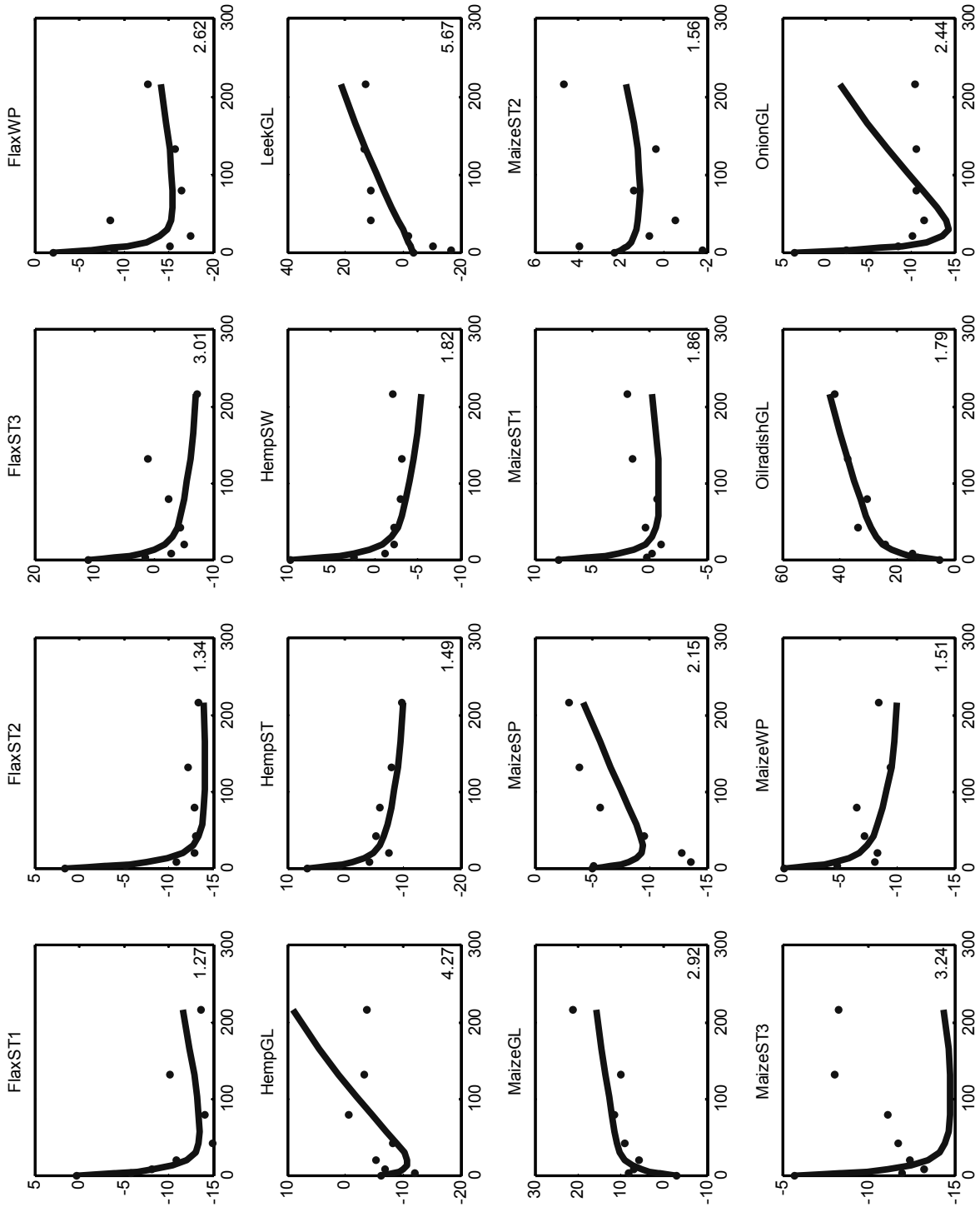


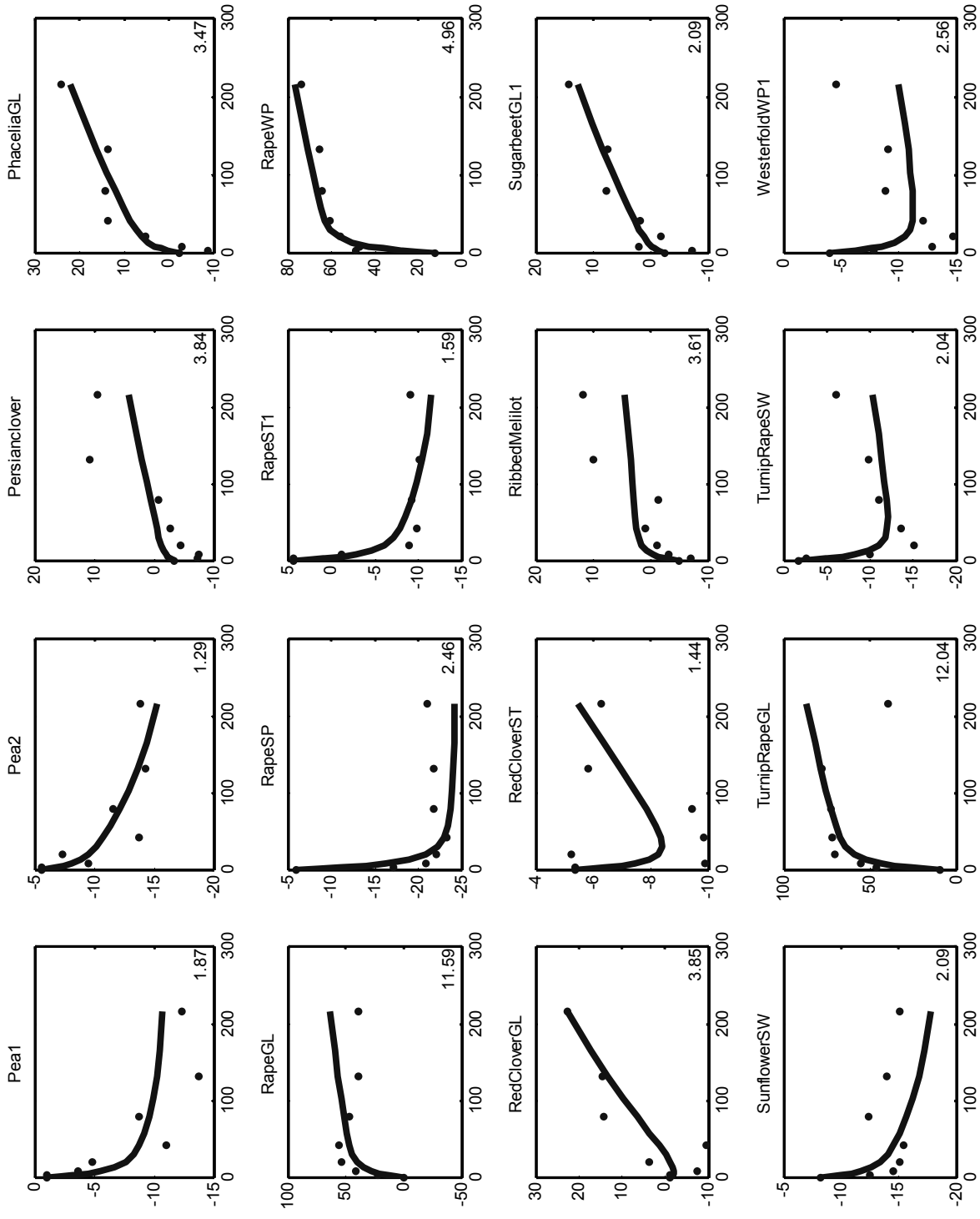


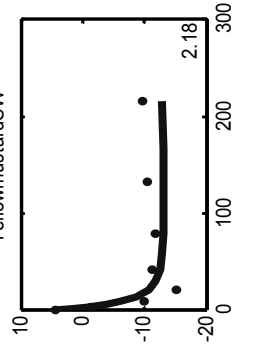
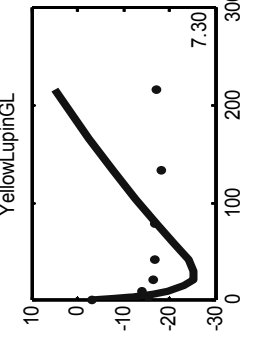
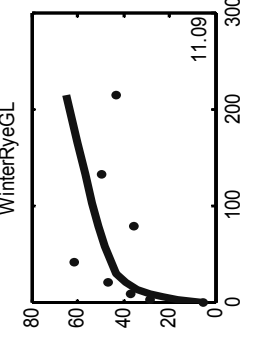
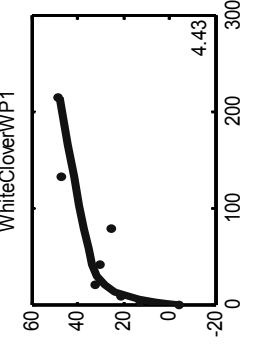
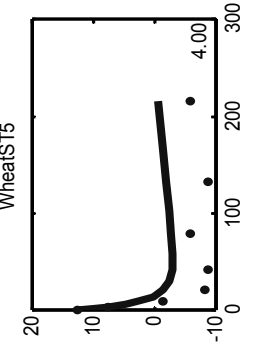
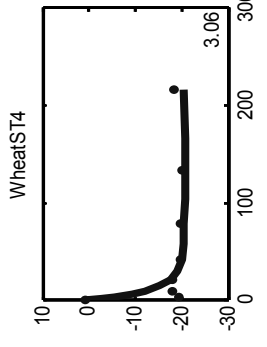
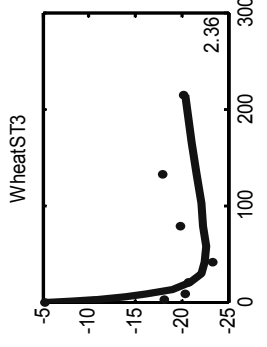
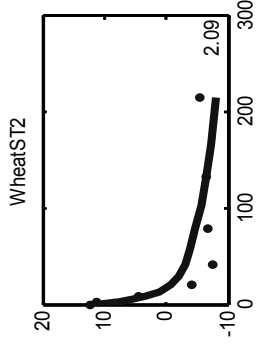
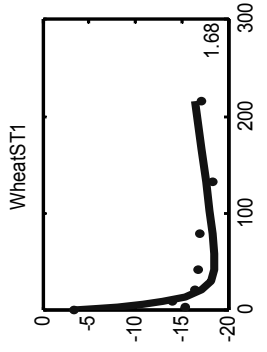
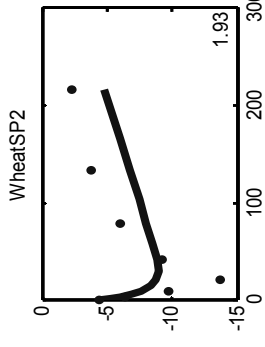
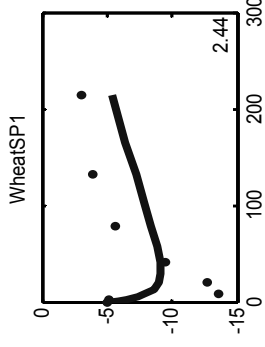
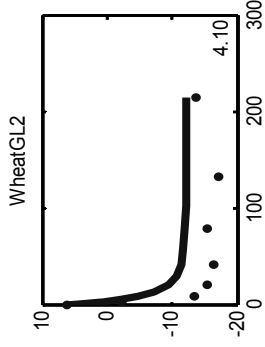
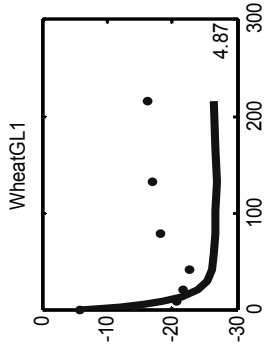


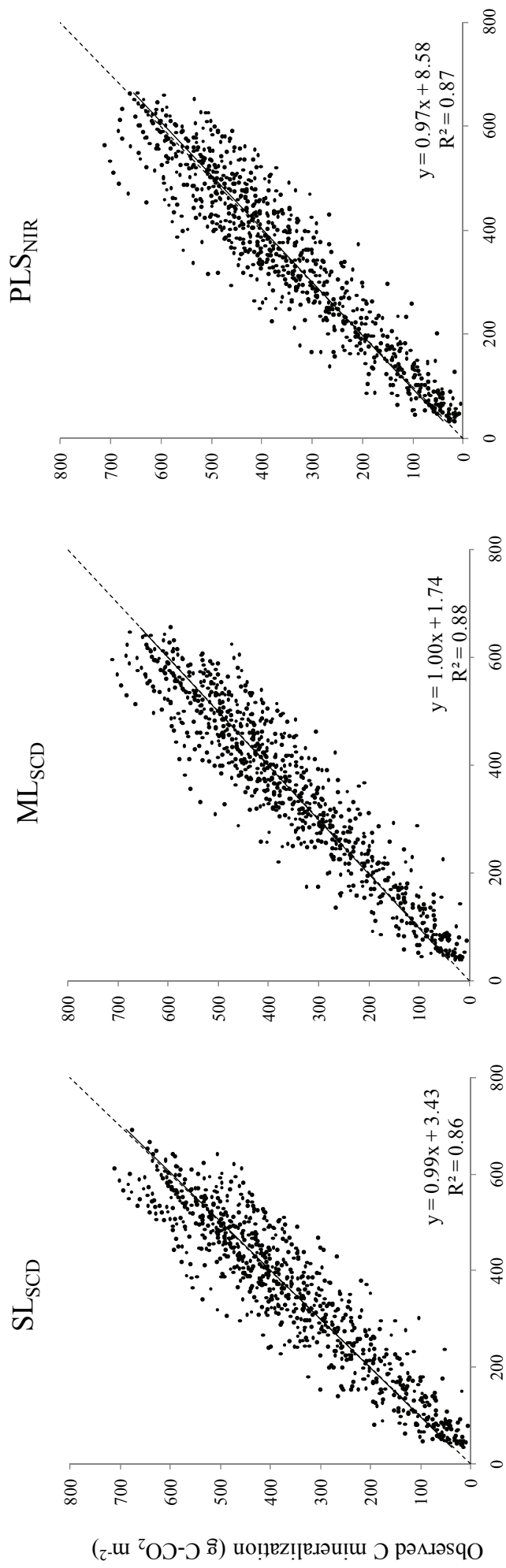
b) N mineralization ($\text{g N}_{\text{min}} \text{m}^{-2}$)





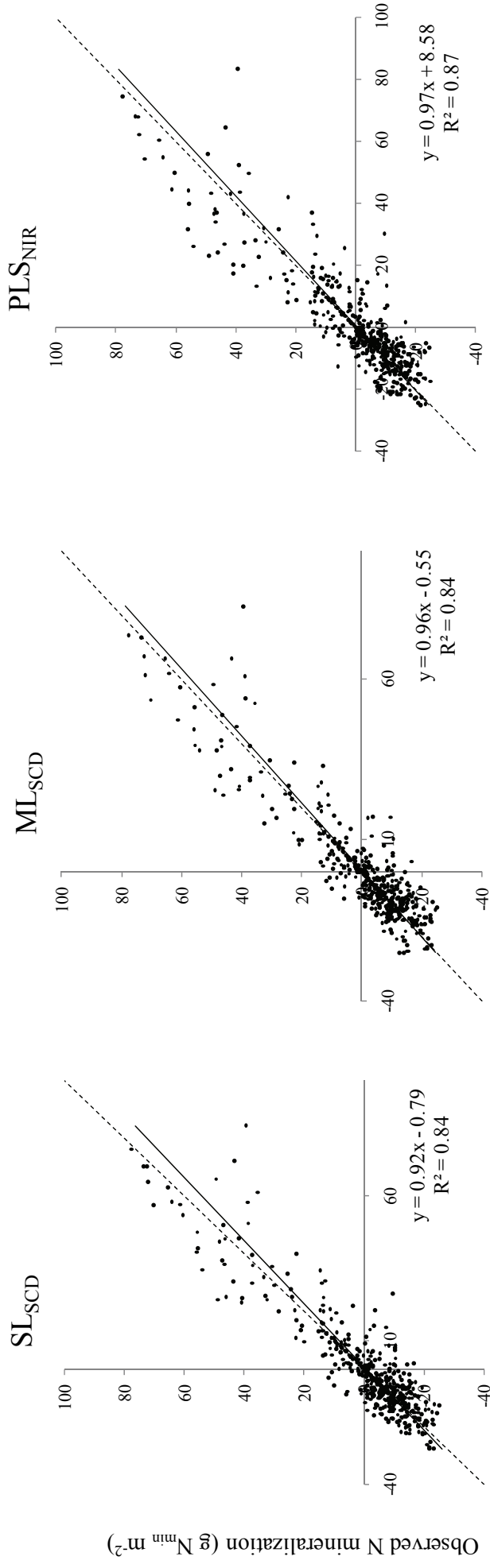






Simulated C mineralization (g C-CO₂ m⁻²)

SM Figure 2 Observed versus simulated C mineralization of the calibration dataset from simulations SL_{SCD}, ML_{SCD}, and PLS_{NIR} using simple-linear and multiple-linear regression based on stepwise chemical digestion data (SCD), and PLS regression based on near infrared reflectance spectroscopy data (NIR) to predict the kinetically-defined the plant litter pool partitioning. Dotted lines (---) represent the 1:1 line of perfect agreement.



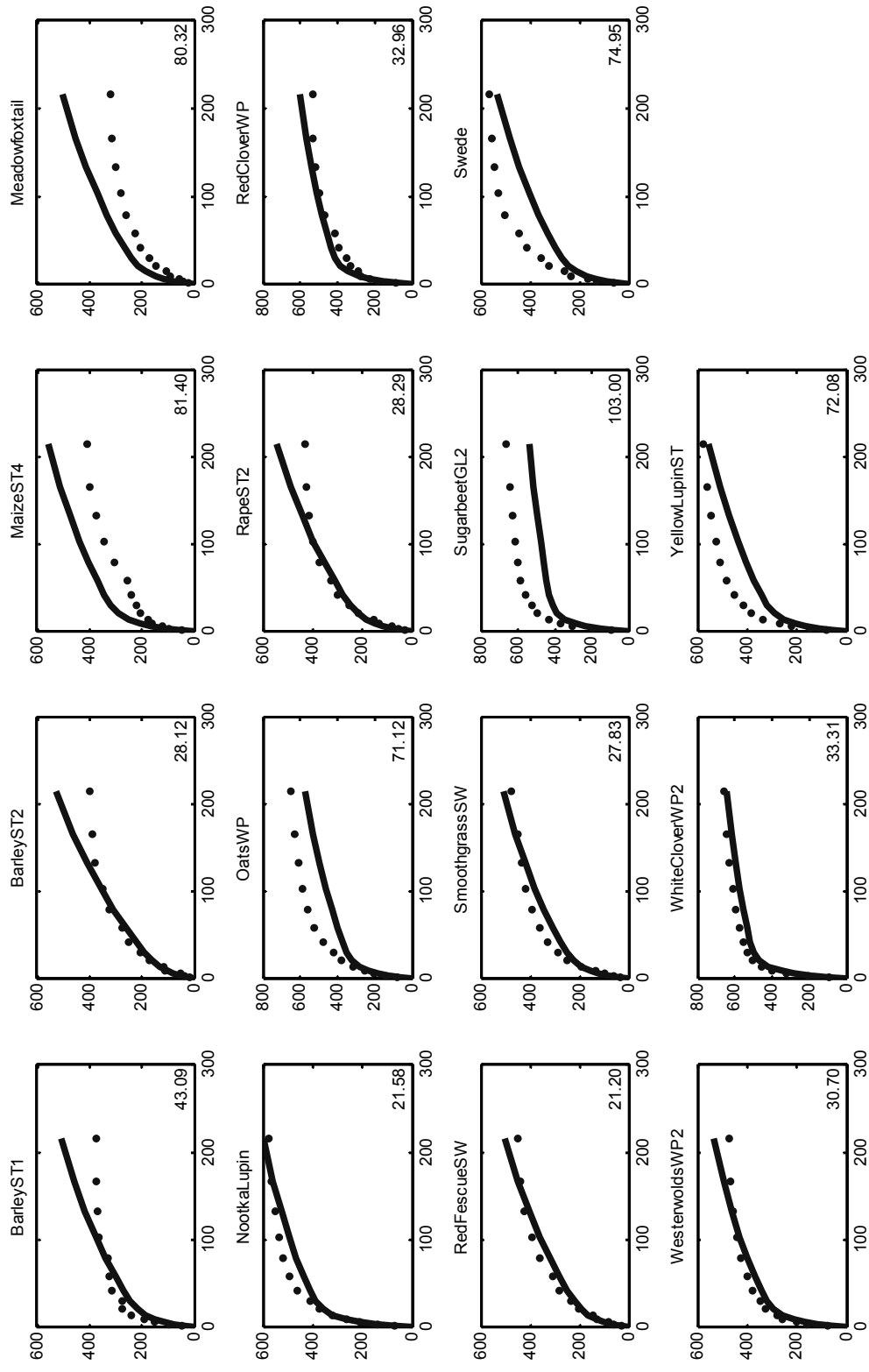
Simulated N mineralization ($\text{g N}_{\text{min}} \text{m}^{-2}$)

SM Figure 3 Observed versus simulated net N ($\text{N}_{\text{min}} = \text{NH}_4^+ + \text{NO}_3^-$) mineralization of the calibration dataset from simulations SL_{SCD}, ML_{SCD}, and PLS_{NIR} using simple-linear and multiple-linear regression based on stepwise chemical digestion data (SCD), and PLS regression based on near infrared reflectance spectroscopy data, NIR to predict the kinetically-defined the plant litter pool partitioning. Dotted lines (---) represent the 1:1 line of perfect agreement.

