Carbon and Nitrogen Dynamics in Agricultural Soils

Model Applications at Different Scales in Time and Space

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Abstract

An understanding of soil organic carbon (C) and nitrogen (N) dynamics is essential for efficient and environmentally sustainable agricultural production. This thesis includes model studies of C mineralization at regional/national level with annual time steps, N balances at field level with annual time steps, and N dynamics at 34 locations within a single field with daily time steps. The same model family (ICBM) was used in all studies. Generally, carbon stocks in mineral soils increased from southern to northern Sweden and were near steady state. Temperature, crop type, and animal density were the main drivers for C fluxes at the regional scale. The inclusion of the changes in soil N stocks in field N balance sheets were necessary for obtaining unbiased estimates of N use efficiency or N surplus. Without these changes in soil N stocks, N surplus in low input systems was underestimated and was overestimated in systems with increasing soil organic matter. The model explained 56% of the total variation in apparent net N mineralization estimated for 34 locations within one field during two growing seasons; however, for a single year, only a small proportion of the variation could be explained. The sources of uncertainty in both measurements and the model at different scales in time and space were addressed, as the precision of available measurements limited model testing and the estimation of critical model parameters. From a decision support perspective, commonly available field data are usually sufficient for models such as ICBM/N in the long-term predicting of the effects of agricultural management on C and N stocks at the field or the regional scale. However, more detailed information and models that are more complex are required for short-term applications at small spatial scales, for example for decision support in a precision farming context.

Keywords: Carbon balances, carbon sequestration, decomposition, ICBM, modeling, nitrogen balances, scaling, SOM, SON.

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Dedication

To my parents Britt-Inger and Karl-Olof.
To my children Josef, Amira, and Jakob.

Vad fan tas överskottet kväve från?
August Strindberg

Contents

List of Publications

This thesis is based on the work contained in the following papers, referred to in the text by Roman numerals:

I Andrén O., Kätterer T., Karlsson T. (2004) ICBM regional model for estimations of dynamics of agricultural soil carbon pools. Nutrient Cycling in Agroecosystems 70:231-239.

II Andrén O., Kätterer T., Karlsson T., Eriksson J. (2008) Soil C balances in Swedish agricultural soils 1990–2004, with preliminary projections. Nutrient Cycling in Agroecosystems 81:129-144.

III Karlsson T., Andrén O., Kätterer T., Mattsson L. (2003) Management effects on topsoil carbon and nitrogen in Swedish long-term field experiments - budget calculations with and without humus pool dynamics. European Journal of Agronomy 20:137-147.

IV Karlsson, T., Delin, S., Kätterer, T., Berglund, K. & Andrén, O. (2011). Simulating site-specific nitrogen mineralization dynamics in a Swedish arable field. Acta Agriculturae Scandinavica, Section B - Soil & Plant Science 61(4), 333-344.

Papers I-IV are reproduced with the permission of the publishers.

The contribution of Thord Karlsson to the papers included in this thesis was as follows:

I Collected and adapted input data for the model, assisted in data analyses and participated in the writing.

II Collected and adapted input data for the model, assisted in data analyses and participated in the writing.

III Adapted model and input data, primarily responsible for analysis of the results and was mainly responsible for the writing, with assistance from co-authors.

IV Adapted model and input data, primarily responsible for analysis of the results and was mainly responsible for the writing, with assistance from co-authors.

Abbreviations

CV	Coefficient of variation; standard deviation/mean
ICBM	Introductory Carbon Balance Model
LFOM	Light fraction organic matter
POM	Particulate organic matter
SOC	Soil organic carbon
SOM	Soil organic matter
SON	Soil organic nitrogen
t	Metric ton, 1000 kg

1 Introduction

In the global biochemical cycle, carbon (C) and nitrogen (N) are major elements. In the soil, there is three times as much C as in the atmosphere, and four times as much as in living organisms (Lal, 2004). These elements have a great impact on the environment, for example, as major greenhouse gases (e.g. CO_2, CH_4 and N_2O) and for eutrophication of water (NO_3^-). The quantification of C pool changes is necessary for national reporting according to international agreements (IPCC, 2006). It is also necessary to quantify how much N is mineralized, both for environmental and for economic reasons, as N is a major plant nutrient and any loss will need to be replaced by expensive N fertilizer.

The cycles of C and N are linked, and in soil, these elements comprise a substantial amount of soil organic matter (SOM), which improves soil fertility due to its influence on soil structure, water-holding capacity, and its content of plant nutrients. However, high SOM contents can also mineralize excess nutrients at times when plants roots are inactive, leading to N losses from agriculture to the environment, which can create major environmental and economic problems (St. Luce *et al.*, 2011).

The crucial step in C sequestration (removal from the atmosphere for a period) is photosynthesis, where CO_2 from the atmosphere is converted to carbohydrates and built into plant biomass. Some N can be fixed from the atmosphere by cyanobacteria or plant-microbe symbiosis, but for most plants, the only source of N is soil. Ultimately, plant biomass ends up in or on the soil, either after wilting, as manure or droppings after being consumed by animals, or as animal carcasses. The biomass (now necromass) is decomposed by microorganisms and soil fauna and CO_2 is returned to the atmosphere. At mineralization, N and other elements are returned to the soil as inorganic compounds and are available for plant uptake again, although depending on the conditions, N can be emitted to the atmosphere in gaseous forms.