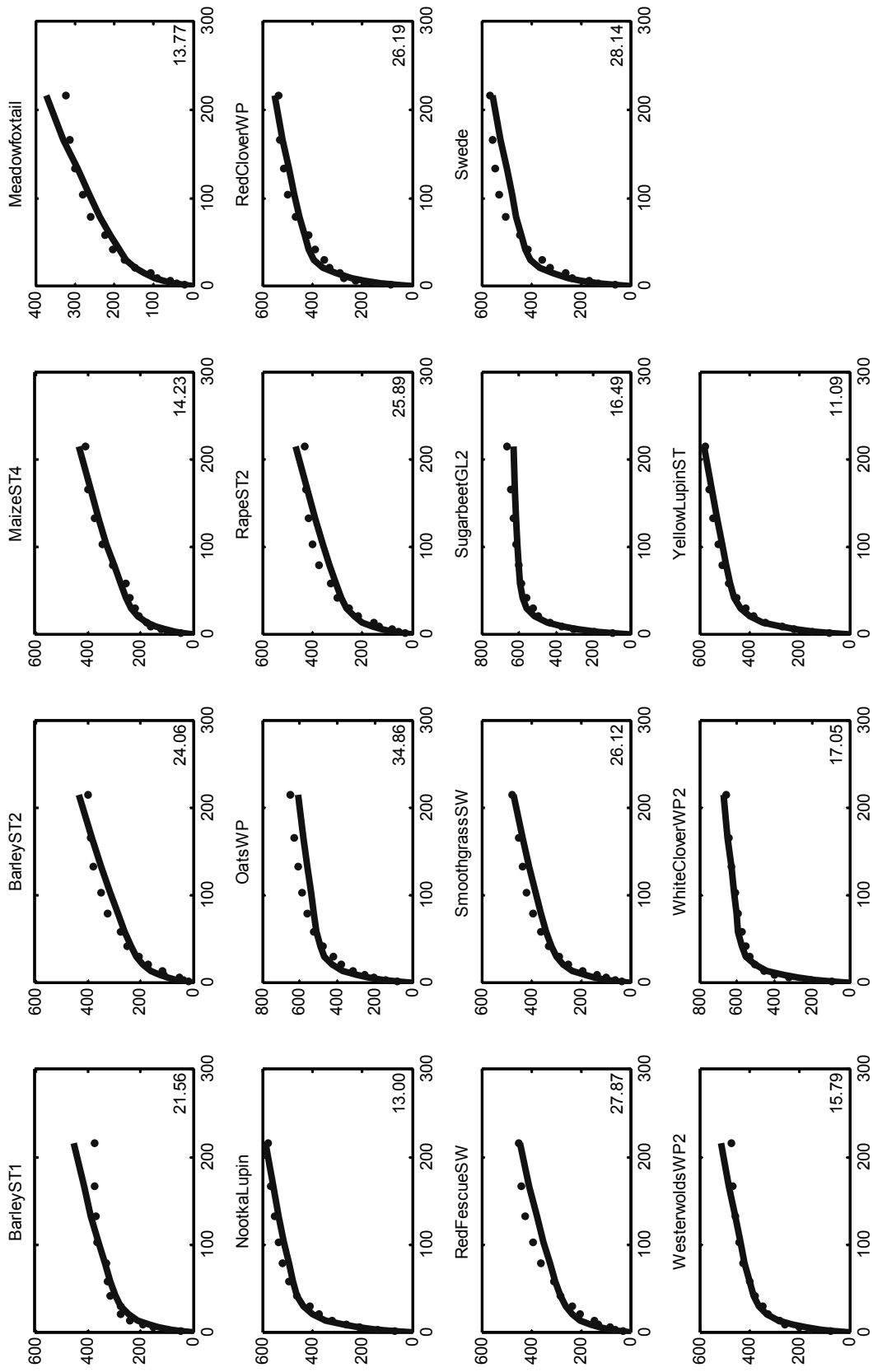
SM Figure 4. Time plots in days of measured (dots) and simulated (lines) CO₂ emission (a) and net N mineralization/immobilization (b) of the validation data of simulations NDS, 'OPT', SL_{SCD}, ML_{SCD}, and PLS_{NIR}. Mean absolute errors displayed in the bottom right corner (g C-CO₂ or N_{min} m⁻²)

a) simulation C mineralization (g C-CO₂ m⁻²)

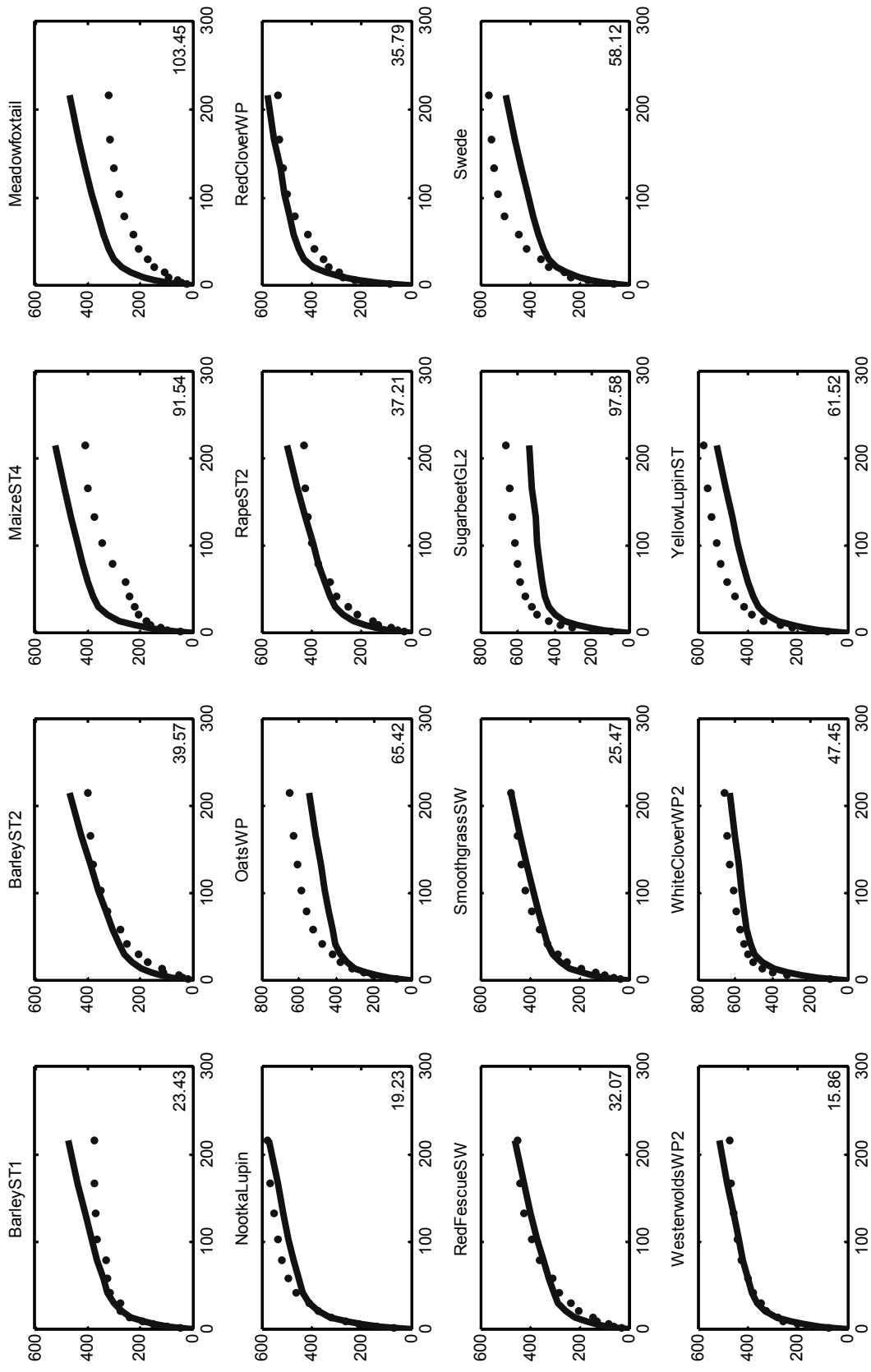
NDS simulation using chemical litter pool partitioning approach of measured NDS-C and -N as litter 1 pool:



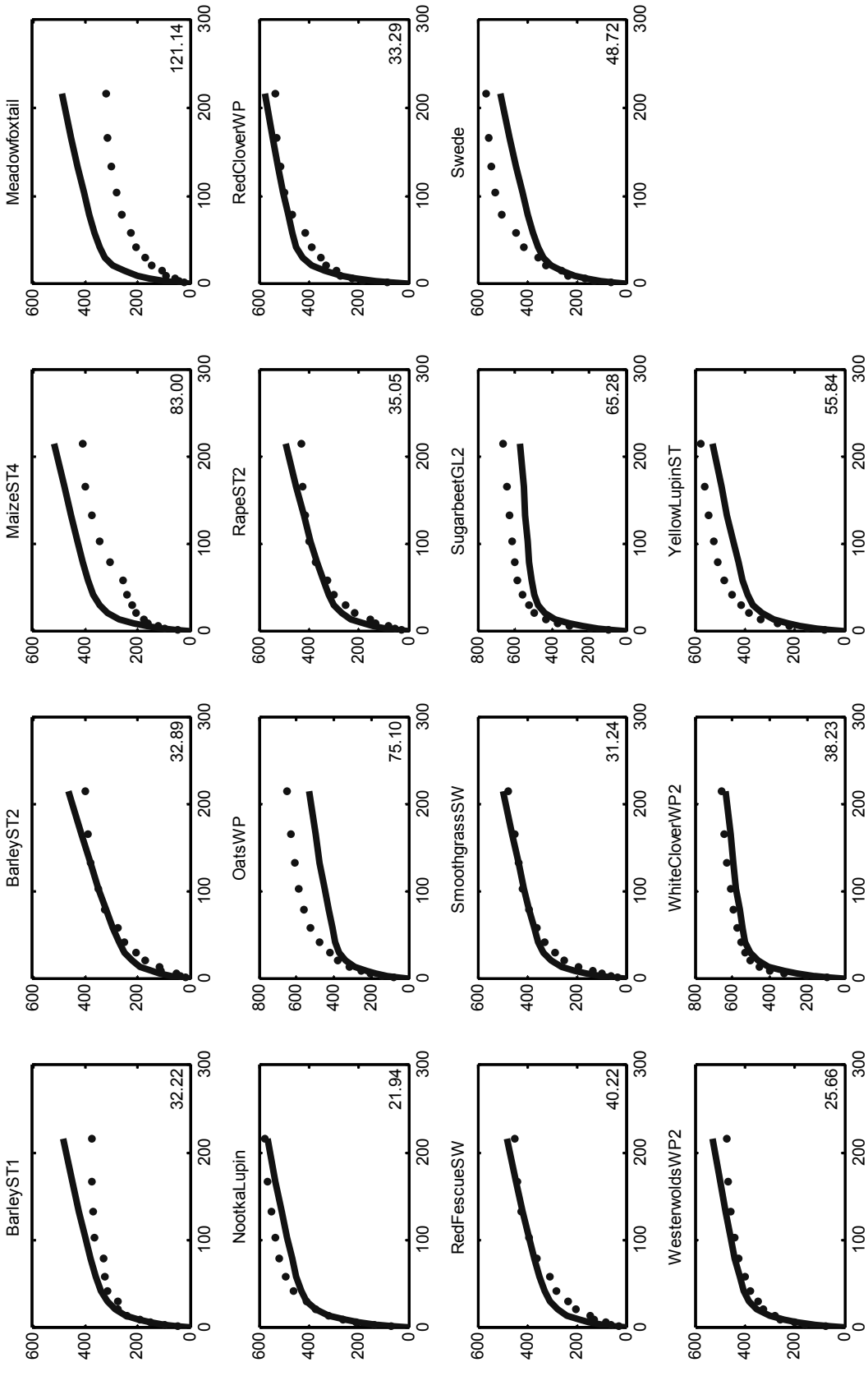
‘OPT’ simulation with optimized litter pool partitioning and global parameters set OPT:



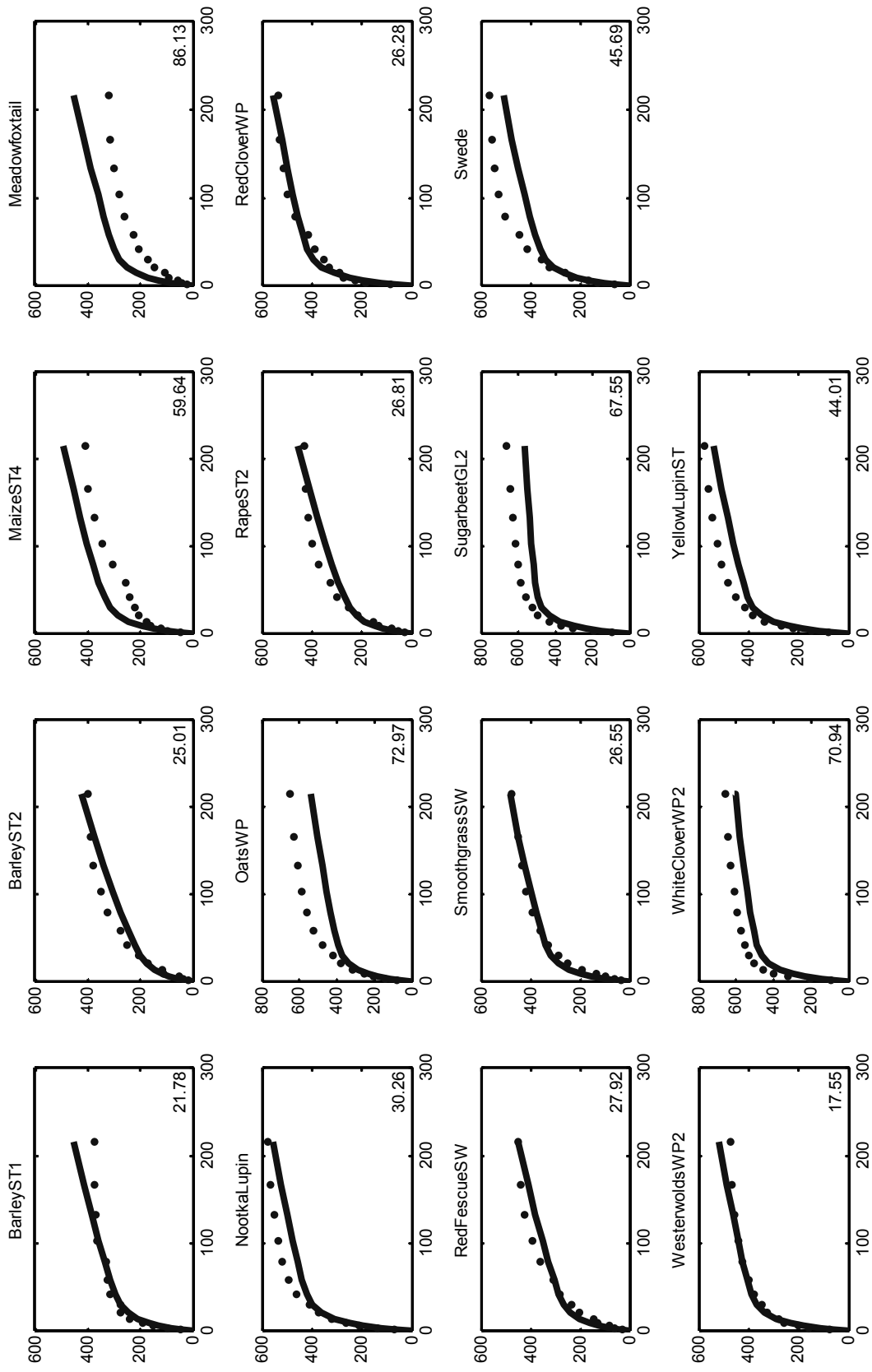
SL_{SCD} simulation using a simple-linear regression model for prediction of the kinetically-defined (optimized) litter pool partitioning:



ML_{SCD} simulation using a multiple-linear regression model for prediction of the kinetically-defined (optimized) litter pool partitioning:

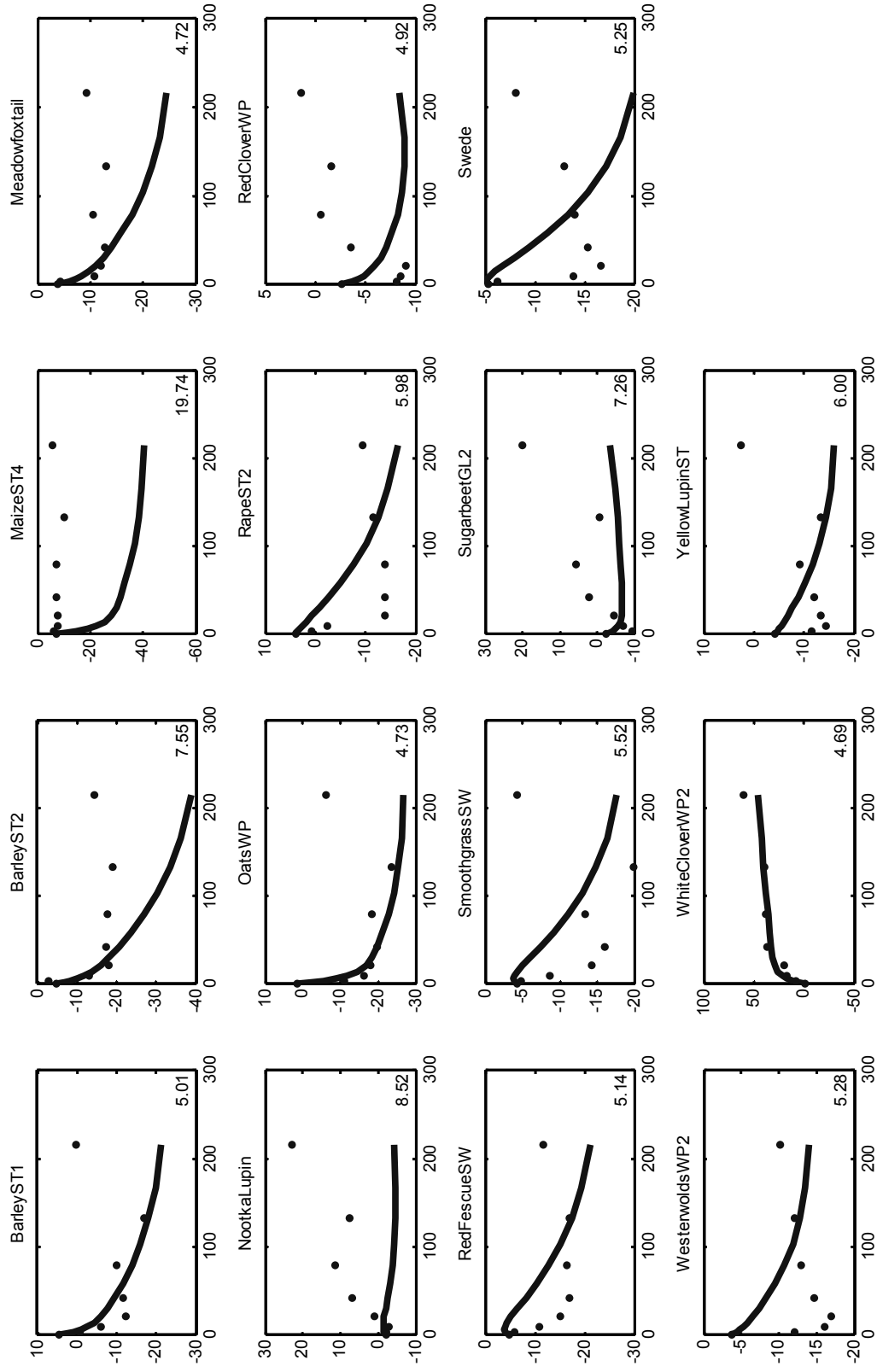


PLS_{NIR} simulation using a PLS regression model based on near infrared reflectance spectra data for prediction of the kinetically-defined (optimized) litter pool partitioning:

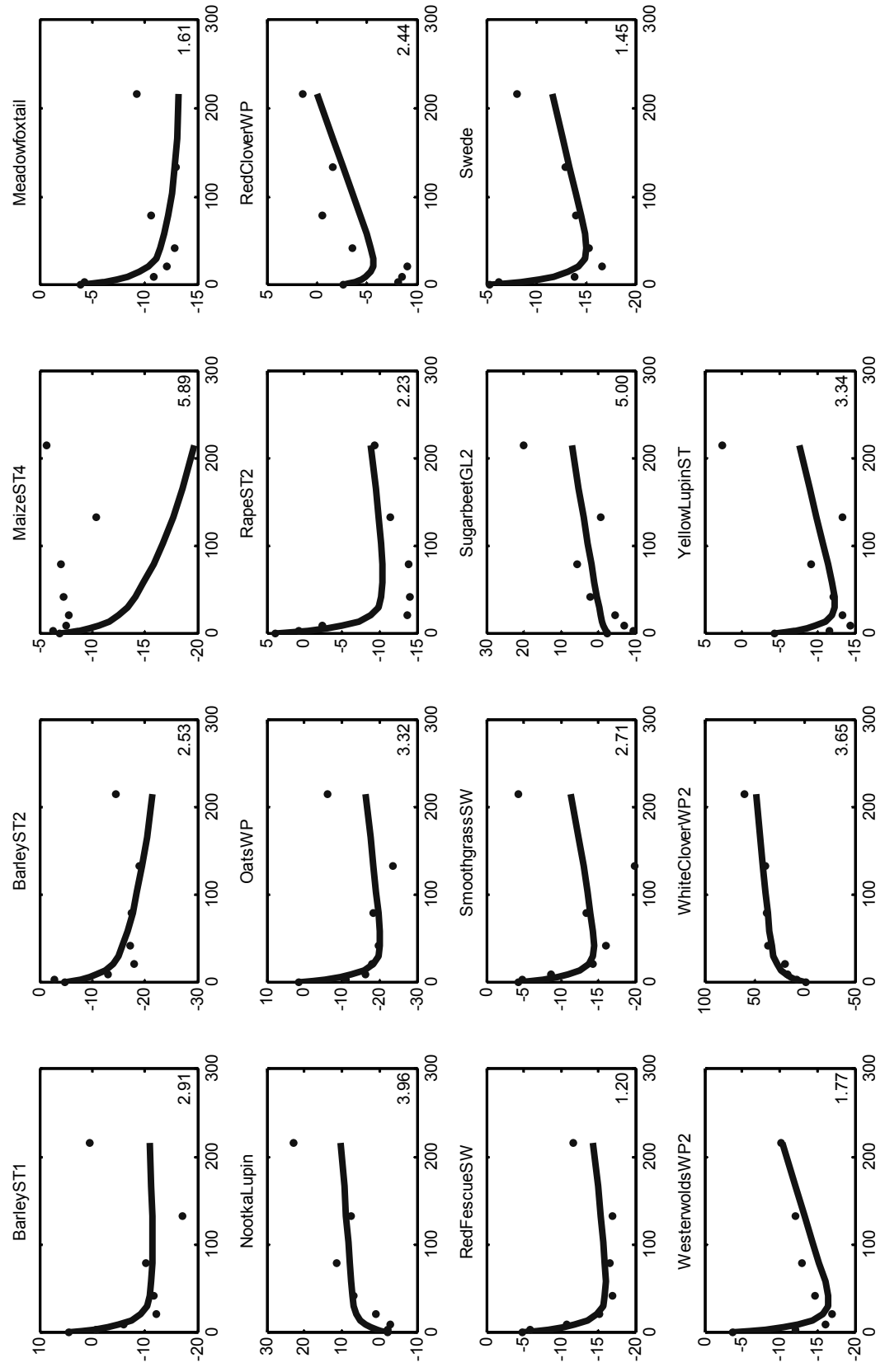


b) simulated net N mineralization ($\text{g N}_{\text{min}} \text{m}^{-2}$)