The fundamental question is how to quantify, describe, and predict changes in soil organic matter. In principle, the measuring of soil organic carbon (SOC) is simple, a soil sample is burnt, and the CO_2 emitted is measured. However, when estimating stock change, a large sum can be subtracted from another large sum to obtain a small difference, which can be compared to measuring a captain's weight by weighing his ship with and without the captain onboard. The precision of the measured difference depends on both successful soil sampling in the field and subsampling prior to laboratory analysis. Although uncertainties in the determination of carbon concentrations are usually low, other variables, including bulk density and soil horizon thickness are needed for estimating C stocks; however, several methodological problems and a large inherent variability in these variables contribute to low precision and often bias in the estimates. Furthermore, measurements do not provide answers about the future. The difficulties in obtaining exact measurements and the complexity of SOM turnover necessitate mathematical models for describing the processes involved and making order out of chaos.

With models, current knowledge can be compiled and compressed to make projections into the future, test alternative scenarios, and answer what-if questions: all of which are necessary features for supporting decision-making processes. Even so, the information available varies considerably from detailed data available from carefully described and monitored long-term experiments to coarsely summarized data available for all cropland within a country. Therefore, a model needs to be able to work with different degrees of detail in parameter estimates.

Calculations of national soil carbon budgets encounter a number of problems, such as, lack of data, low or unclear precision in the data, biased data, and a lack of detailed knowledge about how controlling factors affect, e.g., annual input of C to the soil. One cost-effective approach may be to begin with reviewing available data and deciding how theoretical knowledge can be applied from the amount, resolution, and quality of the data.

Field or farm N balances are often used to identify situations where there is a possible risk of losing large amounts of N to the environment, that is, farms or fields where the calculated N surpluses are high. However, changes in soil organic matter (SOM) between years are seldom included in the balances, even though soil organic N ("humus N", SON) in the topsoil may be of the order of 10 t ha^{-1} (Eriksson *et al.*, 2010), and a 1% annual change corresponds to 100 kg, which in turn is in the same order of magnitude as the annual N fertilization dose. The reason for this oversight is that annual changes in SOM content are usually small in comparison to the total amount of SOM, and changes measured over a few years are difficult to detect due to spatial heterogeneity.

Even if the measurements cover a sufficiently long period to be able to detect statistically significant changes of SOM, a model is still needed for additional forecasting of steady state pools. The lack of focus on SON dynamics can generate errors, such as, N dynamics in the soil are interpreted as N losses, or losses can be attributed to the wrong year and crop in a rotation.

Within a single field, N supply through mineralization and plant demand for N vary in space and time. Accounting for this site-specific variation when applying N fertilizer in arable fields may result in improved economy for the farmer and lower N losses to the environment. However, although it is technically possible to adjust fertilization rates to different parts of a field, the question is whether sufficient information is available for correctly adjusting fertilization rates. The establishment of a well-balanced fertilization rate involves several steps. These steps include the estimation of the crop's present N status and future need of N according to the expected yield, the available mineral N in the soil, the mineralizable N at specified weather conditions, and the economic optimum. In this thesis, the focuses was on the simulation of N mineralization with the use of information commonly available at farms involved in precision farming, i.e., high-resolution soil texture and yield maps from previous years.

2 Objectives

This thesis addresses the quantification of changes in SOC and SON in agricultural land at different scales in space and time. The objectives of the individual studies were to:

- present the dynamics of soil carbon in Swedish arable land during 1990–2004 (Papers I-II).
- evaluate the impact of including changes in SON in field N balances (Paper III).
- test the validity of a model, ICBM/N, for calculating site-specific (sub-plot scale) N mineralization in a field over two years (Paper IV).

In Papers I – II, the focus was on changes in SOC, in Papers III – IV SON was in the focus. The changes with time steps from days (Paper IV) to years (Papers I – III), and spatial scales at national/regional level (Papers I – II), fields (Paper III) to field plots (Paper IV) were considered. The validity of a family of models (ICBM) to describe and explain these changes was investigated.

3 Estimating Changes in Soil C and N Stocks

The content of organic matter in a soil is the result of two counteracting processes, the production and input of organic matter by autotrophs and the decomposition of organic matter by soil heterotrophs. Both processes are influenced by a multitude of factors (Post *et al.*, 2001). The C and N cycles are intimately linked, for example, the plant takes C from the atmosphere and mineral N from the soil and creates organic compounds such as proteins, when soil organisms decompose organic matter, CO_2 is respired and, mineral N is released. SOM comprises approximately 50% C (Pribyl, 2010), with substantial amounts of N, usually equivalent to 8 to 12% of the C content in arable land, this results in a C/N ratio of about 10 (Kirkby *et al.*, 2011).