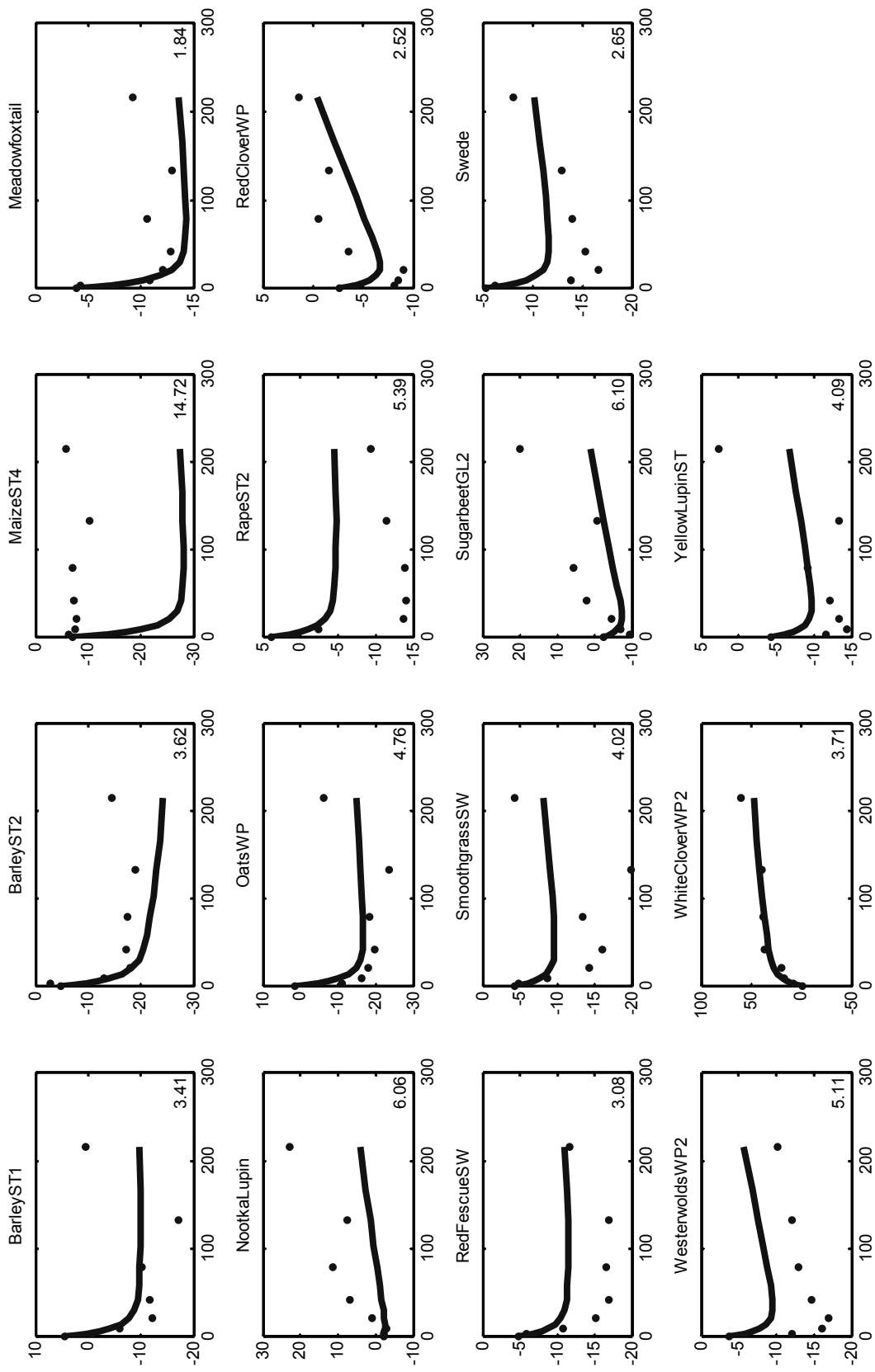
NDS simulation using chemical litter pool partitioning approach of measured NDS-C and -N as litter I pool:



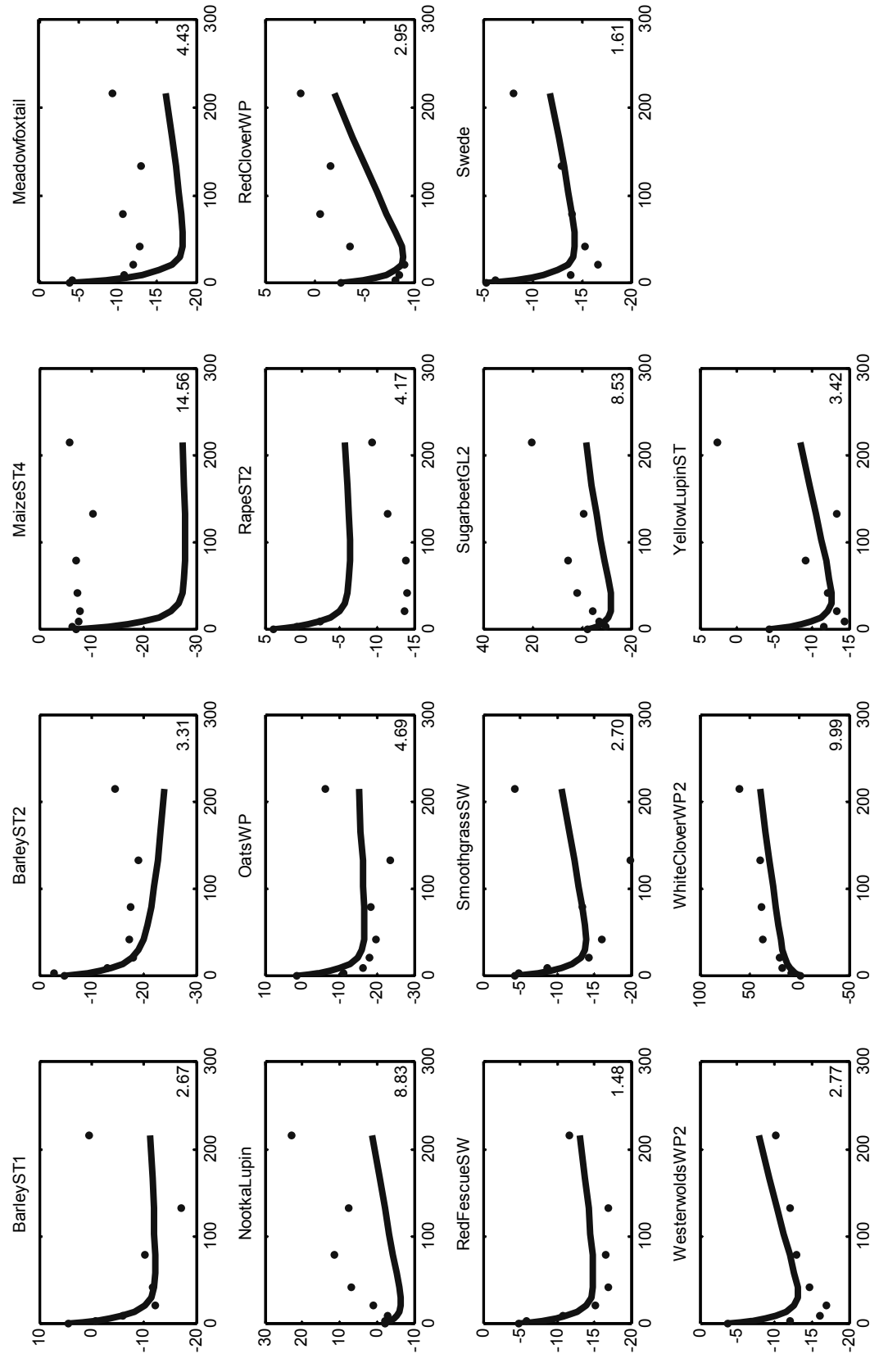
‘OPT’ simulation with kinetically-defined or optimized litter pool partitioning and global parameters:



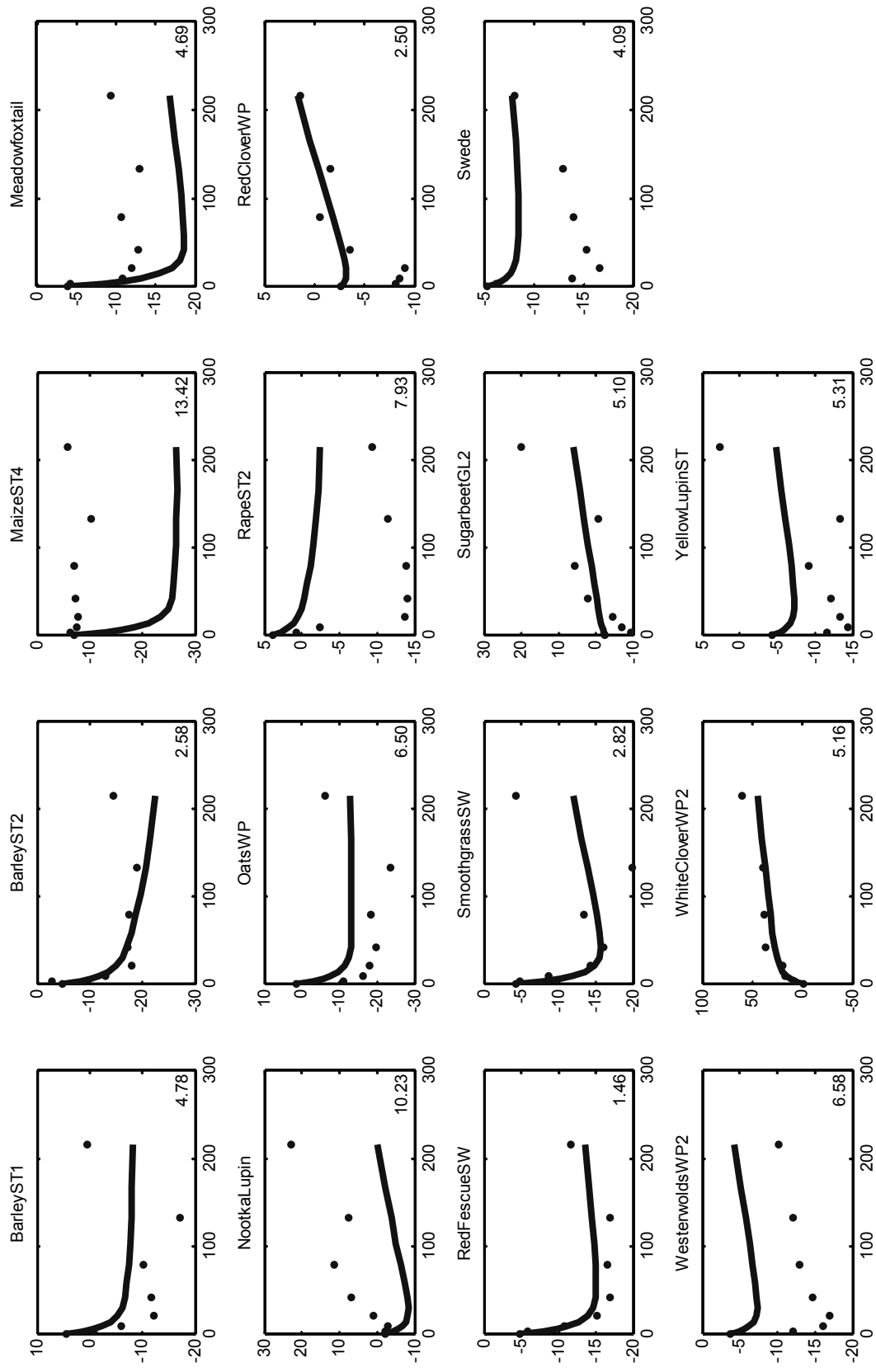
SL_{SCD} simulation using a simple-linear regression model for prediction of the kinetically-defined (optimized) litter pool partitioning:



ML_{SCD} simulation using a multiple-linear regression model for prediction of the kinetically-defined (optimized) litter pool partitioning:



PLS_{NIR} simulation using a PLS regression model based on near infrared reflectance spectra data for prediction of the kinetically-defined (optimized) litter pool partitioning:



Paper II

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Nitrogen dynamics in stockless organic clover-grass and cereal rotations. Submitted to
Nutrient Cycling in Agroecosystems

Nitrogen dynamics in stockless organic clover-grass and cereal rotations

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Abstract

We applied a mechanistic ecosystem model to investigate the production and environmental performances of i) current agricultural practice on two fields of a stockless organic cereal farm in southeast Norway and ii) alternative cereal–ley rotations and plowing time scenarios. Scenarios were simulated using historic weather data and a climate change scenario. Measured and simulated soil mineral N concentrations were generally low (1–4 g N m⁻²) and in good agreement. Simulated nitrate leaching was similar for the two fields, except when an extended period of black fallow weeding was practiced on one of them. Scenario simulations indicated that continuous cereal cropping undersown with a clover–grass winter cover crop performed best when evaluated by whole-rotation grain yield, the ratios N yield/input, N loss/input, and N loss/yield, and greenhouse gas emissions. However, the rotation had the largest soil organic matter losses. The N use and loss efficiency indicators were especially poor when ley years occurred sequentially and under fall plowing. Total greenhouse gas emissions were, however, smaller for the fall-plowed scenarios. Scenario simulation suggested a modest potential for improving stockless systems by management changes in plowing time or crop rotation, which was hardly affected in the climate change scenarios, although nitrate leaching increased substantially in the winter. In conclusion, alternative strategies seem necessary to substantially improve the N-use efficiency in stockless organic grain production systems, e.g., green manure processing by biogas digestion. Abandoning the stockless system and reintegrating livestock should also be considered.

Keywords:

Agronomic productivity; environmental efficiency; management; climate change; modeling.

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Introduction

By means of ecological processes rather than industrial ones, organic farming aims to produce sufficient food of high quality without deteriorating the environment (IFOAM 2007; Lampkin 1994). Increasing consumer demand and government support have moved organic agriculture from being an ideology-driven niche to a large-scale production. This calls for scrutiny of agronomic and environmental performances (Stockdale et al. 2001; Lynch 2009) and a search for possible improvements towards prevailing goals. Furthermore, productivity and nitrate leaching, especially, have been highlighted as problematic (Kirchmann and Bergström 2008) because nitrogen (N) losses per unit grain produced can be larger than under conventional farming practice (Korsaeth 2008; Knudsen et al. 2006). Losses per unit area of organic agriculture are usually smaller than or similar to conventional agriculture (Hansen et al. 2000; Stopes et al. 2002; Stolze et al. 2000), which has also been measured for N₂O emissions (Chirinda et al. 2010).

In organic farming, N is often considered a fairly scarce and valuable resource (Berry et al. 2002; Doltra et al. 2011), which is likely to be the case in southeastern Norway. Subsidy policy has led to a separation of livestock and arable productions, resulting in a predominance of stockless arable farming in the southeast. Ideally, the availability of inorganic N should be in synchrony with crop demand and little mineral N be lost (Myers et al. 1997), but achieving this is a challenge when N is sourced from decomposing plant litter. The complex cause–effect relationships and variability of causal factors, e.g., climate and litter quality, make it difficult to predict the N mineralization from green manure (Dahlin et al. 2005). Understanding the N dynamics in the system under study is crucial because legumes may provide substantial amounts of N (Thorup-Kristensen et al. 2003; Løes et al. 2011), which under wet, relatively mild climatic conditions and a short growing season may be susceptible to off-season leaching (Korsaeth et al. 2003; Dahlin et al. 2005; Dahlin and Stenberg 2010).

Ecosystem models are useful for understanding a specific situation and the complexity of underlying mechanisms. They may also be used to explore possible management improvements for a range of conditions that would be difficult to cover by field trials (Doltra et al. 2011). Moreover, applying models to case studies allows adaptation of generic knowledge to a local context and may thus be a supplement to general advice given on the basis of field experiments. Case studies are not designed to statistically generalize results (Stake 2000). Hence, case-specific results are not necessarily valid beyond the particular case. Nonetheless, analytical generalisation is possible if case-specific conditions are of current societal interest and reliable observations be linked to existing scientific knowledge (Yin 2003), e.g., as formalized in mechanistic ecosystem models.

Our objectives were to investigate the N dynamics in organic arable agriculture relying exclusively on annual green manures and winter cover crop leys for fertilization and to explore management improvements, by applying a simulation model in a case study. We calibrated the mechanistic Soil Plant Nitrogen (SPN) ecosystem model to data collected from two fields that differed in clover–grass ley management on an organic farm. First, we simulated soil mineral N, crop N uptake, nitrate leaching and denitrified N losses on the farm (2000–2009) in order to evaluate the synchronization of mineralized N and crop N uptake. Second, using historic weather data, we simulated crop rotation scenarios that differed in the number and distribution of clover–grass ley years with fall and spring plowing, respectively. Last, the scenarios were simulated with weather data from the IPCC-predicted A2 climate change scenario (IPCC 2000). Effects of crop rotation, plowing season, and climate change were assessed by productivity and environmental indicators such as the ratios N yield/input, N loss/input and N loss/yield, and greenhouse gas (GHG) emissions.

Materials and methods

Field site of the case study

During 5.5 years (2004–2009) we monitored two fields on *Aschjem* farm in southeast Norway (59°4'N, 10°49'E). Long-term mean annual precipitation is 785 mm and mean temperature during the growing season is 14.3°C. Soil texture was classified as a clay loam with a pH of 6.1 and a bulk density of 1.3 g cm⁻¹. Total carbon (C) and N analysis of soil samples taken in December 2007 showed lower organic matter content in Field 1 (1.9% C and 0.18% N) than Field 2 (2.6% C and 0.24% N) in the 0–20 cm soil depth. Field 1 was converted to organic farming in 2000 and Field 2 in 2003. Prior to the organic farming conversion, both fields were cereal monocultures practiced in two systems: spring barley or oats (1980–1994) and winter wheat (1995–1999). Ley management after conversion to organic farming differed on the two fields. On Field 1, leys were removed after cutting; on Field 2 ley cuttings were left on the field. Cereals were consistently undersown in the spring, either with a 15% white clover (*Trifolium repens*) and 85% perennial ryegrass (*Lolium perenne*) seed mixture when the ley served only as a winter cover crop, or with 32% clover (predominantly red clover; *Trifolium pratense*) and 68% ryegrass when the established ley was kept as an annual green manure ley. The 2004–05 green manure ley on Field 2 had 15% alfalfa (*Medicago sativa*), 27% mixed clovers, and 58% ryegrass. See Table 1 for rotations and management details.

Data collection

Yields for grain and leys were collected from farm records and literature values for nearby locations. For clover–grass leys, we supplemented with field sampling to aid the estimation of the cover crop biomass developed during the spring, cereal growing, and fall seasons. Samples were taken (on 8 May, 25 September and 1 December in 2009) in five replicates by cutting plant material including cereal straw and weeds from 0.25 m² plots, as close to the ground as possible. Fresh samples were separated manually into clover, grass, straw, and weed residue fractions, dried at 60°C for at least 48 hours, weighed, and analyzed for total N content after the *Dumas* method (Bremner and Mulvaney 1982) using a Leco CHN 1000 analyzer (LECO Corp., St. Joseph, MI, USA).

The soil sampling took place thrice a year (March–April, August–September and December) from August 2004 to December 2009. On the first 11 sampling occasions (2004–2007), the soil was sampled to 60 cm depth (0–20, 20–40 and 40–60 cm) as one composite sample consisting of seven auger cores. In December 2007 nine replicate samples of four auger cores each were taken in a sampling grid at three depths. This sampling strategy was continued for the last two years (seven sampling events) but at 0–20 cm depth. Samples were analyzed for mineral N (NH₄⁺ and NO₃⁻) by flow injection analysis according to EPA method 352.2 with a FIASTAR analyzer (Tecator, Höganäs, Sweden).

The Soil Plant Nitrogen (SPN) ecosystem model

SPN is a one-dimensional ecosystem model that simulates C and N dynamics in a system of soil, plants and atmosphere on a daily time step. Originally named SOILN (Johnsson et al. 1987), the model has since been developed and renamed SOILN_NO (Vold et al. 1999b) and later SPN (Bleken et al. 2009). The model has been successfully applied for several climatic conditions and agricultural systems (Blomback and Eckersten 1997; Deelstra et al. 2002; McGeehan et al. 2005; Bleken et al. 2009).

The modeling of the most relevant processes is briefly described below; however, for more details, see supplementary material (SM Text 1). The Nitrosim submodel [see Borgen *et al.* (2011) for details], which simulates C and N transformation, has four organic matter pools: two plant litter, one active humus, and one microbial. Each pool decays according to first-order kinetics defined by specific rate constants and decomposition rate modifiers. The modifiers for temperature and soil moisture are given by a Q₁₀ function (Q₁₀ = 2.5) and a power function, respectively. Additionally, simulated N mineralization is affected by soil frost and plowing (SM Text 1.1).

The maximum potential plant N assimilation is modeled by a simple logistic function (SM Text 1.2), which implies that the simulated N uptake is constrained by the available mineral N in the soil during the

growing season (Vold and Sørensen 1997). Details about the fractionation of plant C and N at harvest (SM Text 1.3), residue incorporation (SM Text 1.4; SM Fig. 1) and green manure addition (SM Text 1.5) are available as supplementary material. Heat and water transport is simulated offline by the Coup model (Jansson and Karlberg 2001; Jansson and Moon 2001), which is based on daily temperature, radiation and precipitation and using soil texture and water retention curves for calculations of soil moisture content and temperature. Leaching is calculated as a function of water flow and NO_3^- concentration, and total leaching is the sum of nitrate reaching the drainage below the soil profile of 120 cm (Johnsson et al. 1987). Denitrification is modeled by the NGAS algorithm, which calculates total denitrification as a function of NO_3^- concentration, soil respiration, water-filled pore space, and soil diffusivity (Del Grosso et al. 2000). The $\text{N}_2/\text{N}_2\text{O}$ -ratio is determined by the ratio of soil respiration to NO_3^- concentration and soil diffusivity.

Model calibration

Parameters were generally set as default values or estimated from literature specific to our conditions (SM Table 1). Calibration of the Coup model can be found in SM Text 2.1. The initialization of the humus pool, which determines the level of background N mineralized, was estimated by a pre-simulation for 1973–2000 as suggested by Bruun and Jensen (2002), and using actual cropping history of the fields. The inert soil C pool can vary between 10 and 50% of total soil C (Petersen et al. 2005); we initialized the pre-simulation with the active humus pool at 75% (i.e., 25% inert) of total C and N measured in 2007. The microbial pool that represents microbial biomass and microbial residues was initialized from the steady-state conditions resulting from the pre-simulation.

Based on farmer-reported crops yields, simulated maximum potential N uptake was estimated using the nonlinear regression functions of Vold *et al.* (1999a). The N uptake of winter wheat and spelt during the fall was set at 2 g N m^{-2} (Thomsen et al. 2010). For pea plants, N uptake was calculated using a harvest index of 0.6, grain N concentration of 3.75%, and assuming that the pea plant derived 62% of its N from fixation (Jensen 1996). Estimation of the growth periods is outlined in SM Text 2.2.

Annual clover–grass ley biomass was simulated to be 413 and 542 g DM m^{-2} for the two fields, values well within those reported from field trials in the region (Brandsaeter et al. 2008; Korsæth and Eltun 2000; Steinshamn and Thuen 2008). The proportion of clover biomass in the ley was estimated at 20% and 30% for first and second cuts in the first green manure year, respectively, and at 40% in second green manure year when the ley was plowed under in the spring. The N contents were assumed to be 2.3% in clover and 1.8% in grass (Jensen et al. 2005). For the winter cover crop leys, we applied the mean values of biomass, clover N content, and the clover percentage from the 2008 field measurements (SM

Table 2), which were in line with those reported by Høgh-Jensen (1997). Below-ground biomass (i.e. roots and rhizodeposition) was set at 53% and 43% of total plant N clover and ryegrass, respectively, based on observations by Høgh-Jensen and Schjørring (2001). Clover was considered to have 81% and 68% of the total C and N, respectively, in the rapidly-decomposing fraction (Borgen et al. 2011), as white clover dominated the leys. The fraction of clover N released upon frost killing was set at 20% of the N assimilated during the fall growth period; a conservative estimate within the reported range by Sturite *et al.* (Sturite et al. 2007).

Alternative crop rotations simulated with historic and future climate

The following five-year crop rotations of spring cereals undersown with white clover–grass leys were constructed (Table 2): continuous cereal (CC), one year of ley (1L), two years of ley (2L), and two years of ley separated by one cereal year (2LS). All rotations were simulated with spring (10 May) and fall (30 October) plowing in the cereal years, except for the 2LS rotation, which gave seven scenarios in total. As annual green manure leys are commonly undersown in the cereal the previous year, these years were not fall plowed. The scenarios were run for two 30-year periods with historic weather data from 1980 to 2009 and a climate change scenario from 2071 to 2100. The weather data used for future simulations were based on the A2 IPCC scenario (IPCC 2000), simulated by a coupled atmosphere–ocean general circulation model, HadAM3 from the Hadley Center (Gordon et al. 2000) and down-scaled to the 55 × 55 km² grid by a combination of dynamic and statistical methods (Engen-Skaugen 2007).

SPN was run with the same parameters and inputs for both historic and future climates and no assumptions were made for effects of climate change on plant productivity. However, regardless of a potential climatic effect, plant growth, as simulated here, was limited by available N because the potential crop N uptake was set substantially higher than the realized simulated values for all scenarios. Most input variables were estimated as for the case farm simulation, but with small differences in the growth period and biomass production (SM Text 2.3).

Results and discussion

Simulations of measured field mineral N dynamics

Simulated mineral N concentrations in the 0–20 cm soil profile were low in both fields (Fig. 1), except for the 2003–2004 season of black fallow for mechanical weeding. Simulations agreed well with measured values of the top soil (SM Fig. 2), as well as, in the deeper soil layers (20–60 cm), where mineral N

concentrations were relatively low ($< 1.5 \text{ g N m}^{-2}$; SM Fig. 2). On Field 2 simulated accumulated N mineralization from 2000 to 2009 was 21 g N m^{-2} higher than in Field 1 (102 and 123 g N m^{-2} for Field 1 and 2, respectively). This was primarily due to larger green manure N inputs on Field 2 than on Field 1, rather than the larger initial humus pool values (SM Table 3).

In most of the years, simulated cereal yields were equal to those from farmer's reports ($3500\text{--}4500 \text{ kg ha}^{-1}$), except on Field 1 in 2006, where oats yield were simulated to be 2750 kg ha^{-1} . The reported yields were similar to or in the upper range of those measured for stockless organic arable systems at comparable locations (Korsaeth 2008; Nykanen et al. 2009; Løes et al. 2011).

A freeze–thaw effect on N mineralization (DeLuca et al. 1992) was visible in the field N dynamics as the modeled rapid-N pool pulse was followed by an increase in mineral N for most years (results not shown). The simple soil frost effect in SPN (SM Text 1.1) that allows mineralization to continue down to -1°C , agrees with experimental findings (Cookson et al. 2002; Henriksen and Breland 1999). Although the modeled effect does not consider that net N mineralization can occur at lower temperatures from materials that cause net N immobilization at higher temperatures (Henriksen and Breland 1999; Magid et al. 2004; Magid et al. 2001), it seemed to provide an adequate approximation of the springtime mineral N measured (Fig. 1).

Great variability in the fraction of clover N that is lost during winter was measured in a field experiment in the region (Sturite et al. 2007; Sturite et al. 2006) and our estimate of 20% may be on the conservative side. But a sensitivity test varying this percentage from zero to 100% (equivalent to 0.4 g N m^{-2}) showed that the amount of clover N released due to frost damage, was not crucial for soil mineral N concentrations or NO_3^- leaching as it was a small part in the annual field N dynamics.

Simulated leaching and denitrification N losses

Simulated N losses from leaching were larger than from denitrification. Mean annual leaching for the organic years was similar on both fields (Field 1: $4.3 \pm 1.1 \text{ g NO}_3^- \text{-N m}^{-2} \text{ yr}^{-1}$, Field 2: $4.8 \pm 0.5 \text{ g NO}_3^- \text{-N m}^{-2} \text{ yr}^{-1}$). Our simulated values were slightly higher than measured drainage losses in a similar stockless organic crop rotation (Korsaeth 2008; Korsaeth and Eltun 2000). The intensive mechanical weeding, which lasted from October 2003 to September 2004, resulted in an annual leaching loss of 12.7 g N m^{-2} from Field 1 in 2004 (Fig. 2). Black fallow was initiated by plowing a clover–grass ley, causing an accumulation of N-rich plant residues and high soil mineral N contents (Fig. 1). Consequently, large NO_3^- leaching losses occurred during the subsequent winter (Fig. 2). Field 2 was also under mechanical weed control that year, but it was not initiated by plowing and a ley was sown in June 2004. These results indicate that weeding by repeated harrowing does not necessarily result in large leaching loss if the fallow

is not initiated by plowing and a ley is sown in June. However, the validity of this conclusion depends on if the transient flush of mineral N that is often observed after plowing fallow soil (Silgram and Shepherd 1999; Calderon et al. 2001) was adequately implemented in the model.

On Aschjem farm, weed infestations occurred especially after field peas, which confirms the weak competitive ability of this crop (Lundkvist et al. 2008). Designing a diversified crop rotation is the main strategy to control weeds in organic farming (Lampkin 1994), and our leaching estimates emphasize that mechanical control should be minimized. Pea was mainly grown as a sole crop. Intercropping (e.g., with barley or oats) may have weed suppressing effects (Szumigalski and Van Acker 2005), and thus could alleviate the severe consequences of black fallow, in terms of N loss, absence of plant production and, most probably, accelerated soil erosion and organic matter losses.

Simulated denitrification losses were lower on Field 1 ($1.8 \pm 0.2 \text{ g N m}^{-2} \text{ yr}^{-1}$) than on Field 2 ($2.5 \pm 0.2 \text{ g N m}^{-2} \text{ yr}^{-1}$; mean of the seven organic years), both of which are somewhat higher than values simulated for comparable organic systems (Korsaeth and Eltun 2000; Nykanen et al. 2009; Korsaeth 2008). Mean annual N_2O emission for the organic years were between 0.83 and 1.11 $\text{g N}_2\text{O-N m}^{-2}$ for the two fields, similar to measured fluxes on clover–grass pastures in Germany (Kaiser et al. 1998). The N_2O percentages of total denitrification 44% (Field 1) and 34% (Field 2) were also within the range of values reviewed by Schlesinger (2009). However, although fine-scale temporal fluctuations in N_2O emission are not always captured in simulations, previous testing of our model algorithms supports that treatment means aggregated to annual or greater scales are usually fairly accurate (Del Grosso et al. 2008).

Crop rotation scenarios

Single-year grain yields were highest (4820 kg ha^{-1}) for the rotation with two ley years separated (2LS) and lowest for the continuous grain rotation (CC) where clover–grass was undersown as a winter cover crop only (Fig. 3). In spite of low single-year grain yields, the spring-plowed CC rotation had the highest system productivity (i.e., yearly average of grain yield accumulated during the whole rotation). Thus single-year grain yield increase by annual green manure leys did not compensate the absent grain yields in the green manure years (Fig. 3), corroborating results from an experimental study (Løes et al. 2011).

Nitrogen losses through denitrification were highest for 2LS, which was significantly larger than for the 2L rotations where the two ley years were successive (Fig. 3). This was probably due to the larger N mineralization in the 2LS compared to the 2L of $2 \text{ g N m}^{-2} \text{ yr}^{-1}$ (30-year mean) caused by the more frequent plowing of 2 LS. For nitrate leaching, increasing the number of ley years had no significant effect on NO_3^- leaching, neither for spring nor fall plowing regimes (Fig. 3).

Comparing the N use efficiency indicators for continuous grain and two-year ley rotations revealed interesting differences in the N dynamics. Efficiency for grain production (N yield/input) was highest for continuous grain cropping, reduced with increasing number of ley years, and was smallest for the 2L rotations (Table 3). The same pattern was seen for the N use efficiency regarding losses (N loss/yield). However, the N loss/input ratio showed that plowing season was more influential than number of ley years, as 2L had both the highest and the lowest value for fall and spring plowing, respectively (Table 3). Also, the results indicate that two consecutive ley years in a 5-year rotation significantly limits the utilization efficiency of N added in green manure. Separating the two years of ley (2LS) was better than successive ley years for the yield/input ratio and loss/yield ratio, but not for the loss/input ratio (Table 3). This may be explained by the positive C sequestration and smallest net N-humus mineralization for 2LS (SM Table 2). Although 2LS was plowed more frequently and received larger green manure inputs than 2L, total N input (calculated for the ratios) was smaller because the larger grain yield of 2LS returned more straw to the field, increasing C storage and retaining N in soil organic matter. In the model, the constant C/N ratio of the humus pool ($C/N = 10$) determines that net humus N mineralization is a consequence of humus respiration and thus influenced by C inputs. The substantial mineralization of soil organic matter (i.e., the humus pool) was the main contribution to N sustaining the large yields of the CC rotations (SM Table 5). Thus N inputs from a winter cover crop of clover–grass, as the only fertility-building element, are inadequate for maintaining yields and depreciate the soil humus resource. This is essentially unsustainable in the long term, as the more rapid decomposition of soil organic matter deteriorates soil fertility.

Our results highlight the difficulty of designing stockless organic grain production systems that are productive per area and N input, while maintaining soil organic matter levels and losing little N per grain yield or N input (Kirchmann and Bergström 2008; Korsæth 2008). Doltra *et al.* (2011) concluded from a study in Denmark, encompassing field trials and scenario simulations with the FASSET model, that organic grain yields were N limited and that yields could be increased by N fertilization without significantly increasing N leaching, provided an adequate use of catch crops. In Norway, where temperature-limited mineralization early in the growing season is likely to constrain plant growth, the search for sources of relatively readily plant-available N is particularly relevant. It may be hypothesized that different green manure species could improve the N use efficiency of stockless grain systems. Considering the substantial differences in N mineralization patterns observed for clover species in laboratory incubations (Marstorp and Kirchmann 1991; Jensen *et al.* 2005), it is likely that the litter quality of the green manure influences field N mineralization dynamics and, thereby, grain yield and leaching losses. However, our model testing indicated that effects of different clover species were miniscule (SM Table 4). Consequently, management strategies attempting to optimize production and

environmental efficiency by using specific green manure or clover species do not seem particularly promising. Processing clover-grass biomass by anaerobic digestion for biogas may reduce N losses compared to application of fresh materials. Application of biogas digest was found to increase grain yield and grain N content compared to fresh green manure fertilization (Stinner et al. 2008). However, effects on soil microbial activity and physical properties caused by biogas residue amendment are yet to be determined (Arthurson 2009).

It should be kept in mind, though, that continuous grain cropping with undersown clovers may have several other productivity-related issues that are not accounted for in the model simulations. These may include the accumulation of phytosanitary problems, perennial weed and aphid infestations, and that denser plant stands, with a more humid microclimate, are more conducive to fungal diseases. Thus our results on productivity and N dynamics represent an important but, of course, not the only perspective of a functioning organic cereal rotation.

Plowing season scenarios

The scenario simulations showed that plowing in the spring, rather than the fall, increased grain yields both for the CC and 1L rotations. This was partly caused by the larger green manure inputs of 2.9 and 2.5 g N m⁻² yr⁻¹ for the CC and 1L rotations, respectively (SM Table 5), and also, by an increased N mineralization during the growing season. When switching from fall to spring plowing in the 1L crop rotation, roughly 20% of the total annual N mineralization occurred in the growing season instead of in the fall and, consequently, a better N synchronization was facilitated (Fig. 4). This was reflected in the annual nitrate leaching losses, which decreased by 28% (CC), 32% (1L), and 39% (2L) with spring plowing (Fig. 3). These findings agree with field observations showing less leaching with spring plowing (Korsaeth et al. 2002; Djurhuus and Olsen 1997). Denitrification losses, on the other hand, were substantially larger with spring plowing (Fig. 3). Losses primarily increased during the growing season (Fig. 4), probably because spring plowing simultaneously increased N mineralization and soil microbial respiration in this period compared to fall plowing (Fig. 4). Nitrous oxide emissions were largest in the winter for both plowing times, but spring plowing decreased emissions both in the winter and spring compared to fall plowing (Fig. 4). Furthermore, the percentage of denitrification N losses emitted as N₂O was smaller with spring (47–50%, depending on rotation) than fall (43–44%) plowing scenarios.

Whole-rotation yield N efficiency was improved by spring plowing, especially in the CC rotation (Table 3). The 2L rotation was an exception due to fewer years with fall plowing. However, spring plowing can be a practical challenge as factors related to soil structure and moisture may be negatively affected. Reduced growing season length, increased likelihood of water shortage at early growth stages,

and more difficulties with mechanical control of perennial weeds in autumn are important considerations. The N loss efficiency indicators were smaller for spring than fall plowing (Table 3), because total N losses were similar (SM Table 5); denitrification losses were larger but leaching losses smaller with spring plowing (Fig. 3). Total GHG emissions were larger for the spring-plowed rotations in spite the smaller CO₂ emissions from humus mineralization, which were reduced by 54% and 72% for CC and 1L, respectively (SM Table 5). The direct N₂O emissions made up the majority of the GHG emissions budget (SM Table 5). Our findings support the arguments of Li *et al.* (2005) that managing agricultural systems for C sequestration will increase emissions of N₂O emissions, which are more important in the total GHG budget.

Climate change scenario

Climate change increased grain yields by 1–8% (Fig. 3). This agrees with the biomass (or net primary productivity) increases found in Nordic ecosystems simulated under climate change conditions (Jansson *et al.* 2008). The yield increases could be attributed to the larger N mineralization (3–6%) under the future climate, because the seasonal distribution of the mineralization was hardly affected (Fig. 5). In spite of the larger plant N uptake, leaching losses increased by 9–18% compared to the historic climate (Fig. 3). Losses occurred primarily off season; winter leaching increased by 21% compared to the historic climate in the simulation of the 1L spring-plowed rotation (Fig. 5). Mean annual temperature increased 3.7°C, compared to the historic average (1961–1990), which caused 44 less simulated freeze–thaw events over 30 years. A reduction in such events would decrease the mineral N concentration in the soil, but the prolonged period of off-season water flow outweighed this effect, thus resulting in an overall increase in nitrate leaching.

Denitrification was reduced by 4–7% (Fig. 3) due to the less frequent frost events and drier summers. Freeze and thaw cycles have been held responsible for large annual field fluxes (Johnson *et al.* 2010) possibly due to the release of organic substances (Mørkved *et al.* 2006). However, denitrification was probably affected more by the drier summers because the soil moisture decomposition modifier decreased by 17% and the majority of the annual denitrification losses occurred during the summer (Fig. 5).

The effect of climate change on the N efficiencies indicators was marginal (Table 3). Drier summers and autumn seasons, combined with a rise in temperature, led to a 36% increase in the yearly average value of the decomposition response modifier (Fig. 5). The increased N input (primarily a result of increased humus mineralization; SM Table 5) was proportional to the increase in N losses and N yield, resulting in a small effect on the efficiency ratios. Estimated GHG emissions were slightly reduced, which was primarily the result of reduced direct N₂O emissions.

The increased off-season leaching losses predicted with climate change emphasize the need for maintaining crop cover year round under the Nordic weather conditions. Management options such as plowing time, ley rotation and, especially, weeding strategy will be more important in the future climate in order to avoid large leaching losses and to improve N use efficiency of arable organic farming. Our findings suggest that climate change will deteriorate N synchronization, and the use of catch crops to minimize leaching may become more important.

Conclusions

Model analyzes of the N dynamics and N use efficiency on stockless organic grain production systems showed the challenges associated with simultaneous pursuing short- and long-term productivity as well as environmental goals. Continuous cereal cropping undersown with clover-grass as a winter cover crop plowed in the spring gave the highest simulated whole-rotation grain yield and best N use efficiency (in terms of productivity and environment) but also the largest reductions in soil organic matter compared to rotations including annual green manure leys. This study indicates that the potential to improve stockless organic systems by crop rotation and plowing season is modest and alternative strategies should be sought. Improvements could include using green manure for biogas digestion or recycling municipal waste. Abandoning the stockless system and reintegrating livestock would generate economically-valued products (milk and meat) from the energy and N in clover-grass biomass, as well as produce animal manure. Under future climate simulations, N-use efficiency was marginally affected however management options reducing nitrate leaching will become especially important in organic rotations as N synchronization appears to worsen with the wetter and warmer winters that are expected in this region.

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Table 1 Crop rotation and management for Fields 1 and 2 during the simulation period.

Field 1					Field 2				
Year	Month /day	Arable phase	Month /day	Ley phase	Year	Month /day	Arable phase	Month /day	Ley phase
2000		(Grass ley)	6/20	Grass ley harvested	2000	8/25	Wheat harvest (C)		Stubble
			9/29	Grass ley harvested					
2001	5/16	Oats sown	5/16	Red clover ley sown	2001	5/14	Oats sown (C)	5/12	Plowing
	9/29	Oats harvest				9/17	Oats harvest	7/18	Grass ley sown
2002		(Green manure)	7/13	Ley cut removed	2002	5/8	Wheat sown (C)	5/6	Ley plowed
			8/30	Ley cut removed		8/17	Wheat harvest		Stubble
2003	5/8	Oats sown	5/7	Ley plowed	2003	5/29	Peas sown	5/10	Plowing
	8/26	Oats harvest	5/8	White clover ley sown		9/4	Peas harvest		
			9/6	Ley cut left on field	2004		Black fallow weeding	6/26	Plowing
			10/15	Ley plowed				6/29	Red clover ley sown
2004		Black fallow weeding	5/27	Plowing			(Green manure)	8/13	Ley cut left on field
			9/7	Plowing				8/28	Ley cut left on field
	9/10	Spelt sown			2005		(Green manure)	5/13	Ley cut left on field
2005	8/7	Spelt harvest	4/17	White clover ley sown				5/10	Ley cut left on field
			8/19	Ley cut left on field				6/24	Ley cut left on field
			9/11	Ley cut left on field		9/10	Rye sown	7/19	Ley cut left on field
			9/25	Ley cut left on field				9/8	Ley plowed
2006	5/13	Oats sown	5/12	Ley plowed	2006	5/13	Wheat sown	5/12	Rye plowed up
	8/30	Oats harvest	6/1	White clover ley sown		8/30	Wheat harvest	5/13	White clover ley sown
	9/13	Spelt sown	9/11	Ley plowed	2007	5/4	Oats sown	5/1	Ley plowed
2007	8/6	Spelt harvest	3/22	White clover ley sown		8/22	Oats harvest	6/5	White clover ley sown
2008	5/4	Oats sown	5/1	Ley plowed	2008	5/14	Oats sown	5/13	Ley plowed
	8/22	Oats harvest	6/13	Red clover ley sown		9/22	Oats harvest	6/13	White clover ley sown
2009		(Green manure)	6/20	Ley cut removed	2009	5/2	Peas sown	4/30	Ley plowed
			9/11	Ley cut removed		8/19	Peas harvest	9/16	Plowing
						9/17	Spelt sown		

C: conventional

Table 2 Four alternative crop rotations simulated with historic weather data and a climate change scenario. All rotations were simulated with spring (10 May) and fall (30 October) plowing, except 2LS for which only spring plowing was simulated.

Year	Continuous cereal (CC)	One year ley (1L)	Two year ley (2L)	Two year ley separated (2LS)
1	Spring cereal	Spring cereal	Clover–grass	Spring cereal
2	Spring cereal	Clover–grass	Clover–grass	Clover–grass
3	Spring cereal	Spring cereal	Spring cereal	Spring cereal
4	Spring cereal	Spring cereal	Spring cereal	Clover–grass
5	Spring cereal	Spring cereal	Spring cereal	Spring cereal

Table 3 Nitrogen efficiency indicators (N loss and grain N yield) and greenhouse gas (GHG) emissions from seven rotations in historic and future climate. For crop rotation acronyms, see Table 2.

Crop rotation	CC		1L		2L		2LS
	Fall	Spring	Fall	Spring	Fall	Spring	Spring
<i>Historic climate</i>							
N yield*/input** ratio	0.62	0.67	0.58	0.60	0.50	0.38	0.54
N loss§/yield ratio	0.75	0.59	0.86	0.71	1.11	0.92	0.90
N loss/input ratio	0.47	0.39	0.49	0.43	0.55	0.35	0.48
GHG§§ emissions (g CO ₂ -eq m ⁻²)	297	309	326	353	345	314	392
<i>Future climate</i>							
N yield/input ratio	0.61	0.66	0.56	0.60	0.50	0.40	0.53
N loss/yield ratio	0.78	0.58	0.89	0.70	1.04	0.88	0.90
N loss/input ratio	0.48	0.38	0.50	0.42	0.52	0.35	0.48
GHG emissions (g CO ₂ -eq m ⁻²)	287	308	315	346	324	323	384

*Grain N yields are the mean of 30 years and assumed to be 50% of total plant N assimilated.

**N inputs include: N-fixation (0.2–5.4 g N m⁻² yr⁻¹), net humus (3.0–6.2 g N m⁻² yr⁻¹) and microbial pool mineralization (0.04–1.6 g N m⁻² yr⁻¹), and wet and dry deposition (0.75 g N m⁻² yr⁻¹).

§ N loss is the sum of denitrification and leaching.

§§ GHG emissions include: direct N₂O from denitrification, indirect N₂O assumed to be 1.25% of leached NO₃⁻, and CO₂ emission as the change of soil organic C of the humus pool. The radiating force of N₂O relative to CO₂ is 298.