3.1 C Flows

Carbon is the most abundant element in living matter on Earth. Almost all C entering the soil has first been assimilated from the atmosphere by autotrophs (Figure 1). A fraction of the assimilated C is respired back to atmosphere by the autotrophs, both from green parts and roots. Assimilated C can reach soil directly from autotrophs, e.g. as plant litter and exudates from roots. Carbon assimilated in plant biomass can also be consumed by heterotrophs, which respire CO_2 back to atmosphere: the remaining organic C will finally reach the soil as excreta or as carcasses when the animals die (or when the predator dies that may have consumed the herbivore). Although the biologically mediated C fluxes to and from the atmosphere are larger than the amount of C emitted through the burning of fossil C, the additional C from fossil sources results in a small, but steady increase in atmospheric C, as natural sinks are only partly able to absorb the increase. The 'global warming' debate and proposed remedies are directly connected to C fluxes, but this is not addressed in this thesis.

Microorganisms are crucial for degrading C compounds and finally returning C as CO_2 to the atmosphere. In soil, the final decomposition of C compounds can be delayed for a long time, even several centuries, through resistant compounds formed during decomposition and/or by 'protection' from soil aggregates and organo-mineral complexes (Six *et al.*, 2002; Kleber, 2010; Schmidt *et al.*, 2011).

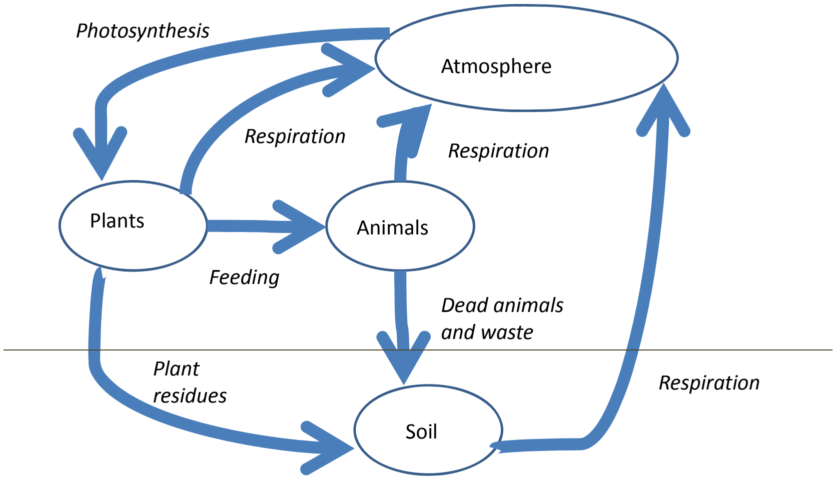

Figure 1. The main C flows in agricultural land.

3.2 N Flows

Nitrogen is essential for life and is a crucial component of amino acids, build proteins, required for respiration, photosynthesis, and nucleic acids that control heredity.

The atmosphere contains 78% N, mainly in the form of inert gas N_2 that is not useful to most organisms. However, some microorganisms can fix N_2 and convert it into biologically accessible forms and lightning can oxidize N into biologically active forms. In modern times, N has been fixed in fertilizer production, and the manmade contribution is now as large as that from terrestrial biological fixation (Galloway *et al.*, 2004). In most terrestrial environments, N is the limiting element for plant production and increased availability of N has increased biological production, and fertilizer N is a foundation for human population increase.

When N-rich organic material decomposes in the soil, N is released as ammonium ions, NH_4^+, which can be converted to nitrate, NO_3^-. For most plants, these inorganic forms are the main N source through root uptake, even if plants can also take up organic forms of N, e.g. as amino acids, directly from the soil (Näsholm *et al.*, 1998; Gärdenäs *et al.*, 2011). Some N is lost from the biological cycle through denitrification and related processes, in which N_2 and N_2O, the potent greenhouse gas, are formed.

3.3 Soil C Input

The amount of organic matter produced (yield and crop residues) in agricultural land depends on crop species and variety, soil conditions, weather and management actions. There can also be input of organic matter from farm-yard manure and other sources, such as sewage sludge.

Reliable estimates of the amounts of organic matter entering the soil are needed for calculating soil C dynamics at regional or larger areas, and for estimating the effects of treatments on SOM mineralization rates in agricultural experiments. However, precise measurements of total organic matter inputs from crops to soils are rarely available (Andrén *et al.*, 1990; Kirchmann *et al.*, 1994; Kuzyakov & Domanski, 2000; Kuzyakov & Schneckenberger, 2004; Wichern *et al.*, 2007; Gan *et al.*, 2009), usually, inputs are estimated from reported agricultural crop yields through allometric functions based on known relationships between yield and other fractions, such as straw, stubble and roots (Bolinder *et al.*, 2007b). Even so, the relation between yield and aboveground crop residues can vary greatly depending on growing conditions, variety etc.

The estimation of the addition of C and N from the roots to the soil is even more difficult. These estimates are uncertain due to the difficulty in extracting roots from the soil and in quantifying extra-root material (exudates and root turnover during a growing season), although these problems can be partially overcome (Bolinder *et al.*, 2007b; Kätterer *et al.*, 2011).

3.4 Decomposition of Organic Matter

Decomposition is mediated by microorganisms and soil fauna and is rate-controlled by environmental factors such as soil temperature, soil water conditions, oxygen concentration, soil chemical properties (mineralogy, pH, available ions), and soil physical properties (e.g. structure and texture). Among these factors, soil temperature and moisture are the most dynamic physical factors controlling SOM turnover (St. Luce *et al.*, 2011).