Figures

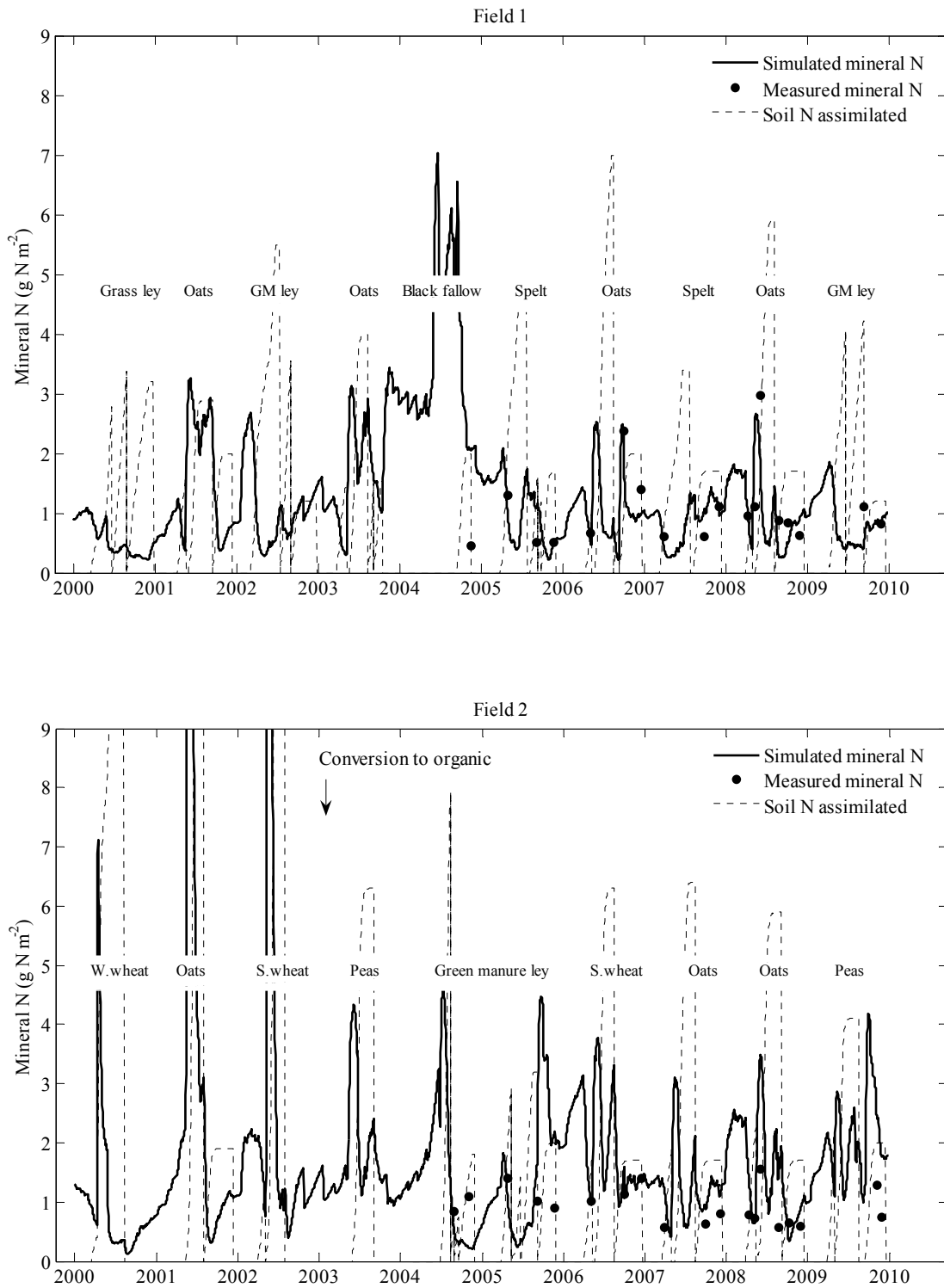


Fig. 1 Measured and simulated soil mineral N on the two fields in 0–20 cm soil depth and simulated plant assimilation of soil mineral N. GM: Green manure.

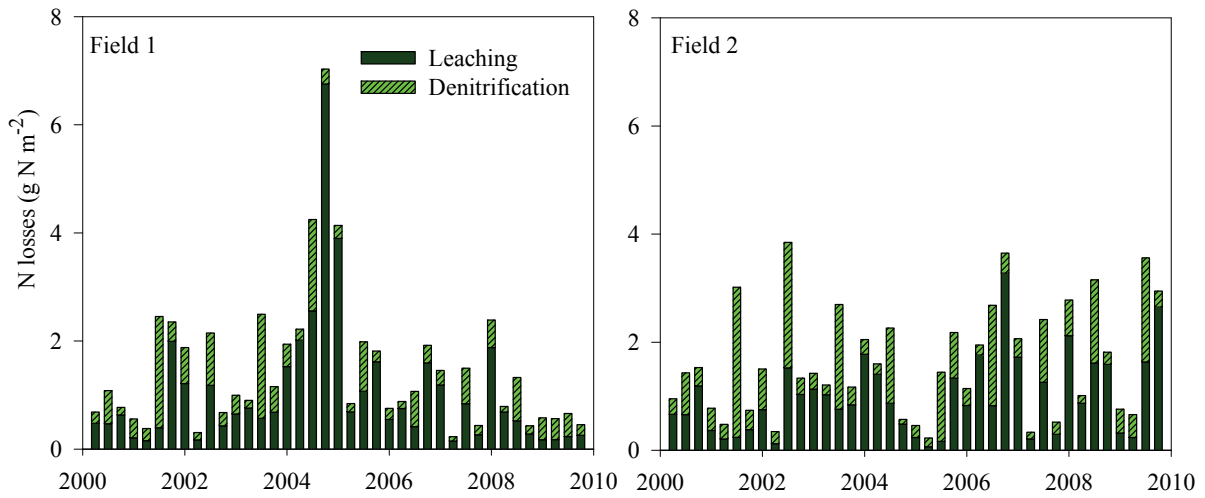


Fig. 2 Leaching and denitrification losses on Fields 1 and 2, summed over spring (15 March – 30 April), growing season (1 May – 25 September), fall (26 September – 30 November) and winter (1 December – 14 March).

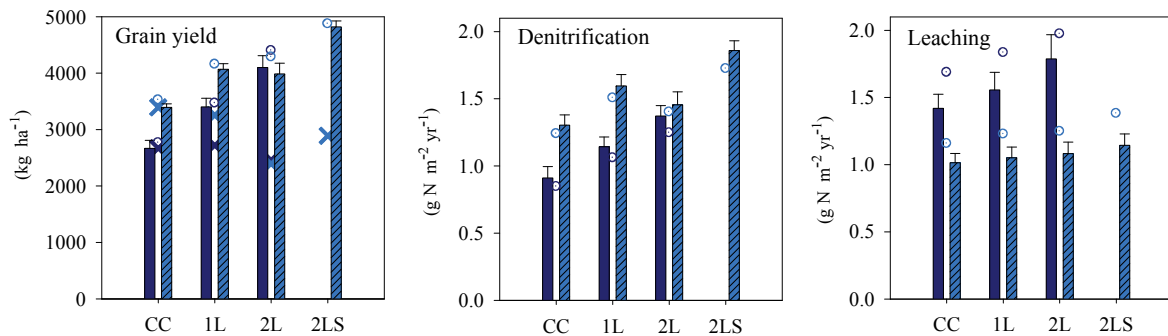


Fig. 3 Predicted cereal grain yields (kg ha^{-1}), denitrification ($\text{g N m}^{-2} \text{yr}^{-1}$), and nitrate leaching ($\text{g N m}^{-2} \text{yr}^{-1}$) of the simulated alternative crop rotations with fall (black bars) or spring (grey bars) plowing. Standard error bars shown with $N = 30$, except for grain yield, for which N equals the number of grain years in the rotation. Dots show values for climate change effects, color coded as the bar. Whole-system productivity is indicated by crosses, showing accumulated grain yield for the whole simulation period divided by its length (30 years). Grain yields reported with water content of 15%.

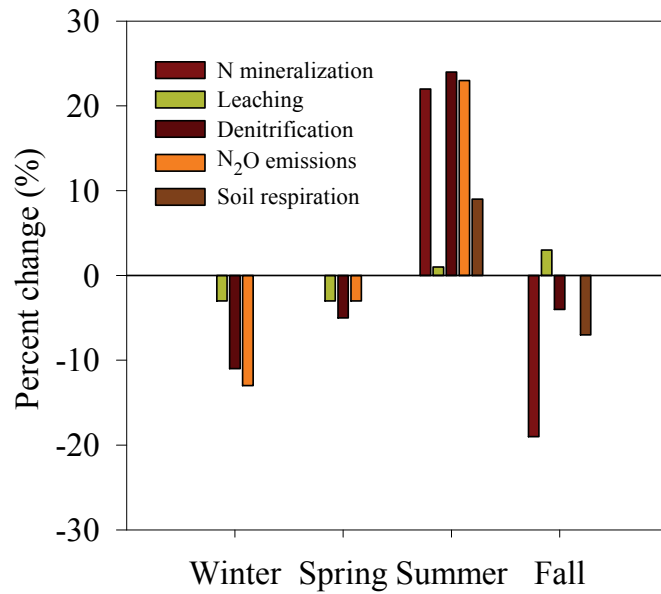


Fig. 4 Effect of spring instead of fall plowing on the seasonal distribution of N mineralization, nitrate leaching, denitrification, N₂O emission, and soil respiration simulated for the 1L rotation.

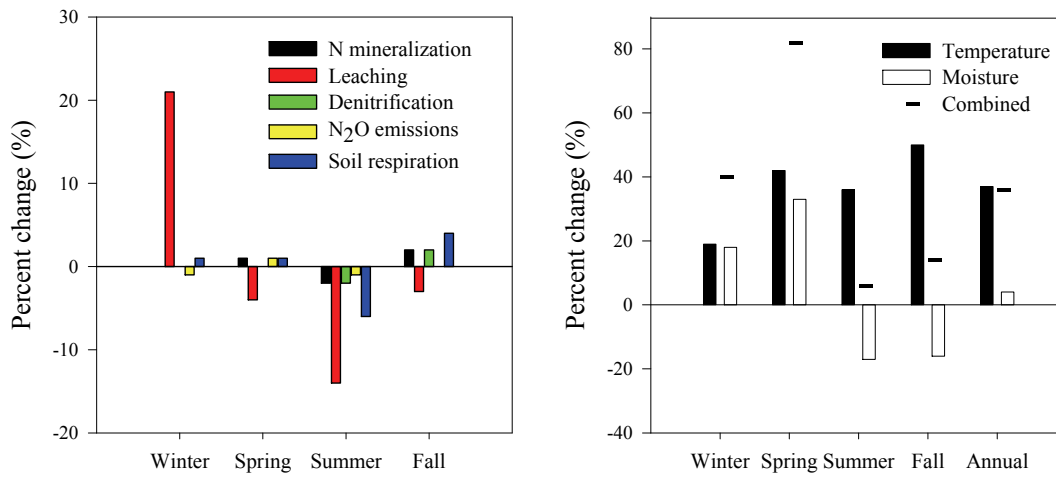


Fig. 5 Climate change effects on N mineralization, leaching, denitrification, N₂O emissions, and soil respiration simulated for the 1L rotation under spring plowing (left) and on yearly average values of decomposition rate modifiers for temperature, moisture and the combined temperature and moisture product (right).

Supplementary Materials

SM Text 1. Description of the SPN (Soil Plant Nitrogen) model

1.1 Frost and plowing events

Two event-driven features are implemented to emulate the response to plowing (Silgram and Shepherd, 1999; Calderon *et al.*, 2001) and soil freeze-thaw events on N mineralization (DeLuca *et al.*, 1992). Upon plowing, 15% of the microbial pool is transferred to a temporary pool with a rapid turnover of 0.2 day^{-1} . The C and N in the rapid pool decay with the same microbial growth yield ($f_c = 0.3$) and flows back to the microbial pool, which results in a noticeable net N mineralization. In the case of soil frost ($T < -1^\circ\text{C}$) for more than five days, 10% of C and N biomass is transferred to this pool.

1.2 Plant N uptake

The maximum projected plant uptake of soil mineral N is modeled by a simple logistic function, where plant N at a given time ($U_{(t)}$) is given by the following equation:

$$U_{(t)} = U_a / (1 + ((U_a - U_b) / (U_b) \times e^{(U_c \times t)})),$$

where U_b and U_c are shape parameters and U_a is the total maximum crop N uptake (Vold and Sørensen, 1997). The simulated N assimilation is constrained by the available mineral N in the soil during the growing season. The logistic N uptake function represents the maximum trajectory for plant N through the defined growth period. When the amount of available N at the beginning of the season is lower than that predicted by the function, this can be compensated for by a higher uptake rate later in the season if mineral N becomes available. Thus, plant N converges towards the trajectory if sufficient N is mineralized.

1.3 Plant fractionation at crop harvest

At the end of a simulated growth period, N in plant biomass is divided into various plant parts, according to the fraction of N assumed to be in living roots (*lr*), dead roots (*dr*), surface residues (*sr*), incorporated residues (*inc*), and harvested material (*hp*; Fig 1). In each fraction, an amount of C is included according to the C/N-ratio of the different plant parts (given by separate parameters). Dead roots (*dr*) and incorporated residues (*inc*) are transferred to litter pools at harvest or end of the growth period. To divide the plant material into the residue N fractions (*lr*, *dr*, *sr*, *inc*, and *hp*), we applied four sets of fractionation parameters which were determined by agricultural and seasonal events: 1) cereal harvest, 2) cereal or ley freezing, 3) ley harvest and removal, and 4) ley cutting without removal. The C/N-ratios for above- and below-ground plant materials were specific to the following three categories: cereals, ley, and plants (cereal and ley) freezing. Each plant material has a specific litter pool partitioning (LPP) parameter that determines the fraction of plant C and N assigned to the

easily-decomposing litter pool. The remaining C and N (1-LPP) is assigned to the slowly-decomposing litter pool.

1.4 Residue incorporation routine

The transfer of plant material to the litter pools is a crucial part of the model, as it determines the effect of crop growth, harvest, and tillage on the seasonal distribution of N mineralization and immobilization. Plant residues, as modeled, enter the litter pools in two ways: via continuous decay of live roots and surface residues or as immediate transfer at harvest or during soil tillage. The C and N in living root material and surface residues flow continuously into the litter pools from the temporary *SurfRes* and *RootRes* pools (Fig 1) as a constant daily fraction (0.015 day^{-1} and 0.10 day^{-1} , respectively). Upon tillage, these pools are emptied and all C and N are transferred to the litter pools. If there is no tillage between two (or more) subsequent crops, the temporary pools accumulate. For ley, each period between two harvests is treated as a separate crop. Thus, there are four ‘crops’ per year in the AGM ley: one crop from spring to the first harvest, two crops between the two harvests, and the final crop from the last harvest to plant growth arrests in the late fall or onset of winter. For the winter cover crop ley, assimilation takes place in two stages, from cereal harvest to onset of winter and from spring thawing to plowing.

1.5 Green manure addition routine

The simulation of legumes and their biological N fixation (BNF) is simple, requiring total clover-grass biomass, C and N content, and percentage of N derived from the atmosphere as inputs. The biomass derived from BNF enters the litter pools as a single input of green manure at ley harvesting, plowing, or frost. The plant N assimilation and residue incorporation of the non-BNF-derived biomass (conceptually, the grass crop since we assumed clover derived 100% of its N from fixation) is simulated as described above. The clover quality is given by the LPP parameters, which for green manure may be different for C and N, and C/N-ratios of the green manure entering the two litter pools (CN_{L1} and CN_{L2} ; SM Table 1). This feature of Nitrosim was advantageous, compared to keeping the same LPP for C and N, when simulating C and N mineralization from plant litter of various quality (Borgen *et al.*, 2011).

SM Text 2. Model Calibration

2.1 The heat and water transport model

The heat and water transport model; Coup, was calibrated using daily temperature, precipitation data and calculated potential evapotranspiration from a nearby weather station for 1973–2009. The pF

curves applied were taken from a nearby experimental field with similar soil texture (clay content 18%) with water volume of 33 and 9.2% for field capacity and wilting point, respectively.

2.2 Growth periods in the case study simulations

Cereal growing period started 10 days after sowing data and terminated 15 days before harvest, thus assuming that all uptake of mineral N had ceased at grain maturity. The growing period for the subsequent clover-grass ley, which had been undersown together with the cereal, was modeled to start immediately after grain maturity. The onset of the spring growth period was marked by soil temperatures above 0 °C without further soil freezing (occurred between 7 March and 15 April). The end of the growing period was marked by snow cover or soil temperature below 0 °C and not followed by more than a 1 °C increase (occurred between 27 November and 24 December).

2.3 Scenario simulations

The growing period for spring cereal was set from 15 May to 15 September with the same assumptions for seed germination and grain maturity as for the case study simulations. Fall plowing (30 October) allowed sowing 10 days earlier than the spring plowing (10 May). The end and beginning of the fall and spring growth period were fixed; N assimilation stopped on 1 November and resumed on 31 March. The N concentration of clover and grass and the winter cover crop biomass were estimated as for the case study simulations. Annual green manure leys were estimated at 550 g DM m⁻² yr⁻¹ from two cuttings (20 June and 10 September) with clover assumed to comprise 41 to 70 % of the ley biomass, depending on the time of the year. The soil organic matter pools (active humus and microbial biomass) were initialized as per Field 1.

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Supplementary Tables

SM Table 1 Default and estimated model parameter values

Parameters	Value	Parameters	Value
Residue routine		Nitrosim submodel	
<i>C/N-ratios of plant material arriving from:</i>		Decay of litter 1 pool (k_{L1})	0.099 day ⁻¹
Grain roots	50	Decay of litter 2 pool (k_{L2})	0.0025 day ⁻¹
Grain ARES	61	Decay of humus pool (k_H)	0.000085 day ⁻¹
Grass roots	50	Decay of microbial pool (k_B)	0.002 day ⁻¹
Grass ARES	38	Microbial growth yield (f_c)	0.30
Ley roots	33	Humification fraction (f_h)	0.34
Ley ARES	33	Humus pool C/N-ratio (CN_H)	10
Green manure to litter 1	19	Microbial pool C/N-ratio (CN_B)	7.1
Green manure to litter 2	22		
<i>LPPs of plant material arriving from:</i>		Logistic crop N uptake function	
Grain root	0.4	Max daily assimilation	0.08 day ⁻¹
Grain ARES	0.49	U_b (shape parameter)	0.10
Grass roots	0.4	U_c (shape parameter)	0.15
Grass ARES	0.52		
Ley roots	0.4	Atmospheric N deposition	
Ley ARES	0.43	Dry	0.000423 g N day ⁻¹
<i>Temporary pool for frost and plow effects</i>		Wet	0.000767 g N L ⁻¹
Decay rate (k_F)	0.20 day ⁻¹		
<i>Continuous residue transfer</i>		Nitrification	
Fraction of surface residues	0.10 day ⁻¹	NO_3^-/NH_4^+ -ratio	10
Fraction of roots	0.015 day ⁻¹	Nitrification rate	0.05 day ⁻¹

ARES: aboveground residues, LPP: litter pool partitioning parameters, i.e. fraction of plant C or N assigned the easily-decomposing litter 1 pool.

SM Table 2 Measured clover and grass N content and biomass estimates (mean \pm SE). Means for the two fields of total clover and grass biomass was used to estimate simulated winter cover crop productivity. Number of observations $N=9$.

	N content (%)				Biomass (g DM m ⁻²)						
	Clover		Grass		Clover		Grass		Total (clover + grass)		
	Field 1	Field 2	Field 1	Field 2	Field 1	Field 2	Field 1	Field 2	Field 1	Field 2	Mean
May	4.7 \pm 0.3	3.7 \pm 0.05	3.6 \pm 0.3	2.6 \pm 0.1	36 \pm 2.7	10 \pm 6.7	26 \pm 11	76 \pm 21	62	86	74
Sep/Oct	3.4 \pm 0.1	3.6 \pm 0.2	2.9 \pm 0.1	3.0 \pm .05	3 \pm 1.1	13 \pm 4.8	18 \pm 3	18 \pm 3.3	21	31	26
Dec	3.5 \pm .01	3.5 \pm 0.2	3.0 \pm 0.1	3.4 \pm 0.1	7 \pm 4.1	5 \pm 2.6	34 \pm 5	38 \pm 3.2	41	43	42

SM Table 3 Simulated cumulative N mineralization over three time periods for Field 1 and Field 2, and Field 2* when the initial humus values of Field 1 were applied. Green manure inputs were greater on Field 2 than Field 1 during 2005 to 2009.

Period	Field 1	Field 2	Field 2*
	N mineralization (g N m ⁻²)		
2000-2009	102	123	120
2000-2005	57	60	61
2005-2009	43	66	59

SM Table 4 Differences in grain yield, nitrate leaching and N mineralization when spring plowed scenario 1L was run using either red or white clover litter pool partitioning (LPP) parameters estimated by (Borgen *et al.*, 2011).

	Grain yield (g DM m ⁻²)		Leaching (g NO ₃ ⁻ -N m ⁻² yr ⁻¹)		N mineralization (g N m ⁻² yr ⁻¹)	
	White	Red	White	Red	White	Red
Mean \pm SE	236 \pm 5.7	238 \pm 5.4	1.05 \pm 0 .08	1.07 \pm 0.08	11.80 \pm 0.34	11.91 \pm 0.35

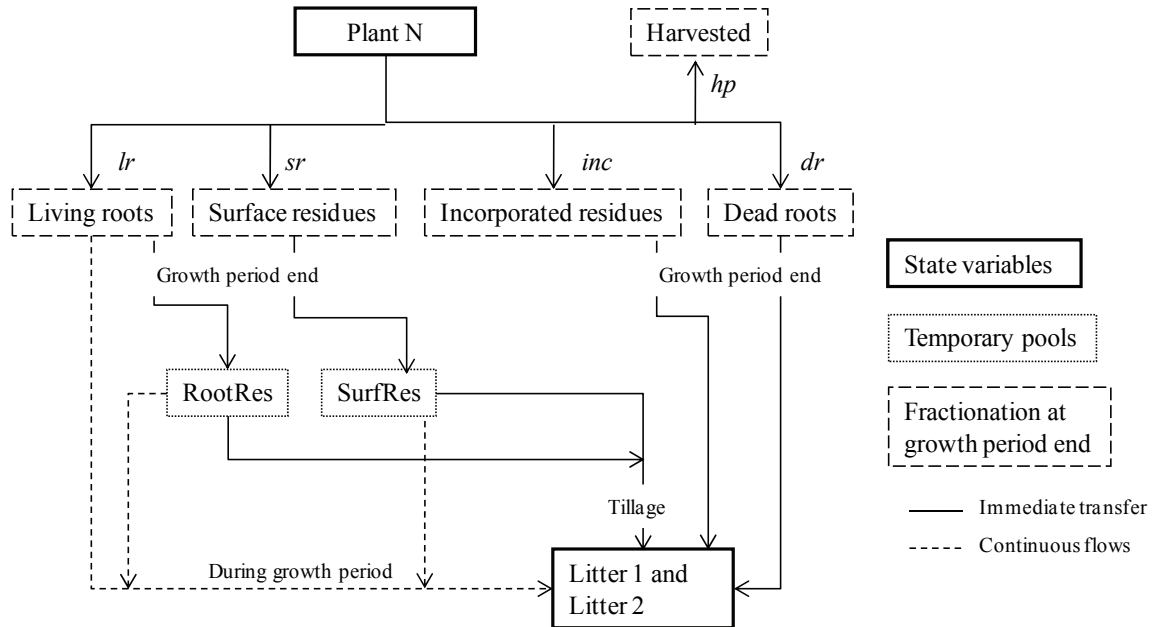
SM Table 5 Calculations for N use efficiency indicators and GHG emissions for all scenario simulations.

Crop rotation	CC		1L		2L		2LS
Plowing time	Fall	Spring	Fall	Spring	Fall	Spring	Spring
<i>Historic climate</i>							
(30-year mean values) (g N m ⁻² yr ⁻¹)							
N fixation by green manure	0.20	3.10	1.80	4.30	3.30	5.30	5.40
Net microbial mineralization	1.60	0.81	1.23	0.49	0.79	0.55	0.06
Net humus mineralization	2.50	1.33	1.77	0.73	1.00	0.70	0.13
Total inputs (including deposition)*	5.06	6.01	5.56	6.28	5.85	7.31	6.35
Grain N yield**	3.15	4.00	3.20	3.80	2.90	2.80	3.40
N loss (denitrification + leaching)	2.38	2.36	2.75	2.69	3.21	2.58	3.05
Greenhouse gas emissions: (g CO ₂ -eq m ⁻² yr ⁻¹)							
Indirect N ₂ O§	8.5	6.1	9.3	6.3	10.6	6.5	6.9
Direct N ₂ O	217	270	267	332	309	293	390
CO ₂ from change soil humus C	72	33	50	14	25	14	-5
<i>Future climate</i>							
(30-year mean values) (g N m ⁻² yr ⁻¹)							
N fixation by green manure	0.20	3.10	1.80	4.30	3.30	5.30	5.40
Net microbial mineralization	1.60	0.84	1.25	0.48	0.79	0.51	0.04
Net humus mineralization	2.77	1.57	2.03	0.93	1.30	0.97	0.33
Total inputs (including deposition)*	5.33	6.27	5.84	6.47	6.15	7.54	6.54
Grain N yield**	3.25	4.15	3.25	3.90	3.10	3.00	3.45
N loss (denitrification + leaching)	2.53	2.40	2.89	2.73	3.22	2.65	3.11
Greenhouse gas emissions: (g CO ₂ -eq m ⁻² yr ⁻¹)							
Indirect N ₂ O§	8.4	7.8	10.4	8.6	7.7	8.1	11.1
Direct N ₂ O	201	264	250	320	286	297	375
CO ₂ from soil humus C	77	36	55	17	30	18	-2

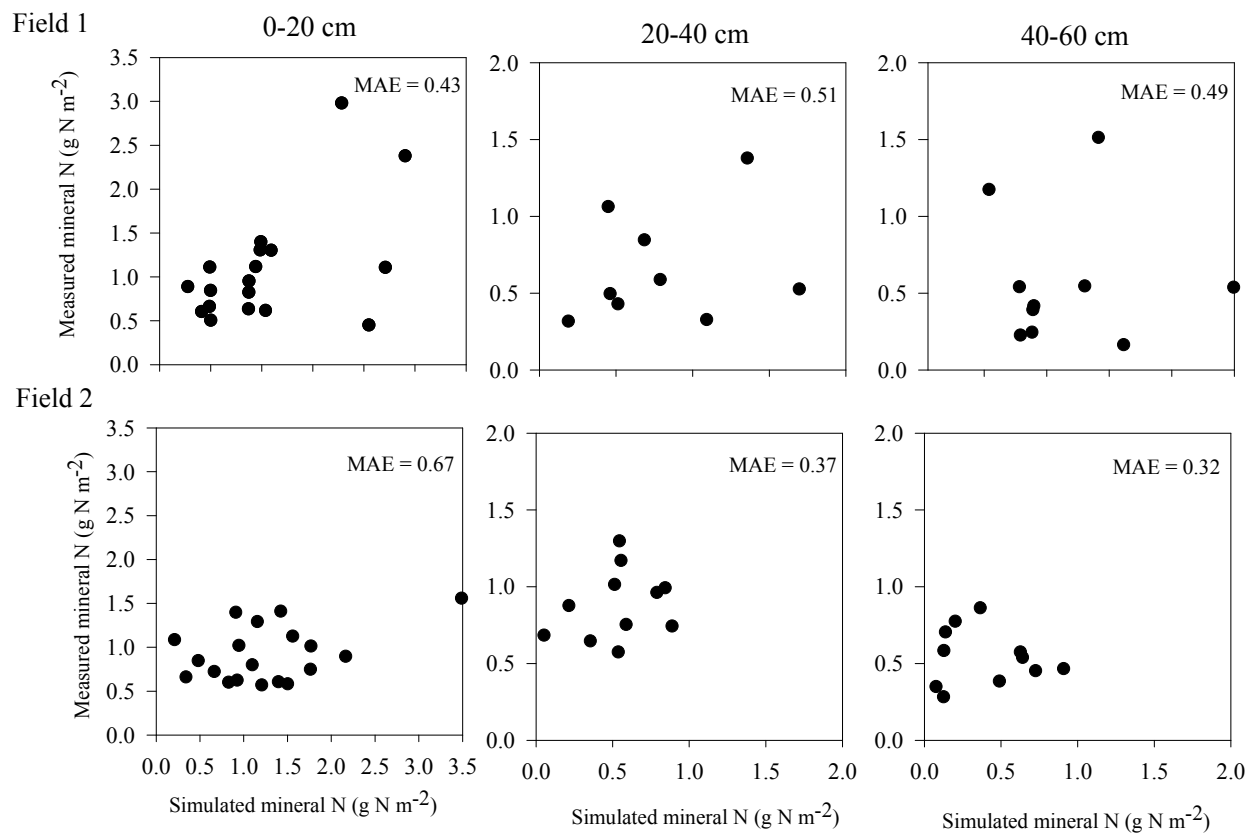
*N input include: N fixation by green manure, net mineralization from humus and microbial pool, and wet and dry atmospheric N deposition (0.75 g N m⁻²). ** 50% of total plant N was harvested as grain.

§ Indirect N₂O emissions assumed to be 1.25% of leached NO₃⁻ is assumed to be emitted as N₂O. Radiation capturing force relative to CO₂ of N₂O is 298.

Supplementary Figures



SM Fig. 1 Illustration of the plant residue incorporation routine of the SPN model conceptualized by immediate and continuous transfers of C and N and fractionation into plant parts by partitioning coefficients lr , sr , inc , dr , and hp upon ended growth periods.



SM Fig. 2 Measured versus simulated mineral N (g N m^{-2}) on Field 1 (top) and 2 (bottom) in 0–20, 20–40, and 40–60 cm soil depth. MAE: Mean absolute error (g N m^{-2}) calculated as $MAE = \sum_{n=1}^N \left(\frac{|y_i - \bar{y}_i|}{N} \right)$, where N is number of sample ($N = 19$), y_i each measurement and \bar{y}_i each model prediction of mineral N.

Paper III

Borgen, S.K., Grønlund, A., Andrén, O., Kätterer, T., Tveito, O.E., Bakken, L.R., and Paustian, K. (2011). **CO₂ emissions from cropland soils in Norway estimated by IPCC default and Tier 2 methods**. Submitted to *Greenhouse Gas Measurement and Management*.

CO₂ emissions from cropland in Norway estimated by IPCC default and Tier 2 methods

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Abstract

Monitoring changes in soil organic carbon is not only linked to atmospheric CO₂ dynamics, but also to the sustainability of agricultural systems, maintaining food security, reducing water pollution, and soil erosion. In accordance with the IPCC methodology, a Tier 2 method for estimating CO₂ emissions from cropland on mineral soils in Norway was developed and the results compared with those of the default Tier 1 method. The soil C balance model (ICBM) was used to calculate country-specific SOC stock change factors for cropland management systems. Annual CO₂ emissions from cropland management were substantially greater when estimated by the default Tier 1 method (313 Gg CO₂ yr⁻¹) compared with Tier 2 (139 Gg CO₂ yr⁻¹). The difference between the two methods was caused by the default Tier 1 stock change factors for crop rotations without manure application predicting greater CO₂ emissions compared with the ICBM-based Tier 2 factors. Reduction in livestock numbers and reduced manure application to arable land was the main cause of net emissions for both methods. Policies to stabilize or increase livestock numbers could reduce soil CO₂ emissions, although the impacts on other agricultural emissions sources, particularly methane from livestock, would need to be considered.

Keywords: Greenhouse gas accounting, arable agriculture, carbon stock change factors, C sequestration, animal manure

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1. Introduction

As of October 2010, a total of 192 nations have signed the Kyoto Protocol and are required to produce inventory reports accounting for greenhouse gas emissions (GHG), which are to be delivered to the United Nations Framework Convention on Climate Change. To facilitate compliance with the commitment and to create a common reporting format, the Intergovernmental Panel on Climate Change (IPCC) produced a three-tiered approach for national GHG inventories. The three tiers increase in potential accuracy of estimation but also in complexity and data requirements (IPCC, 2006d). For a Tier 1 method, information of management effects on soil carbon are given by IPCC default stock change factors, whereas for a Tier 2, country-specific data are used to estimate the factors. A Tier 3 requires substantial input data sets and detailed model simulations and/or measurement-based inventories. Most countries are currently using Tier 1 for CO₂ emission estimates from agricultural soil (UNFCCC, 2011; Lokupitiya and Paustian, 2006). Reasons why country-specific methods seldom are applied may be inadequate information about the extent and type of management practices (i.e., activity data), as well as too few measurements of carbon (C) stock changes for estimating emission factors.

Since Norway signed the Kyoto Protocol in 1993 (and ratified its commitment in 2002), there has been no methodological development for estimating CO₂ emission from mineral soils. The national inventory reports assume that mineral soils of cropland are in steady state, implying that recent and current changes in agricultural practices (e.g., manure applications and crop rotations) do not significantly affect soil organic carbon (SOC) stocks (CPA, 2010). However, Norwegian agriculture has undergone significant changes in land use and management in recent decades (see below) and it is well documented that agricultural management (such as tillage frequency and organic matter inputs) influences SOC turnover (Paustian *et al.*, 1997; Smith *et al.*, 2006). In addition climate variables, including, temperature and soil moisture, as well as soil biophysical properties are key controllers of the biogeochemical cycling of C (McLauchlan, 2006). Norwegian agricultural land stretches from 58°N to 71°N and thus has a strong gradient in temperature and seasonality and diversity in soil types. Although annual crops, leys and grazing land are broadly distributed over much of Norway's agricultural area, the vast majority of annual cropping occurs in few counties, mainly in the south, while animal production is concentrated in other regions (SSB, 2011). Hence, it is likely that regional interactions between soil, climate and agricultural management of cropping systems and animal manure availability, as well as temporal trends in land use and management, are changing the soil C balance of the country as a whole.

Soil C storage is typically greater in cooler climates with low decomposition rates. In Norway, the C sequestration potential of agricultural land was estimated at 806 Gg C yr⁻¹ assuming improved agricultural practices (Singh and Lal, 2005). However, current changes in SOC of Norwegian cropland have not been adequately assessed. Such an assessment is needed to evaluate the potential for soil C

sequestration and, more importantly, to provide a detailed estimate of emissions from mineral soils that accounts for differences in agricultural management related to residue inputs, crop rotations and tillage.

Our objective was to develop a Tier 2 method to estimate CO₂ emissions from mineral soils in Norwegian cropland and to compare the results with a Tier 1 method. Stock change factors and reference soil C stocks were generated for relevant crop rotations with and without manure and straw amendments using the Introductory Carbon Balance Model (ICBM; Andrén and Kätterer, 1997; Andrén et al. 2004). Agricultural activity data of crops and livestock, collected for 31 agrozones, were compiled and estimates were calculated for the inventory period 1999-2009.

2. Methods

We developed a Tier 2 method for Norwegian cropland and compared CO₂ emission estimates with those of Tier 1. First, climate, soils and agricultural activity data were compiled and analyzed to identify relevant climate regions, soil types and management systems. Second, the ICBM was used to estimate CO₂ emission factors (i.e., C stock change factors) and C stocks under reference steady-state condition. Third, agricultural activity data were applied to the IPCC Tier 1 and 2 methods, respectively, and CO₂ emissions were estimated.

Tier 1 and 2 IPCC methodology

The IPCC method for calculating CO₂ emissions from mineral soils holds two basic assumptions. First, that the annual rate of change in C stocks (ΔSOC) over an inventory period is equal to the C stock (SOC) difference between the start (t) and end ($t+1$) of the period, where D is the time dependency factor of the stock change factors (Eq. 1). The second assumption is that C stock changes occur as a function of changes in land use and management under specific climate and soil conditions. For a defined management system the C stock is equal to the product of the reference C stocks (SOC_R), stock change factors (F) and the area (A) under the same climate and soil combination at time t . (Eq. 2). The stock change factor is defined as the fractional change in soil C stocks relative to the reference SOC stock level, over a fixed time period D , which is the time assumed between the two equilibriums states of before and after the management change. The stock change factor is the product of land-use, tillage management and C input effects (i.e., $F = F_{LU} \times F_{MG} \times F_I$).

$$\Delta SOC = \frac{SOC_{(t+1)} - SOC_{(t)}}{D} \quad (1) \quad SOC_{(t)} = SOC_R \times F \times A_{(t)} \quad (2)$$

Equations 1 and 2 are the same for Tier 1 and 2 but the reference stocks, stock change factors and definition of management systems, climate regions and soil types can differ. In Tier 1, global climate regions, soil types and land use and management factors are defined with corresponding SOC_R and F

values as listed in the IPCC guidelines (IPCC, 2006b). The stock change factors have a 20-year dependency. In Tier 2, more detailed information relevant to a specific country or region is used to estimate reference stocks and stock change factors specific to defined management systems.

Climate and soils input data

Norway was divided into 31 agrozones (AZ) based on a combination of counties and climate zones used by the National Agricultural Authorities (SLF; Statens Landbruksforvaltning) to allocate subsidies (Figure 1). Climate data, i.e., air temperature, precipitation and potential evapotranspiration (Penman-Monteith equation) for 1980-2009 were estimated for 32,000 grid points covering arable land, applying the spatial interpolation approach described by Tveito *et al.* (2005). For each AZ, the climate variables were averaged to daily means. Climatic differences between the AZs and the overall cool climate is illustrated by a span in mean annual air temperature of -0.2 to 7.1°C, and the mean annual precipitation ranged from 576 to 2461 mm (Table 1).

A database holding approximately 600,000 soil samples was used to calculate the distribution of soil textures within each agrozone. Translation of the Norwegian classification system of 12 mineral soil classes into the 11 of the USDA scheme (Supplementary Material; SM Text 1) gave the following national distribution: 37% loamy sand, 15% sandy loam, 15% sand, 12% silt loam, 10% silt clay loam, 4% silt, 3% loam, 2% clay loam, 1% silt clay, 0.5% clay and 0.2% sandy clay loam. Mean C concentrations estimated from ignition loss measurements were: 4.1% C (loamy sand), 3.5% C (sandy loam), 4.6% C (sand), 2.8% C (silty loam), 2.2% C (silty clay loam), and 2.2% C (loam). The samples (n = 125,611) were taken on arable land between 1991 and 2007 to facilitate fertilizer management planning.

Agricultural activity data

Areal statistics for major crop types [small grains (cereals and oilseeds), root crops (potatoes and rutabaga) and leys] were collected for 1999 and 2009 and showed permanent cropland areas ranging from 2.8 to 686 km² per agrozone (Table 1). Seven crop rotations were defined: three ley-grain (LG) rotations named 1:1 LG, 1:2 LG and 2:1 LG (where 2:1 LG means two years of ley and one year of grain etc.), two with root crops: 1:2 root crop-grain (RG) and 1:2 root crop-ley (RL), and continuous cropping of grain (GR) and leys (LE). Root crops were in rotation with the more dominating of either grain or ley in the specific AZ. The grain percentage of the total ley-grain area determined the dominant LG rotation for each AZ by: > 65% grain = 1:2 LG, 35-65% grain = 1:1 LG and < 35% grain = 2:1 LG. Continuous grain cropping was modeled both with straw removal and retention, and all crop rotations could have animal manure applied (Table 2).

Mean grain yields of the major cereals (spring and winter wheat, barley and oats, occupied 98% of the grain area) were used to calculate C input based on the C mass of harvested yield (Y_C ; kg C ha⁻¹), as follows: below-ground = $570 + 0.2 \times Y_C$, above-ground stubble residues = $500 + 0.15 \times Y_C$, and straw = $140 + 0.83 \times Y_C$ (Kuzyakov and Domanski, 2000). For root crops mean potato yields were used per county and C inputs (kg C ha⁻¹) calculated as below-ground = $0.2 \times Y_C$ and residue = $0.42 \times Y_C$ (Kuzyakov and Domanski, 2000). To obtain ley yields per agrozones, ley yields were first multiplied by a yield index, assuming the relative productivity differences between the agrozones within counties are the same for leys as for cereals (for which agrozone-specific data was available). Carbon inputs were then calculated as belowground inputs = $0.4 \times Y_C$ and surface residue = $0.6 \times Y_C$ (Bolinder *et al.*, 2007) corresponding to a root/shoot ratio before harvest of 0.30. Carbon concentration was assumed to be 45% of dry mass in all plant material.

Available manure (Mg DM) was estimated from livestock numbers. Cattle slurry = $0.95A + 1.17B + 0.95C$, pig slurry = $0.29D + 0.43E$, and poultry manure = $0.2F + 0.02G$ where the letters A-G represent heads of dairy cattle, feeding cattle, other cattle, breeding swine, slaughter swine, hens and chicken, respectively (Raadal *et al.*, 2008). Cattle and pig slurry quantities were calculated with 6% DM, 45% C in DM and an application rate 45 Mg (wet mass) ha⁻¹ yr⁻¹. Poultry manure is generally applied in a more solid form, thus assuming 30%DM, 48%C in DM and an application rate of 9 Mg ha⁻¹ yr⁻¹, the same annual C inputs from all manure types of 1.3 Mg C ha⁻¹ yr⁻¹ is reached. An analysis of almost 4,000 farms, producing about 50% of all manure in Norway showed that cattle slurry was produced primarily in combination with ley cultivation, while farms with pig and poultry were grain and root crop producers (SM Text 2). The areas of the crop rotations receiving manure were as follows: cattle slurry was prioritized to the LE and RL rotations, while pig slurry and poultry manure were prioritized to the RG and LG rotations but with any surplus (only pig and poultry manure) allocated to RL and leys.

Introductory Carbon Balance Model (ICBM)

The ICBM calculated annual soil C changes for 30 years after a management change to the 16 defined management systems for all agrozones and soils. The model was chosen due to its simplicity (can be solved analytically as well as dynamically simulated) and because it was developed for Swedish arable agriculture, hence climatically similar to Norway. Furthermore, it has been thoroughly tested under these conditions and applied for other climates as well (Andrén *et al.*, 2004; Kätterer and Andrén, 2001; Juston *et al.*, 2010; Andrén *et al.*, 2007; Bolinder *et al.*, 2008; Salazar *et al.*, 2011). ICBM is a compartmental SOM model (Andrén and Kätterer, 1997) where total soil C is the sum of a young (Y) and an old (O) carbon pool. The two pools Y and O decay by first order and the decay rates are products of default decay rates ($k_Y = 0.8 \text{ yr}^{-1}$ and $k_O = 0.006 \text{ yr}^{-1}$) and an external factor (r_E), which depends on climate, soil and

tillage management. Thus, the decay rates of Y and O are $k_Y \times r_E$ and $k_O \times r_E$, respectively. Organic inputs (roots, litter residues and animal manure) enter Y , while input to the O pool is a fraction (h) of the decay of Y . The humification coefficient (h) is a weighted mean of the values for plant residue ($h_{res} = 0.13$) and manure inputs ($h_{man} = 0.30$), i.e., $h = (i_{res} \times h_{res} + i_{man} \times h_{man}) / i$, where i is the sum of all C inputs. When the model is solved analytically the amounts of Y and O can be calculated by Eq. 3 and 4 where Y_0 and O_0 are the initial values of the pools:

$$Y(t) = \frac{i}{k_Y r_E} + \left(Y_0 - \frac{i}{k_Y r_E} \right) e^{-k_Y r_E t} \quad (3)$$

$$O(t) = h \frac{i}{k_O r_E} + \left(O_0 - h \frac{i}{k_O r_E} - h \frac{k_Y r_E Y_0 - i}{r_E (k_O - k_Y)} \right) e^{-k_O r_E t} + \left(h \frac{k_Y r_E Y_0 - i}{r_E (k_O - k_Y)} \right) e^{-k_Y r_E t} \quad (4)$$

Solving the differential equations for steady state (i.e. when the state variables Y and O are constant over time) and by summing the expression for Y_{SS} and O_{SS} we get total organic C at steady state (C_{SS}).

$$Y_{SS} = \frac{i}{k_Y r_E} \quad O_{SS} = \frac{h k_Y Y_{SS}}{k_O} = \frac{h i}{k_O r_E} \quad C_{SS} = \frac{i}{r_E} \left(\frac{1}{k_Y} + \frac{h}{k_O} \right) \quad (5, 6 \& 7)$$

Calculation of r_E is performed by a separate water and temperature balance model programmed in SAS software and running on a daily time step, while the ICBM calculations were made annually in Excel. The annual r_E value (Eq. 8) can be set as the mean over N years of the daily external decomposition response factor [$r_e(d)$] where $r_e(d)$ is equal to the product of the daily response factors for temperature, soil moisture and soil cultivation (Eq. 9) as described by Andrén *et al.* (2004). The cultivation factor (r_C) is determined by default values respective to crop type as 1 for grain, 0.9 for ley (Kätterer *et al.*, 2008) and 1.13 for root crops (Andrén *et al.*, 2008). The r_E values were normalized to the original dataset, for which decay rates were calibrated, as described in Andrén *et al.* (2008), by dividing all calculated r_E values with 0.1.

$$r_E = \sum_1^N \frac{r_e(d)}{N} \quad r_e(d) = r_T(d) \times r_W(d) \times r_C(d) \quad (8 \& 9)$$

Soil temperature (T_{soil}) is a function of air temperature and leaf area index, which also includes a correction for the effect of snow cover on soil temperature by calculation of surface temperatures (Bolinder *et al.*, 2008; Kätterer and Andrén, 2009). The response factor for temperature (r_T) was derived from the Ratkowsky function of T_{soil} on a daily time step (Ratkowsky *et al.*, 1982), where the minimum temperature for decomposition (T_{min}) is -3.8 (Kätterer *et al.*, 1998) as shown below (Eq. 10).

$$r_T(d) = \frac{(T_{soil}(d) - T_{min})^2}{(30 - T_{min})^2} \quad (10)$$

The soil water response factor (r_W) is determined by the relative water content (θ_r ; Eq. 11) between field capacity (θ_{fc}) and the minimum water storage, which is a fraction α of wilting point (θ_{wp} ; Eq. 12).