The temperature dependence of decomposition is the result of several processes such as adsorption, desorption and diffusion of substrates and exo-enzymes, uptake mechanisms of microbial cells, and metabolic pathways within cells that may have different dependencies (Thornley & Cannell, 2001; Ågren & Wetterstedt, 2007). Moreover, different SOM pools may react differently to changes in temperature, although consensus has not been reached in this discussion (Bosatta & Ågren, 1999; Liski *et al.*, 1999; Fang *et al.*, 2005; Knorr *et al.*, 2005; Reichstein *et al.*, 2005; Davidson & Janssens, 2006; Haddix *et al.*, 2011). In most C models, a Q10 value of ca. 2 is assumed at intermediate temperatures (5 – 35°C), meaning a temperature increase of 10°C doubles the decomposition rate (Ratkowsky *et al.*, 1982; Kätterer *et al.*, 1998). Soil temperature follows air temperature, but with some delay and depending of the surface cover, and with spatial variation in surface slope and aspect (Bennie *et al.*, 2008).

Besides temperature, soil moisture is the major factor influencing microbial activities. Microorganisms need water for their life processes, for movement, and for the diffusion of substrates, exoenzymes, and nutrients, thus, soil moisture strongly affects the microbial community structure (Brockett *et al.*, 2012). Generally, decomposition rates increase when soil moisture is at peak value, and then decline due to oxygen limitation. The water content above which decomposition rates decrease depends on the soil texture and SOM (Schurgers *et al.*, 2006; Moyano *et al.*, 2011). Soil water content can be expressed in several ways: mass based or gravimetric, water fraction (θ_m), volumetric water fraction (θ_v), fraction of water content at saturation (θ_s), and the logarithm of water potential or tension (ψ_{log}). The variables θ_s and ψ_{log} are more versatile predictors of microbial respiration as θ_s is related to optimal air space and ψ_{log} is related to water energy status (Moyano *et al.*, 2011).

The spatial variability of soil water is usually greater than the variability in soil temperature (Drury *et al.*, 2003). Precipitation in itself is not evenly distributed, and there is redistribution both through surface runoff, depending on the slope and surface roughness, and below ground, depending on slope and variation in soil water conductivity. The amount of water a given volume of soil can hold (water retention capacity) and crop water uptake by roots are other factors contributing to spatial variability (Romano & Palladino, 2002).

3.5 N-transformation and N Cycling

The ammonium ions, NH_4^+, released during SOM decomposition can be converted to nitrate, NO_3^-, through nitrification (Figure 2). Nitrate is usually the main source of nitrogen for agricultural crops. Ammonium can also be converted to NH_3 gas and lost through volatilization, but this loss is usually smaller than nitrate losses through denitrification and leaching (Janzen *et al.*, 2003; Rochette *et al.*, 2009).

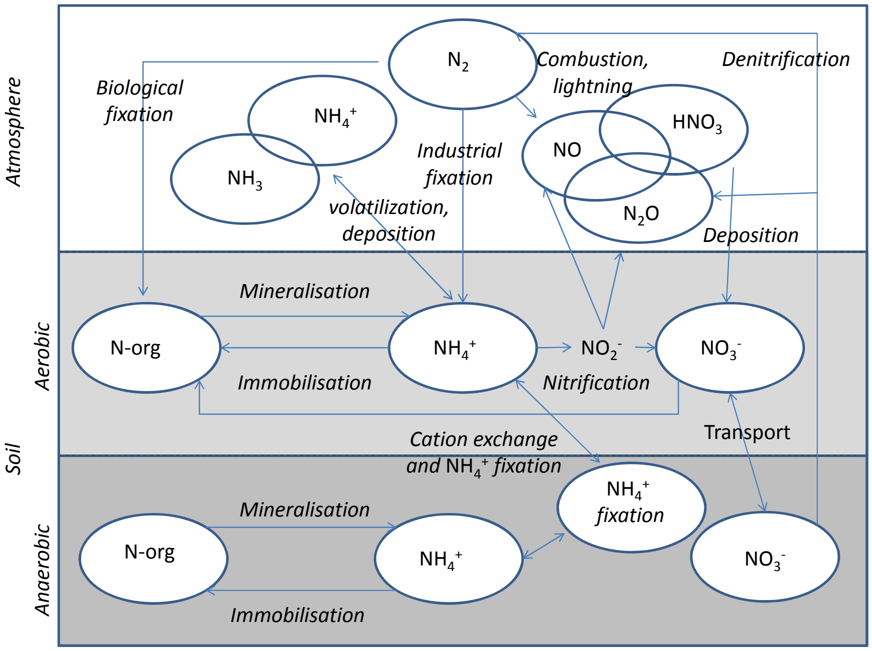

Figure 2. Biological fixation, fertilizers and deposition add N to arable land. Crop removal, leaching, denitrification and NH_3 volatilization remove N. Mineralization, immobilization and nitrification are examples of processes transferring N between different chemical forms or pools. (redrawn from Kätterer (2011)).