The exponent γ was set at 1.3 according to Lomander *et al.* (1998). Pedotransfer functions proposed by Kätterer *et al.* (2006) were used for estimating θ_{fc} and θ_{wp} from soil C and clay concentrations.

$$r_w(d) = \theta_r(d)^\gamma \qquad \theta_r(d) = \frac{(\theta(d) - \alpha\theta)^2}{(\theta_{fc} - \alpha\theta)^2} \qquad (11 \ \& \ 12)$$

ICBM calculations of stock change factors

We predicted the annual response of SOC to a change in management from a reference condition for each of the 16 defined systems for each agrozone and soil type. The stock change factors were calculated as the relative change in SOC at the end of the simulation compared to initial SOC stock. As the reference condition by definition is in equilibrium, the initial SOC stock could be calculated as the steady state solutions (Eq. 5-7) of the reference condition. Continuous ley cropping with a moderate manure application ($0.5 \text{ Mg C ha}^{-1} \text{ yr}^{-1}$) was defined as the reference condition, because it was likely to have been present throughout the whole country in the past. The long cultivation history of Norwegian soils made continuous ley a more appropriate reference than the native soil (pre-cultivation) condition as used in the IPCC Tier 1. Continuous grain may also have been an appropriate choice, but climate restricts grain cultivation in the Northern AZs. IPCC recommends keeping a constant reference condition throughout the GHG accounting, also across land-use categories, and thus ley cropping was chosen. For each of the major soil types 31 reference stocks and associated stock change factors, with a 30-yr dependency (i.e., $D = 30$ yrs) was computed. Increasing D to 30 instead of the default of 20 years was done because the cool temperature climate can be expected to decrease decomposition rates and increase the time required to reach an equilibrium state.

Application of Tier 1 and 2

First, the agricultural activity data and manure availability was organized for dividing the areas of leys, grain and root crops in each agrozone between the crop rotations. To do this we used the following assumptions for both methods. Straw was considered to be removed on 5% of the monocropped grain area, which is the current area used for biofuel production (PFI, 2007). In 1999 straw burning on the field is likely to have occurred but not in recent years. On the remaining areas straw was assumed to be left in the field. Only one type of manure was considered to be applied to a given area, according to the application preferences described above. The estimated changes in the area of each management systems between the start (1999) and the end (2009) of the inventory period are shown in SM, Table 1.

Second, the calculations using Eq. 1 and 2 were made for each management system, soil type and AZ. For Tier 2, the ICBM-estimated reference stocks and stock change factors were applied. C input levels

and tillage effects implicit in the Tier 2 stock change factors were used for each management system. To account for soil texture effects in Tier 2, we multiplied the change in SOC stocks per agrozone and major soil types (loamy sand, sand, sandy soil, silt loam, and silty clay loam) with the fraction of cropland under each soil type (SM, Table 2).

For Tier 1, the reference C stocks were determined by soil and climate according to the IPCC guidelines (IPCC, 2006a). The European Soil Database, described by Panagos *et al.* (2011) classified all arable land (excluding grasslands) in Norway as soils with high-activity clays, i.e., Albeluvisols, Cambisols, Fluvisols, and Phaeozems, (JRC, 2011). The IPCC climate classification identified two climate regions: cool moist temperate climate for AZs 1-30 and boreal moist climate for AZ 31 (IPCC, 2006a). Thus, the reference stocks are 95 Mg C ha⁻¹ for cool moist temperate and 68 Mg C ha⁻¹ for the boreal moist agrozones according to IPCC (2006b).

Default stock change factors were taken from Table 5.5 of the IPCC guidelines and defined as shown in Table 2. The land-use factor was assigned to be 0.69 for long-term cultivation for all systems. Tillage was considered to occur annually (*full* tillage level) for grain monoculture and rotations with root crops but reduced for LG rotations and continuous leys. Input level definition is likely to have a large impact on estimated CO₂ emissions, thus we used national mean yields per crop rotation to categorize the input levels for each management system as low, medium, high, and very high when annual C inputs were less than 2 Mg C ha⁻¹, 2.0-2.5 Mg C ha⁻¹, 2.5-3.0 Mg C ha⁻¹, and > 3 Mg C ha⁻¹, respectively.

3. Results and discussion

Reference C stocks

Compared to the IPCC default C reference stock (SOC_R) for temperate moist climate of 95 Mg C ha⁻¹, the mean SOC_R estimated by ICBM was similar, 98 ± 2.6 Mg C ha⁻¹ in 30 cm depth. However, across all agrozones, SOC_R ranged from 76 to 133 Mg C ha⁻¹ (Table 1). The combination of less favorable decomposition conditions (low r_E values) and relatively large C inputs produced the largest reference stocks, while the smallest reference stocks occurred in agrozones with large r_E values and relatively small C inputs (Table 1). Soil texture influence on SOC_R was especially visible for sandy soil. The SOC_R was 105.8 Mg C ha⁻¹ for sandy soil and 94 Mg C ha⁻¹ for silt loam and loamy sand (Table 3). The differences in SOC_R were caused by the soil texture effect on the external decomposition factor (r_E), which was lowest for sandy soil. The r_E value depends on the water content at field capacity, which is derived from measured C concentration (Kätterer *et al.*, 2006). Measured C concentration for the sandy soil was fairly high (4.6% C) in our soils database. Furthermore, sampling depth was variable; probably 15-20 cm on grass ley and 20-25 cm on grain fields, hence the C content may be overestimated at the bottom of the 30

cm soil layer. In Norway sandy soils are often under ley cropping where C inputs in form of roots and animal manures may be substantial. Arable sandy soil were also found to have larger C concentrations than clay soil in a study from Denmark, which was partly explained by the cultivation history (Schjøning *et al.*, 2007), whereas in Sweden, sandy soils have lower soil C concentration than finer textured soils (Kätterer *et al.*, 2006).

Carbon stock change factors

For all rotations without manure application, the Tier 1 default stock change factors (i.e., the relative change in SOC between the equilibrium states of the new management system compared to the reference condition defined as continuous ley with a small manure application) were smaller than the ICBM-based Tier 2 factors as means of all agrozones and soil texture types are shown in Figure 2. For continuous grain with straw removal (GR) the Tier 1 factor value was also smaller than the Tier 2 when manure was added. Generally, the default method predicted higher losses relative to the reference condition, compared to the Tier 2 method in the unamended rotations, whereas when manure was applied (except, the GR rotation) the stock changes factors were marginally different between the two approaches. Soil texture affected the stock changes factors differently when manure was applied (Table 3). Without manure, sandy soil had the largest stock change factors, whereas with manure application they had the smallest (compared with the other soil textures). Manure effects on SOC stabilization were larger for the heavier soil types (mean factor value increase of 11-12%) than for the sandy soils (9% increase), corresponding with the theory that formation of physically-protected SOC occurs less in sandy than in fine-textured soils (Six *et al.*, 2002; Hassink *et al.*, 1997).

ICBM-calculated C sequestration rates for manure application were similar to those reported in the literature. Rates for continuous grain with straw incorporation (and manure) were lower (106-179 kg C ha⁻¹ yr⁻¹, depending on soil texture) than reported for a similar treatment in 34-year long field trial in Italy (Triberti *et al.*, 2008), whereas for leys, the estimated sequestration rates for manure application (134-230 kg C ha⁻¹ yr⁻¹) were slightly higher than those measured in a 50-year long Swedish trial (Bolinder *et al.*, 2010). The effect of manure in the long-term Ås trial in Norway was 85-195 kg C ha⁻¹ yr⁻¹ depending on rotation and a 37 or 48 year time period (Uhlen, 1991; Singh *et al.*, 1996; Yang *et al.*, 2004). Significant manure effects were reported for the Møystad long-term trial in Norway where larger FYM amounts were added (Uhlen, 1976; Riley, 2007) and also in other European trials (Ekwue, 1992; Blair *et al.*, 2006; Paustian *et al.*, 1992; Kätterer and André, 1999).

ICBM predicted a smaller manure effect (mean increase in stock change factor values for rotation with manure compared to those without: 0.11) than the default Tier 1 stock change factors (0.26). Carbon stabilization in soil from application of FYM was shown to be larger compared to slurry (Triberti *et al.*,

2008; Bertora *et al.*, 2009; Kirchmann and Bernal, 1997) and C concentrations may vary substantially between manures (Moral *et al.*, 2005). This advocates generation of specific stock change factors for different manure types and application rates by calibrating the humification coefficient for manure in ICBM (h_{man}) to the prevalent manure application practices regionally or per agrozone. However, we did not have sufficient information or data available for calibrating the h_{man} value. We reduced the default ICBM manure humification coefficient from 0.35 to 0.30 in these simulations because the original calibration was based on cattle FYM (Andrén and Kätterer, 1997), and in Norway manure is mainly applied as slurry.

Estimated CO₂ emissions from cropland

When estimated by the default Tier 1 method, net annual CO₂ emissions for Norwegian cropland were 313 Gg CO₂ yr⁻¹, which was twice the amount, 139 Gg CO₂ yr⁻¹, estimated by the Tier 2 method (Table 4). Tier 2 estimated emissions (0.139 Tg CO₂ yr⁻¹) from cropland on mineral soils represents less than 0.5% of the total C sequestration (28.6 Tg CO₂ yr⁻¹) estimated from the land-use, land use change and forestry category in the 2010 National Inventory Report (CPA, 2010). Related to the total emissions from the agricultural sector in Norway (4.4 Tg CO₂ equivalents with 10% as CO₂ from fossil fuel combustion), the presented cropland emissions are not completely negligible (CPA, 2010). For the cropland (remaining cropland) category, estimated emissions of 82 Gg CO₂ yr⁻¹, including all C sinks and sources, i.e., above-ground biomass sequestered in orchards, mineral and organic soils and liming, was reported for Norway in 2010 (CPA, 2010). It is difficult to compare with this value because ley farming is not included in the cropland category but instead in the grassland category. This seems uncalled for because more accurate estimates of C input are available for ley than for uncultivated pastures or grazing lands, and also because leys are often in rotation with grains, which influences management aspects such as tillage frequency. Substantial C losses from undisturbed soils can result from a single plowing event (Conant *et al.*, 2007) and differences in the tillage frequency of ley-grain rotations versus permanent pastures is likely to affect CO₂ emissions from the system (Paustian *et al.*, 2000). Although plowing frequency can differ in ley farming, this was not directly accounted for in the ICBM modeling. Instead we assumed that potentially larger CO₂ losses caused by more frequent plowing would be compensated for by increased biomass productivity.

For the whole country, estimated C loss rates by Tier 2 were less than half of those estimated by Tier 1 (Table 4). The highest C loss rates of 444 kg C ha⁻¹yr⁻¹ (Tier 1) and 209 kg C ha⁻¹yr⁻¹ (Tier 2) were calculated for AZ 10 (SM Table 3). It should be noted that although differences between methods seem to be large, all losses were small compared to the actual stocks, i.e., 209 kg C ha⁻¹yr⁻¹ is only 0.2% of an

initial C stock of 98 Mg C ha⁻¹. Measured SOC loss of arable cultivation on a long-term research farm in Norway was estimated to be declining at 1% yr⁻¹ of initial SOM levels (Riley and Bakkegard, 2006).

Emission differences between agrozones

There was great variation in CO₂ emissions between agrozones (Figure 3). For several agrozones net emissions were close to zero (AZ 2, 19, 20, 21) and Agrozone 4 alone was responsible for 25% of the national net emissions. Agrozone 4 is the second largest grain-producing agrozone (AZ 1 being number one) and the cessation of manure addition on large grain areas was the cause of these emissions. This was also case for the large C losses from agrozones 1, 8 and 13 (Figure 3; SM Table 1). Nationally, livestock numbers were reduced significantly between 1999 and 2009 (SSB, 2011), and for agrozones 4 and 10 this implied a reduction of 46% and 58% in the area being applied manure (Figure 4). The two agrozones (7 and 27) that experienced a rise in animal numbers, and thus available manure for soil amendment, were also the only zones with negative net emission (CO₂ removal from the atmosphere) estimated by both methods. For agrozone 5, net emissions were positive when estimated by Tier 1 but negative by Tier 2 because a large reduction in the area under ley-grain with manure (LG+) occurred during the inventory period, and the ICBM-based stock change factors were closer to 1 for this management system than the default factor values. Hence SOC stock changes were smaller for LG+, which combined with the increased area of continuous grain with manure, resulted in net C sequestration when using the Tier 2 method.

Ley farming and livestock numbers are generally positively correlated. However, in the southeast of Norway, ley areas increased (while grain decreased) but still livestock numbers were reduced (Figure 4). Organic agriculture has been increasing in the southeastern counties and ley farming (green manures) occupy 60-90% of organically farmed agricultural land (DEBIO, 2010). This corresponds to an area about the same size as that of the ley increase. Foreid and Høgh-Jensen (2004) showed that conversion to organic farming in Northern Europe increases the potential for C sequestration. Our results suggest that this will indeed depend on whether livestock is included or not.

Manure-related assumptions

Regional differences in manure production and application are crucial for accurate CO₂ emission estimates (by the IPCC approaches) as they influence the areal changes upon which the SOC stock changes are calculated. Because areal changes are determined per agrozone, potential manure import and export between the AZs would influence the calculations. A farm-level analysis of manure production and available area for application, indicated that 32% of manure produced on farms could not be spread on the arable farmland, and thus may be considered exported. We assumed that excess manure is exported to the

permanent grazing pastures, however; this may not be realistic because of the distances between farm and pasture but also for practical reasons related to spreading manure on hilly fields. Also, differences in application rates were found between regions, being largest in Hedmark, Oppland and the northern counties (SSB, 2001). Recommended annual application rates (in wet mass) are between 30 and 50 Mg ha⁻¹ yr⁻¹ (Tveitnes, 1993), but there are no government restrictions or penalties for surpassing this amount. Hence farmers may choose to do so for fuel efficiency optimization during spreading. Although some information about manure quality and application practices has been collected, there is a lack of hard data on a regional or agrozone level regarding manure distribution, application rates, and export/import. Specifically for the Tier 2, the assumed C input of the manure rotations determines the ICBM-based stock change factors. The C input of 1.3 Mg C ha⁻¹ yr⁻¹ that was assumed for rotations with animal manure amendments may be on the low side. Bonesmo and Sjelmo (2008) estimated a national mean value of 1.9 Mg C ha⁻¹ yr⁻¹ based on manure production and including permanent grazing land, the latter not being included in our analysis. Thus CO₂ emissions may be underestimated by the Tier 2 method. However, the reduction in manure availability during the inventory period may have been overestimated. Quantities of manure excretion per animal may be related to the amount of meat produced per head of livestock. In Norway, livestock numbers declined but meat production has remained stable and therefore the manure reduction could have been overestimated.

Implications of estimated emissions

Our results showed that net CO₂ emissions during 1999-2009 from arable mineral soils in Norway were primarily driven by reduced manure applications. Reversing the trend of declining animal husbandry or at least maintaining current numbers would reduce net CO₂ emissions. If such a strategy is desired for C sequestration, agricultural policy must be implemented accordingly (Smith *et al.*, 2005). In Norway, previous policies (accompanied with financial incentives) have been effective, e.g., for agro-environmental schemes imposed to reduce soil erosion (Arnoldussen, 2005) and for subsidized grain production on the most fertile soils in the country. The latter caused a separation between grain and livestock production through the country. Allocating subsidies for a reintegration of livestock with grain production (for human consumption to comply with the government goals of increasing self-sufficiency of cereals) would be a reasonable option for reducing CO₂ emission from cropland. It would also improve N use efficiency and nutrient cycling of organic grain production systems.

However, it is likely that other potent GHG (methane and nitrous oxide) have a larger impact on the total emissions budget than CO₂. Increasing livestock numbers may well enhance C sequestration, but would also increase methane emission from enteric fermentation by ruminants. We estimated methane emission from dairy and other cattle using IPCC emission factors (IPCC, 2006c) for the number of cattle

that was reduced during the inventory period. Estimated methane emissions (259 Gg CO₂-eq yr⁻¹) would more than outweigh potential C sequestration benefits from added manure supplied by these animals. It seems that although manure application has several well-documented benefits on soil fertility, it should not be considered an efficient GHG mitigation strategy because emissions not only methane but also (and perhaps of greater importance) of N₂O from increased denitrification rates, would have a substantial negative effect on the overall budget (Li *et al.*, 2005). It must be mentioned that a full GHG account should be made before political incentives are instigated.

4 Conclusions

Our study showed that decreased availability of animal manure during 1999-2009 was the main cause of net CO₂ emissions from cropland on mineral soils in Norway. Ignoring such changes in manure management (as done in the Norwegian national inventory report) gives biased results. The Tier 1 method estimated greater emissions compared to Tier 2 because the ICBM-estimated stock change factors resulted in lower decomposition rates (and net emissions) than estimated by the default Tier 1 factor values. Increasing the accuracy and determining the uncertainty of both Tier 1 and 2 would require investigations on a regional or agrozone level of manure application practices, such as actual application rates, crop preferences, and export and import on farms. Emission from mineral soil on cropland may give a small quantitative contribution to the overall C budget of all emission sectors. But even for countries with relatively small cropland areas (such as Norway), net emissions can be sizable (per area) due to changes in manure practices. Reducing cropland CO₂ emissions for Norway could be done by increasing livestock numbers to previous levels. However, methane and N₂O emissions accompanying animal husbandry would counterbalance reduced CO₂ emissions from soils. The need for integrated GHG emissions budgets for policy development to mitigate climate change by C sequestration is highlighted.

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Tables

Table 1. Cropland area, climatic descriptors (mean annual temperature, MAT; precipitation, MAP; potential evapotranspiration, PET), and the decomposition factor (r_E), C inputs (Mg C ha⁻¹ yr⁻¹) and estimated soil C reference stocks (SOC_R in Mg C ha⁻¹, 30 cm depth) for reference condition as a mean of five major soil types.

Agrozone	County	Area (km ²)	MAT (°C)	MAP (mm)	PET (mm yr ⁻¹)	r_E value	C input (Mg C ha ⁻¹)	SOC _R (Mg C ha ⁻¹)
1	Østfold	686	5.7	981	461	0.99	3.33	91
2	Østfold	2.8	4.5	909	455	0.89	2.62	83
3	Akershus/Oslo	148	5.7	979	473	1.00	3.26	89
4	Akershus	573	4.5	867	462	0.90	3.42	103
5	Hedmark	317	3.6	749	444	0.82	3.15	105
6	Hedmark	410	3.7	764	450	0.84	2.84	94
7	Hedmark	232	0.9	720	411	0.56	2.40	123
8	Oppland	355	3.3	853	440	0.77	3.09	111
9	Oppland	452	1.7	784	417	0.60	2.87	133
10	Buskerud	138	5.2	939	468	0.97	2.78	80
11	Buskerud	147	4.7	840	462	0.92	2.63	81
12	Buskerud	144	2.6	867	429	0.67	2.53	108
13	Vestfold	369	6.2	1176	460	0.99	3.25	89
14	Telemark	112	5.7	992	461	0.92	2.64	82
15	Telemark	94	3.9	1089	435	0.76	2.48	93
16	Aust-Agder	94	6.1	1456	450	0.97	2.59	76
17	Vest-Agder	144	6.2	1982	439	0.92	2.89	87
18	Rogaland	259	7.2	1723	458	1.04	3.38	88
19	Rogaland	28	6.5	2404	450	0.91	2.54	80
20	Rogaland	158	7.1	2261	458	0.98	2.81	81
21	Hordaland	214	6.4	2461	456	0.90	2.71	85
22	Sogn og Fjordane	275	5.6	2364	446	0.81	2.95	101
23	Møre og Romsdal	438	6.1	2004	455	0.84	3.00	100
24	Sør Trøndelag	345	4.5	1303	447	0.74	3.05	113
25	Sør Trøndelag	289	3.4	1264	431	0.65	2.64	116
26	Nord-Trøndelag	516	4.6	1151	455	0.79	3.14	109
27	Nord-Trøndelag	260	4.1	1506	445	0.72	2.53	100
28	Nordland	452	4.2	1725	439	0.68	2.34	100
29	Troms	188	2.3	1135	425	0.57	1.82	98
30	Troms	27	1.6	796	415	0.53	1.82	106
31	Finnmark	80	-0.2	579	407	0.47	1.69	113

Table 2. Management systems defined by crop rotation, manure application, tillage factor (r_c), and annual C inputs for the Tier 2 and the Tier 1 defined tillage levels and input levels.

	Acronym	Crop rotation	Manure	Tier 2		Tier 1	
				Tillage (r_c)	C input (Mg C ha ⁻¹)	Tillage	Input level
1	GR	Grain (- straw)	No	1.00	1.55	Full	Low
2	GRS	Grain (+ straw)	No	1.00	2.83	Full	High
3	1:2RG	1:2 root-grain	No	1.07	2.35	Full	Medium
4	1:2RL	1:2 root-ley	No	1.00	1.93	Full	Low
5	1:2LG	1:2 ley-grain	No	0.97	2.56	Reduced	High
6	1:1LG	1:1 ley-grain	No	0.95	2.61	Reduced	High
7	2:1LG	2:1 ley-grain	No	0.93	2.54	Reduced	High
8	LE	Leys	No	0.90	2.25	Reduced	Medium
9	GR+	Grain (- straw)	Yes	1.00	2.85	Full	High
10	GRS+	Grain (+ straw)	Yes	1.00	4.13	Full	Very high
11	1:2RG+	1:2 root crops-grain	Yes	1.07	3.65	Full	Very high
12	1:2RL+	1:2 root crops-ley	Yes	1.00	3.23	Full	Very high
13	1:2LG+	1:2 ley-grain	Yes	0.97	3.86	Reduced	Very high
14	1:1LG+	1:1 ley-grain	Yes	0.95	3.91	Reduced	Very high
15	2:1LG+	2:1 ley-grain	Yes	0.93	3.84	Reduced	Very high
16	LE+	Leys	Yes	0.90	3.55	Reduced	Very high

Table 3. Tier 2 reference C stocks (SOC_R) as mean \pm standard error ($n = 31$), the external decomposition response factor r_E and mean stock change factors for the whole country per soil texture type. Standard errors over the agrozones for stock change factors were $< 0.5\%$ of the mean value.

	Loamy sand	Sand	Sandy loam	Silt loam	Silty clay loam
	Reference C stock				
SOC_R (Mg C ha ⁻¹)	93.8 \pm 2.6	105.8 \pm 2.7	97.6 \pm 2.5	93.6 \pm 2.6	97.3 \pm 2.6
r_E value	0.84	0.74	0.81	0.85	0.81
	Mean stock change factors for all agrozones in Norway				
Without manure	0.93	0.94	0.93	0.93	0.93
With manure	1.05	1.03	1.04	1.05	1.04

Table 4. Net CO₂ emissions and mean SOC loss rates for Norwegian cropland estimated by the default Tier 1 and the model-based Tier 2 methods.

	Net emissions	Removals	Emissions	C loss rate
	(Gg CO ₂ yr ⁻¹)			(kg SOC ha ⁻¹ yr ⁻¹)
Tier 1	313	-18	331	107
Tier 2	139	-9	148	39

Figures

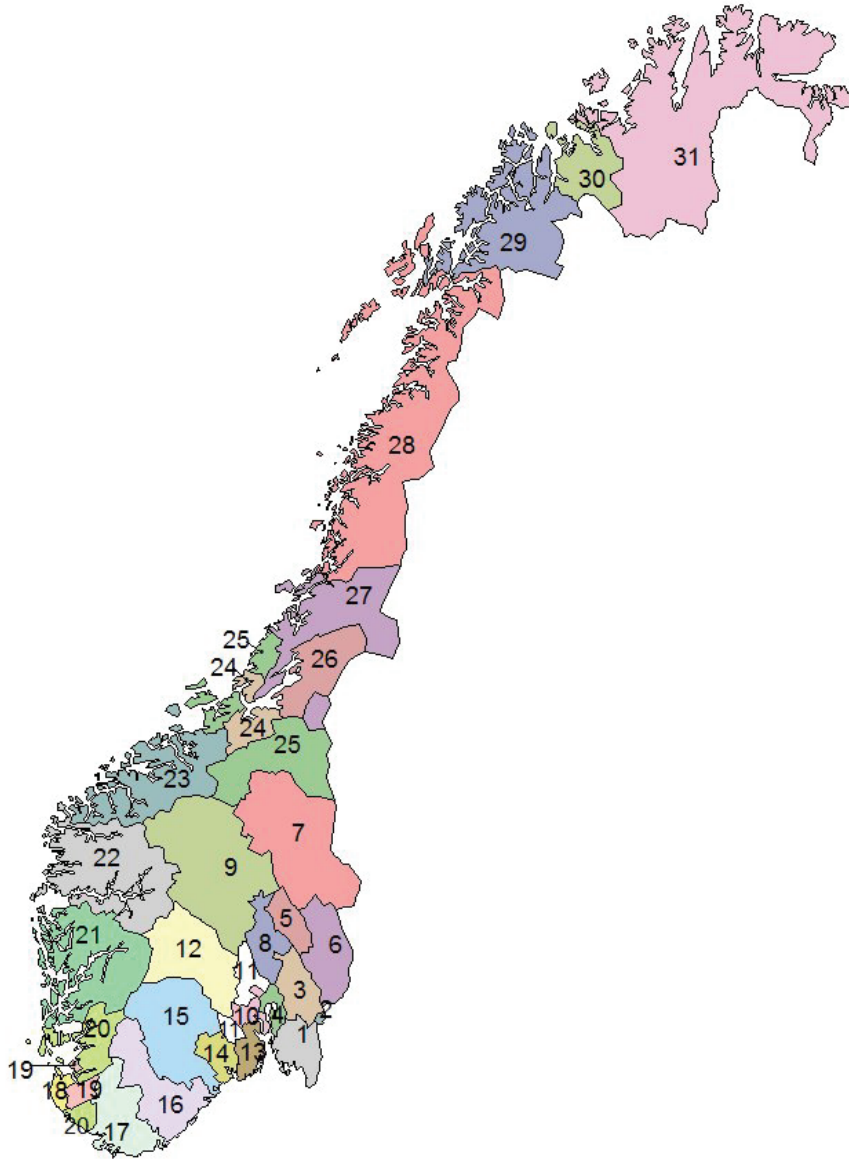


Figure 1. Norwegian agrozone division based on counties and climate zones. See Table 1 for county names of each agrozone number.

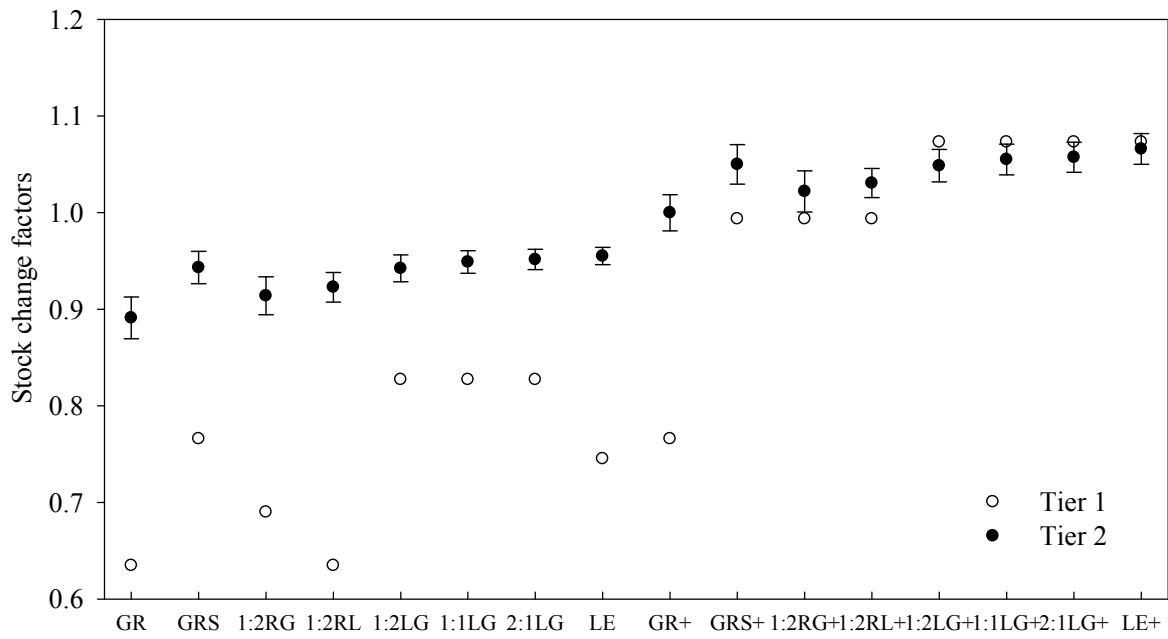


Figure 2. Mean national Tier 1 and 2 stock change factors per management systems. For the Tier 2, mean factor values are displayed of all agrozones and soil texture types with standard deviation are calculated for the agrozones with $n = 23$ (as grain is not cultivated in eight agrozones), except for 1:2 RL and LE where $n = 31$. See Table 2 for explanation of management system acronyms.

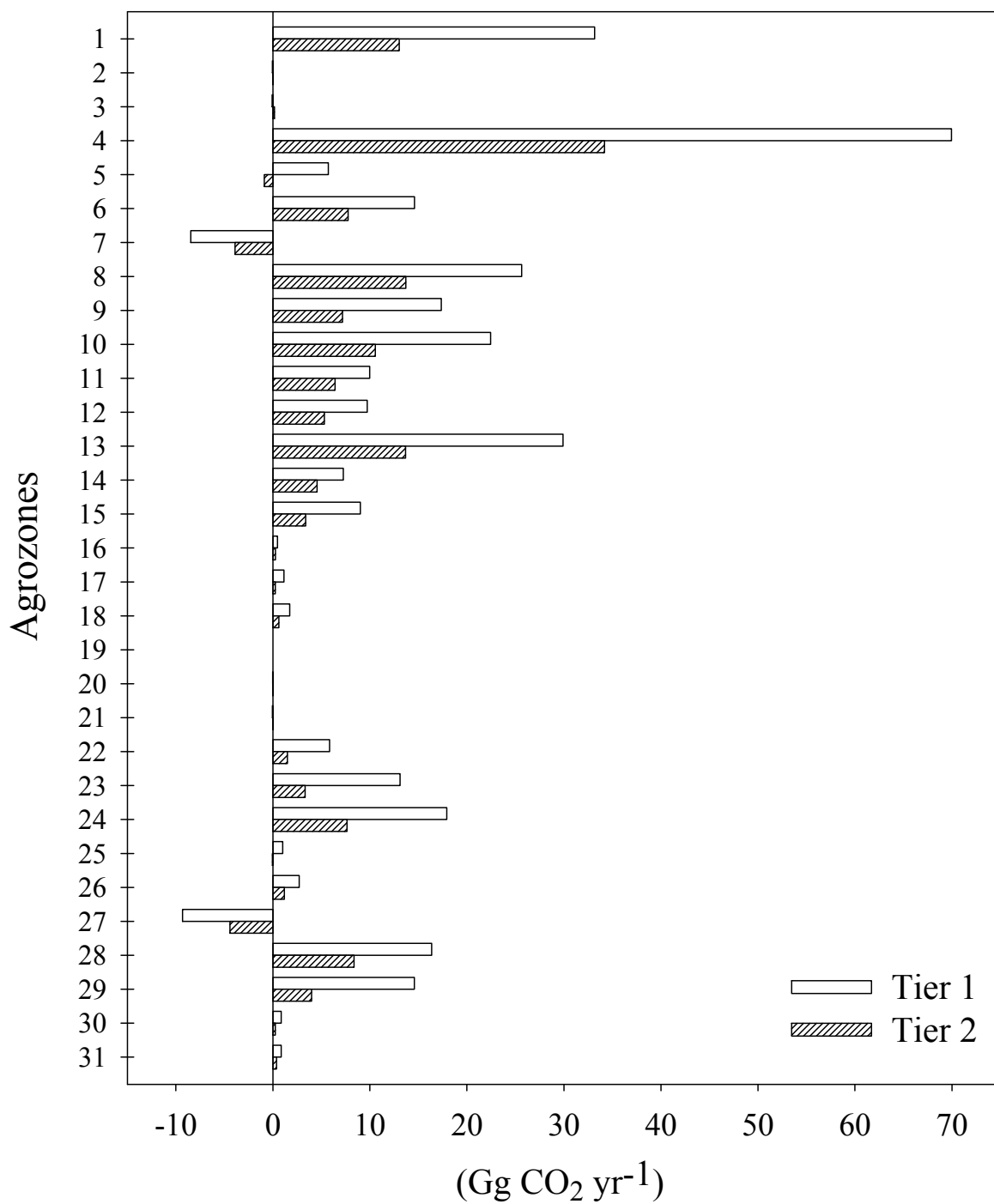


Figure 3. Annual CO₂ emission (Gg CO₂ yr⁻¹) during 1999-2009 calculated by Tier 1 and Tier 2 methods. Negative values indicate CO₂ removals.

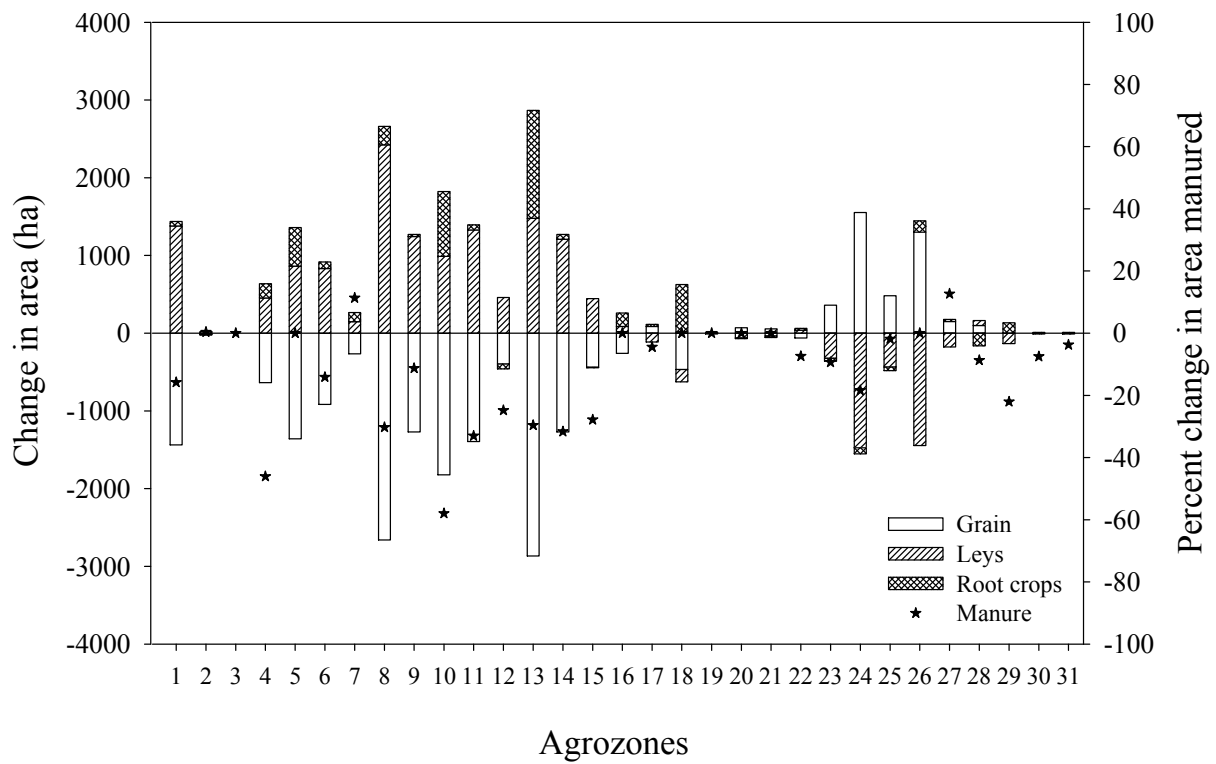


Figure 4. Changes between 1999 and 2009 in the area of major crops and the area estimated to be applied with manure (right axis).

Supplementary Material Texts

SM Text 1: Soil textures translation of Norwegian into USDA classification

To transfer the Norwegian systems of soil texture distribution to the USDA classification scheme their respective texture triangles were overlaid. But some Norwegian classes consisted of several USDA classes (e.g., Norwegian classes 9-12) and others were grouped together, e.g. Norwegian classes 1-3 are classified by the USDA system as sandy soil. A subsample (n = 2939) from the soils database contained information about the clay, silt and sand contents of the soil samples within each Norwegian class, which was used to determine the percentage of the USDA classes within the Norwegian classes. USDA soil textures were assigned the Norwegian classes as shown in Table 1.

Table 1.1 Soil texture types of the Norwegian texture classes and their distribution within the USDA texture classification system.

Norwegian class	Texture type	USDA texture	Norwegian class
1	Coarse sand	Clay	12
2	Medium coarse sand	Clay loam	11
3	Fine sand	Loam	9
4	Silty coarse sand	Loamy sand	4 & 5
5	Silty medium coarse sand	Sand	1 & 2 & 3
6	Silty fine sand	Sandy clay	11 & 12
7	Sandy silt	Sandy clay loam	9 & 11
8	Silt	Sandy loam	9 & 10
9	Light clay	Silt	8
10	Silty light clay	Silt loam	7 & 10
11	Medium clay	Silty clay	11 & 12
12	Heavy clay	Silty clay loam	10 & 11

SM Text 2: Animal manure distribution preferences on crop types

The purpose of this data analysis was to determine potential relationships between crop type cultivation (leys, grain and potato) and type of manure produced (cattle, pig or poultry). All farms with livestock in 2009 were selected (n = 3937) and these represented 69% of total cropland area, 100% of the manure was produced, and 87%, 31% and 32% of total areas grown with leys, grain and potato (Table 2.1). Manure application rates were assumed to be 4 Mg DM ha⁻¹ of cattle slurry and 3 Mg DM ha⁻¹ for pig slurry and poultry manure.

Table 2.1 Livestock farms used in the manure distribution and type analysis

	Area (ha)	Manure quantity (Mg DM)				Area (ha)		
	Cropland	Total	Cattle	Pig	Poultry	Ley	Potato	Grain
All total farms	1008435	1872858	1364654	220277	287926	480285	13741	297061
Selected farms	700302	1872858	1364654	220277	287926	420094	4423	92409
% of total	69 %	100 %	100 %	100 %	100 %	87 %	32 %	31 %

The results showed that the majority (62%) of all manure produced could cover the leys areas and 32% of all manure could be assumed to be exported because, given the assumed application rates, there was no land available for spreading (Table 2.2). For poultry, 80% of the manure did not find application area on the farm where it was produced (Table 2.2). Analyzing the specific manure types showed that cattle slurry was mainly produced on farms that grow leys whereas pig slurry and poultry manure were produced on farms with large grain areas (Table 2.2).

Table 2.2 Distribution of manure between ley, potato, grain and surplus (i.e., exported) with manure amount produced as the total

	Ley	Potato	Grain	Surplus
Total manure	62 %	0 %	6 %	32 %
Cattle slurry	79 %	0 %	2 %	19 %
Pig slurry	22 %	2 %	27 %	50 %
Poultry manure	9 %	1 %	10 %	80 %

A larger percentage of the total cultivation of potato compared to grain occurred on livestock farms, especially pig productions (Table 2.3). The area under ley could absorb 94% of all cattle slurry produced.

Table 2.3 Distribution of cattle, pig and poultry manure within leys, potato and grain areas with total crop area as 100%.

	Crop area of total	Cattle	Pig	Poultry
Ley	69 %	94 %	4 %	2 %
Potato	62 %	26 %	43 %	31 %
Grain	39 %	19 %	54 %	27 %

In conclusion, the results confirm that cattle manure is primarily applied to ley fields and that grain cultivation is connected more with pig and poultry production and cattle rearing. However, the available data do not provide information about cropland on stockless farms that receive imported manure and the destiny of exported manure (especially relevant for poultry manure). The fact that the majority of potato cultivation is done in combination with livestock may indicate farmers' preference of applying manure to potato than to grain crops. Thus manure import may be mostly applied to potatoes. Other considerations related to manure import/export preferences may be that poultry manure have higher potassium and phosphorous concentrations than cattle slurry. Hence, specific nutrients may set the upper limit for the actual application rate applied in practice.

Supplementary material tables

SM Table 1 Percent of soil samples distributed on soil texture type

Agrozone	County	Loamy sand	Sand	Sandy loam	Silt loam	Silty clay loam
1	Østfold	10 %	4 %	6 %	20 %	60 %
2	Østfold	37 %	2 %	16 %	35 %	9 %
4	Akershus/Oslo	10 %	2 %	5 %	30 %	52 %
3	Akershus	14 %	4 %	2 %	27 %	53 %
5	Hedmark	72 %	3 %	7 %	11 %	7 %
6	Hedmark	21 %	3 %	23 %	51 %	2 %
7	Hedmark	33 %	7 %	31 %	29 %	0 %
8	Oppland	73 %	2 %	3 %	17 %	5 %
9	Oppland	67 %	5 %	16 %	11 %	2 %
10	Buskerud	23 %	3 %	5 %	27 %	42 %
11	Buskerud	20 %	4 %	9 %	27 %	39 %
12	Buskerud	65 %	10 %	17 %	8 %	1 %
13	Vestfold	39 %	12 %	6 %	22 %	21 %
14	Telemark	16 %	7 %	22 %	43 %	12 %
15	Telemark	51 %	24 %	8 %	12 %	4 %
16	Aust-Agder	50 %	21 %	12 %	12 %	4 %
17	Vest-Agder	47 %	45 %	6 %	1 %	0 %
18	Rogaland	96 %	1 %	0 %	0 %	3 %
19	Rogaland	70 %	27 %	3 %	0 %	0 %
20	Rogaland	48 %	42 %	10 %	1 %	0 %
21	Hordaland	61 %	13 %	24 %	2 %	0 %
22	Sogn og Fjordane	60 %	21 %	16 %	2 %	0 %
23	Møre og Romsdal	52 %	37 %	10 %	1 %	0 %
24	Sør Trøndelag	39 %	12 %	23 %	14 %	13 %
25	Sør Trøndelag	52 %	21 %	20 %	5 %	2 %
26	Nord-Trøndelag	20 %	3 %	11 %	29 %	37 %
27	Nord-Trøndelag	34 %	20 %	16 %	19 %	10 %
28	Nordland	28 %	51 %	10 %	8 %	3 %
29	Troms	46 %	31 %	17 %	5 %	1 %
30	Troms	35 %	20 %	36 %	9 %	0 %
31	Finnmark	30 %	27 %	27 %	13 %	2 %

SM Table 2 Soil organic C loss rates (Mg C ha⁻¹yr⁻¹) during the inventory period 1999-2009 per agrozone estimated by the default Tier 1 and the ICBM-based Tier 2 methods.

Agrozone	SOC loss rates (kg C ha ⁻¹ yr ⁻¹)	
	Tier 1	Tier 2
1	132	52
2	-50	-3
3	-1	3
4	333	163
5	49	-8
6	97	52
7	-99	-46
8	197	105
9	105	43
10	444	209
11	186	119
12	185	101
13	221	101
14	177	111
15	263	99
16	14	8
17	22	5
18	18	7
19	1	0
20	0	0
21	-1	0
22	58	15
23	82	21
24	142	60
25	10	0
26	14	6
27	-98	-46
28	99	51
29	212	58
30	86	26
31	30	13

SM Table 3 Area changes (ha) of each management system (see main text Table 2 for description) between 1999 and 2009

Agrozones:	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
GR	1941	-3	0	-45	0	-137	0	0	0	-101	-209	0	733	54	0	0
GRS	8904	-57	0	21391	0	-2609	0	0	0	3243	-423	0	10185	1019	0	0
1:2RG	0	-1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1:2RL	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1:2LG	0	60	0	0	0	8533	0	0	0	0	5482	0	0	0	0	0
1:1LG	0	0	0	5047	0	0	0	10756	0	4849	0	0	0	2472	0	0
2:1LG	0	0	0	0	0	0	-2697	0	1903	0	0	3470	0	0	999	0
LE	0	0	0	0	0	0	-287	0	3112	0	0	0	0	0	1624	0
GR+	-2157	0	-28	0	206	0	0	-224	0	0	0	0	-828	-184	0	0
GRS+	-12999	0	-527	-22249	3909	0	0	-4259	0	-5164	-3553	0	-11973	-3495	0	0
1:2RG+	169	1	555	0	1492	250	0	-367	0	2508	201	0	4166	190	0	0
1:2RL+	0	0	0	0	0	0	351	0	80	0	0	-188	0	0	-21	517
1:2LG+	4141	0	0	0	-21991	-6037	0	0	0	-7380	-1497	0	-15725	0	0	0
1:1LG+	0	0	0	-4144	16385	0	0	-5906	0	2046	0	0	13442	-55	0	0
2:1LG+	0	0	0	0	0	0	1899	0	-5714	0	0	-4663	0	0	-2313	-778
LE+	0	0	0	0	0	0	734	0	619	0	0	1380	0	0	-288	261
Agrozones:	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	
GR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GRS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1:2RG	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1:2RL	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1:2LG	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1:1LG	0	0	0	0	0	0	0	6352	0	0	0	0	0	0	0	0
2:1LG	0	0	0	0	0	0	0	0	0	0	-3285	0	0	0	0	0
LE	281	0	0	0	0	1519	3470	0	304	0	0	4415	3733	232	326	0
GR+	0	0	0	0	0	0	0	0	0	16	0	0	0	0	0	0
GRS+	0	0	0	0	0	0	0	0	0	302	0	0	0	0	0	0
1:2RG+	0	0	0	0	0	0	0	0	0	2574	0	0	0	0	0	0
1:2RL+	82	1876	8	-24	-57	66	-109	-233	-140	0	79	-489	401	-28	-28	0
1:2LG+	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1:1LG+	0	0	0	0	0	0	0	-3248	0	-2892	0	0	0	0	0	0
2:1LG+	258	-1400	0	0	0	0	1081	0	1449	0	3739	296	0	0	0	0
LE+	-622	-476	-8	24	57	-1585	-4441	-2871	-1613	0	-533	-4222	-4135	-205	-298	0