Under anaerobic conditions, NO_3^- or NO_2^- (nitrite) can be reduced to either N_2 or gaseous N oxides and be lost to the atmosphere. The process of denitrification is carried out by facultative anaerobic microorganisms and occurs under anaerobic conditions in the soil, e.g., when the soil is waterlogged or when a large supply of fresh material induces high microbial oxygen consumption. A supply of easily degradable organic material is necessary for denitrification to occur. In a heterogeneous soil matrix, different habitats can exist within small distances. In one area, there may be sufficient O_2 for aerobic decomposition and release of NH_4^+, which after conversion to NO_3^- can diffuse to a nearby area with anaerobic conditions, where it is converted to N_2. Due to the interplay of the necessary conditions, denitrification at high rates only occurs during a short period and in small limited volumes within the soil matrix. This variability renders it difficult to measure and calculate a valid average rate, such as flux ha^{-1} $year^{-1}$ without having a high number of measurements per area and time, and a clever system for interpolation. Therefore, useful denitrification data are often lacking, and budget calculations rely on general averages that may deviate significantly (orders of magnitude) from the actual fluxes (Nielsen & Revsbech, 1998). During nitrification and denitrification, nitrous oxide (N_2O) can also be formed as well as N_2. As N_2O is a powerful greenhouse gas, the N cycle need to be fully understood to be able to reduce the climatic impact of agriculture.

In many agricultural areas in cold temperate regions, nitrate leaching to groundwater and streams constitutes a large N loss, due to high precipitation when plant uptake is low, spring flooding due to snowmelt, and the high mobility of NO_3^-. In agricultural fields, there is generally more NO_3^- than NH_4^+ in soil solution, thus, the risk of NO_3^- leaching is higher in soils with low water holding capacity, such as sandy soils. In Sweden, N leaching from agricultural soils is estimated to be approximately 18 kg ha^{-1} $year^{-1}$ (Johnsson *et al.*, 2008).

3.6 Measuring Stock Changes

Measuring changes in organic matter pool sizes is a method for estimating decomposition rates over longer periods, especially for changes in SOC and SON pools at a certain spatial and temporal scale, e.g., change in topsoil C per m^2 and year. To estimate the C or N pool, the elemental concentration, soil volume and mass and/or bulk density, and the thickness of the topsoil layer need to be known, and gravel and rock fragments have to be compensated for, assuming these fractions do not contain SOC or SON. Then determination of elemental concentration, soil layer depth, and dry bulk density includes pitfalls in the estimation, and high precision estimates are difficult to obtain. Estimations are further complicated, as the annual change is usually very small compared with the total mass (Goidts *et al.*, 2009).

SOM is a mixture of organic compounds that vary in molecular structure and resistance to decomposition and in their content of elements. This heterogeneous mixture has various physical locations in the soil, such as particles in the soil solution, adsorbed to clay minerals, or on the external or internal surface of aggregates. The location of the organic compounds together with the chemical composition and particle size affect the availability of the compounds for the decomposing organisms (Schmidt *et al.*, 2011; St. Luce *et al.*, 2011).

The mixture of different substances in a variety of locations can be and is classified into fractions through various physical, chemical or biological analyses (Ros *et al.*, 2011). Among the physical fractions, light fraction organic matter (LFOM) and particulate organic matter (POM) are often determined. LFOM and POM are partially decomposed plant residues that are not bound to soil particles and SOM in these fractions has a relatively rapid turnover rate in the soil (Six et al., 2002).

Chemical fractions defined and used in research are hot-water- and hot-KCl-extractable SOM and includes fractions of SOM with a longer turnover time than LFOM and POM. The methods for estimating microbial biomass, which is considered the most biologically active and labile fraction in soil (Deng *et al.*, 2000), measure microbial activity through both aerobic and anaerobic incubation for different times. Although there are indications the differences in recalcitrance in SOM depend more on the interaction between the SOM properties and surrounding soil environment than on the chemical structure of SOM, there are conflicting views of the proportion between chemical and other recalcitrance factors (Schmidt *et al.*, 2011).

In models, SOM is often divided into several pools, each with different properties, such as size and turnover rate. Another approach is to consider the decomposition of SOM as a quality continuum, along which SOM is moved downwards as decomposition progresses (Bosatta & Ågren, 1985; Ågren & Bosatta, 1987).

It is generally difficult to interpret the various measurable fractions directly in terms of conceptual pools in the models or to quantify the exact quality of SOM (Magid *et al.*, 1997; Andrén *et al.*, 2008). However, for obtaining a reasonable description of the changes in SOM, models appear to require a minimum of two pools; one with rapid turnover and one with slower turnover (Manzoni & Porporato, 2009).

3.7 Variability and Uncertainty

3.7.1 Uncertainties in SOC and SON Stock Change Estimation

For all parameters and variables needed to describe SOC and SON dynamics, there is considerable spatial variation, and often a temporal variation, on different time scales. During sampling, measurement, and analysis, random and systematic errors can be introduced: random errors lead to low precision and systematic errors generate biased results. Sometimes it is not possible to measure the property of interest and it becomes necessary to correlate the property with another known entity, this creates further uncertainty. Often calculations are at a different scale than the actual measurements, for example, there are no direct measurements of national carbon budgets. The recalculation to the desired scale can reduce precision compared to measuring at the ‘right’ scale. Models can also be too simplistic or even incorrect, and some are commonly used outside their validity range.

There are several ways of expressing statistical variation and one common method is to calculate the coefficient of variation (CV), which is the standard deviation divided by the mean of the measurements. For measurements distributed over an area, geostatistical methods suggest whether the variation is small or large scale, for example, in a semivariogram (Figure 3), the range indicates the maximum distance where spatial dependences exist (Post *et al.*, 2008; Goidts *et al.*, 2009; van Wesemael *et al.*, 2011).

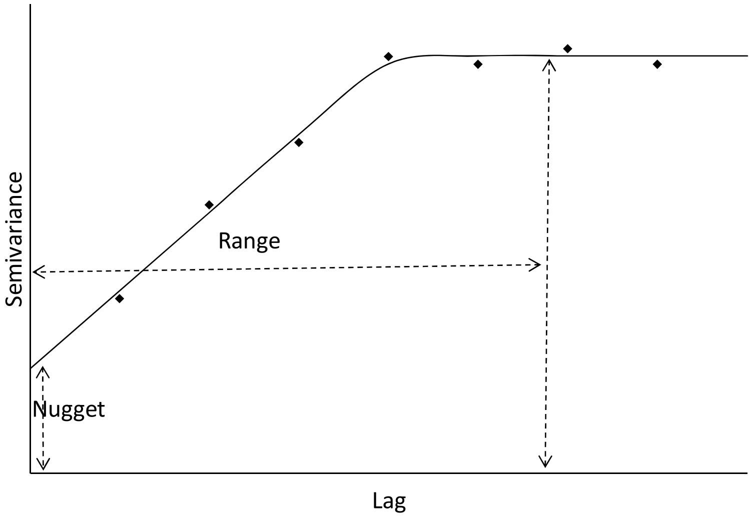

Figure 3. Schematic example of a semivariogram. Lag is the distance between sampling points. The points shown in the variogram are mean values for all pairs separated by a certain distance. The range indicate the distance where spatial dependence exists.

3.7.2 Variation in Soil Properties

SOC and SON Concentration

Soils are the current results of climate, parent material, geological and hydrological processes, topography, vegetation, and cultivation, and this has created a multitude of different varieties of soils. The individual soil type is not a homogeneous medium; instead it is a mixture of solid matter, water with solute substances, gas, and different living organisms, from the smallest microorganism to soil-living vertebrates, and residues from living organisms in the form of organic matter. The processes operating at different scales, from large-scale geological processes and climate fluctuations to millisecond chemical processes in soil micropores create variability at all scales and in all soil properties (Andrén *et al.*, 2008).

The spatial variability of organic carbon concentrations and stocks in soil is scale dependent. In grassland soils in the USA, Conant & Paustian (2002) identified a decrease in the CV for concentrations with scale: 39% at county scale and 63% at national scale. However, Kätterer *et al.* (2004) found a considerably lower CV at sampling points within one square meter (3 soil cores, CV 2.6 – 3.6%) than within a whole field (CV 3.5 – 20%). In contrast, Amador *et al.* (2000) and Stark *et al.* (2004) observed high variability in SOC stocks even at a centimeter scale; however, the majority of studies on the spatial variability of SOC neglect small scale variability by not sampling at distances below 1 m (Simfukwe *et al*., 2011).

To obtain a reliable estimation of the changes in SOC and SON concentrations due to different treatments or at regional and national scale, a carefully designed sampling and monitoring system is required (Goidts *et al.*, 2009; van Wesemael *et al.*, 2011; Raczkowski *et al.*, 2012). In Sweden, such a system is now in place. A total of 2034 sampling points with exact coordinates are sampled and they will be sampled every 10 years. (Eriksson *et al.*, 2010).

Even at small scales, there is considerable variability; therefore, the various properties should be measured in the same soil volume, if possible (Western & Blöschl, 1999). As this requires special consideration in experiments that continue over several years, a possible solution to including and dealing with spatial variation would be the annual sampling of several subplots that represent a common larger plot.

Mineral N Concentrations

Heterogeneity of soil properties causes local differences in mineralization rates within a field and variable weather conditions cause temporal variations at hourly, daily, and yearly scales. These differences affect crop growth and crop demand for N. Thus, soil mineral N concentrations often vary, with greater variability at small-scale than SOM concentrations. In samples taken within a distance of 40 and 90 m, Giebel *et al.* (2006) Baxter *et al.* *(*2003) found detectable spatial correlations, which means these samples are more similar than samples taken at wider distances. However, other studies present contrasting results, for example, correlations over much shorter distances (Bogaert *et al.*, 2000), no detectable spatial pattern (Ilsemann *et al.*, 2001; Haberle *et al.*, 2004), and a CV for samples from experimental plots (4.5 x 24 m) of the same magnitude as the CV from whole fields (Lindén (1981).

C and Mineral N Variation in a Meadow at Ultuna

In May 2005, we sampled a 2.60 x 3.16 m rectangular plot in a meadow at Ultuna, Uppsala, Sweden (17°39.989' E, 59°50.149' N). Single soil samples (n=121) were taken, with a distance of 0.3 m between each sample. The C concentration was analyzed in the soil sample from 0.1 – 0.3 m depth. The mean average total soil carbon concentration was 2.84% (CV 9.47%): the minimum SOC concentration was 2.33% and the maximum was 3.70%, thus, the maximum concentration was 61% larger than the minimum concentration (Figure 4). Between the two neighboring sampling points, the maximum difference in carbon concentration was 46%, three-quarters of the maximum variation in the sample plot. This high variability was reflected in a variogram (not presented), which showed no spatial correlation.

The variability in soil mineral N concentration was larger than the variability for total SOC. The mean soil mineral N concentration was 15.5 kg ha^{-1} with a CV of 99.6% (Figure 5); however, no spatial correlation was apparent in the variogram (not presented). There appeared to be accumulations of high concentrations, for example in the upper right corner of Figure 5, whereas, the neighboring points had very low concentrations, however, generally, it was not possible to distinguish any spatial patterns.

Estimation of Soil Bulk Density and Hydraulic Properties

Direct measurements of bulk density and soil hydraulic properties are labor intensive, time-consuming, tedious, and expensive (Vereecken *et al.*, 2007; Suuster *et al.*, 2011). Therefore, empirical functions are often developed and utilized for estimating bulk density and hydraulic properties from other soil properties such as texture and SOM (Kätterer *et al.*, 2006; Børgesen *et al.*, 2008).

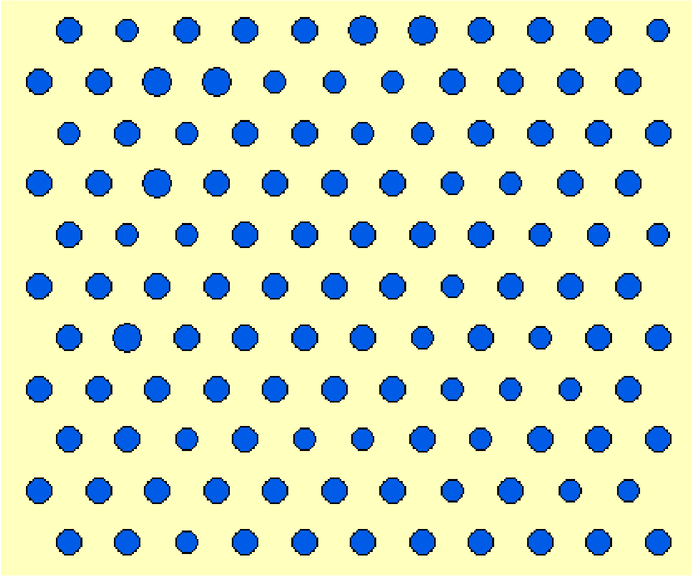

Figure 4. Variation of total C concentration in a 2.60 x 3.16 m plot at Ultuna, Uppsala, Sweden. The diameter of each dot is proportional to the C concentration at that spot, at 0.1 – 0.3 m depth. Distance between sampling points is 0.3 m.

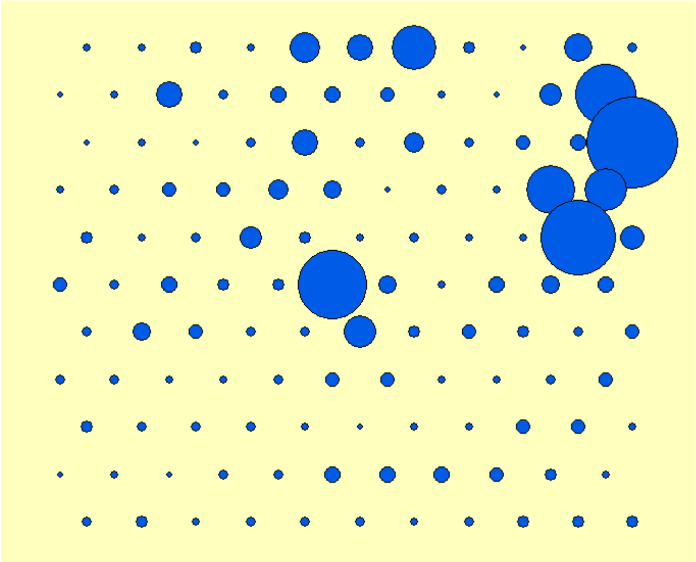

Figure 5. Variation of NO_3^- concentration in a 2.60 x 3.16 m plot at Ultuna, Uppsala, Sweden. The diameter of each dot is proportional to the NO_3^- concentration at that spot, at 0.1 – 0.3 m depth. Distance between sampling points is 0.3 m.

3.7.3 Modeling

Why Models?

Models are necessary for extending observations from single or compiled field experiments to other conditions, for instance to regional scale, or for making projections. SOM turnover involves many factors that are difficult to estimate, and the interaction of these factors with each other means they all cannot be measured outside of large projects. Thus, models are necessary for understanding and generalizing the main processes and to filling the gaps where data are not available (Molina & Smith, 1997; Gabrielle *et al.*, 2002; Shibu *et al.*, 2006; Post *et al.*, 2008; Juston *et al.*, 2010; Ros *et al.*, 2011).

Model Types

Models are categorized in several ways (Shibu *et al.*, 2006; van Wesemael *et al.*, 2011), but are basically, although not exclusively, of two types: process-based (mechanistic) or functional (empirical) (Viaud *et al.*, 2010). Process-based models attempt to describe several or many of the actual processes through model algorithms representing the basic mechanisms, whereas, functional models are based on the relationship between different factors or variables, for example, multiple linear regressions can be used to describe how climate, soil type and land use affect the amount of carbon. Empirical models constrain the conditions from which they are derived and new external factors outside their validity range cannot easily be included in functional models, nor can they make predictions about the future.

Process-based models usually require more data than functional models; however, some crucial parameters are often difficult to quantify, particularly in highly complex models: the model can only be as precise as the input data and included functions. Consequently, the models have to be calibrated to specific sites through adjusting the rate constants and pool sizes to fit locally measured data (Benbi & Richter, 2002).

Precision and Uncertainties in Models

Model uncertainty is mainly due to uncertainty in parameter values, and in the correctness or validity of the functions included. Functions are simplifications of reality and will always be incomplete. Moreover, different processes govern mineralization at different scales, thus, a model's precision is affected by the processes included in the model (Pringle *et al.*, 2008; Manzoni & Porporato, 2009; Franko *et al.*, 2011).

Parameter uncertainty derives from errors in the measurements that are the basis of parameter values, in scaling-up from point values to model scale, and in the estimation of parameter and input values via indirect values for parameters that cannot be directly measured (Post *et al.*, 2008).

4 Materials and Methods

4.1 ICBM and Parameter Estimation

The Introductory Carbon Balance Model (ICBM) was developed as a minimum approach for calculating soil carbon balances over a 30-year period (Andrén & Kätterer, 1997). ICBM is based on generally agreed core concepts such as first-order decomposition kinetics and a low number of C and N pools (Henin & Dupuis, 1945). The basic idea was to create a simple, analytically solved model for use at different levels of complexity. In ICBM there are two C pools, young (Y) and old (O), two decay constants, and parameters including 'litter' input (i), 'humification coefficient' (h), and external influences (Figure 6). Crop residues and manure are input (i) to Y, and during decomposition of this material, some C will be respired and lost as carbon dioxide and some will enter the O pool according to the value of the humification coefficient (h). Outflows from the pools follow first-order kinetics, and the rate constants k_y and k_o are modified by a factor (r_e), which accounts for all external driving variables, such as soil water and temperature status.

The model is analytically solved, that is simulation techniques are not necessary and the model properties can be mathematically analyzed and the model run and optimized in an ordinary spreadsheet program (e.g. Excel®). Equations for steady-state conditions, i.e., when the pools are constant in size and the inputs and outputs balance, are also included. However, it is also possible to run the model as a simulation, with i, h and r_e as driving variables, i.e., with different values for each time step (Kätterer *et al.*, 2004). The model and the instructions and supporting literature can be downloaded from www.oandren.com.

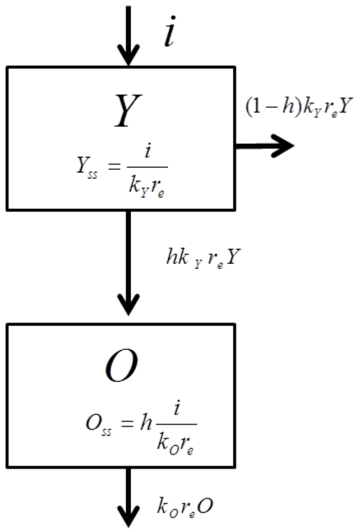

Figure 6. Structure of ICBM. *i*=input, *Y*=young carbon, *O*=old carbon, k_Y, k_O=decomposition constants, *h*=humification coefficient and r_e=external control

The basic ICBM model has been expanded to fulfill different needs. Examples of features that have been added are functions to; describe the changes in SON, provide a more precise description of the initial stages of decomposition, and explicitly model organism C and N (Kätterer & Andrén, 2001). Therefore, the model can be readily adapted to different needs, such as predicting at different scales and application in different environments (Andrén *et al.*, 2007; Bolinder *et al.*, 2007a; Juston *et al.*, 2010; Salazar *et al.*, 2011; Borgen *et al.*, 2012; Lokupitiya *et al.*, 2012). The different components in the ICBM family of soil C and N models are described in detail by Andrén & Kätterer (1997), Kätterer and Andrén (1999), Kätterer & Andrén (2001), Andrén *et al.* (2004) and Fortin *et al.* (2011).

In the studies in this thesis, ICBM was used in Papers I - II, ICBM/2N was used in Paper III, and ICBM/N was used in Paper IV. In ICBM/N, two N pools have been added to the original ICBM model, one to the 'young' pool (*YN*) and one to the 'old' pool (*ON*). C in crop residues (*i*) are inputs to *Y* and N in crop residues (*i/qi*) are inputs to *YN*. During decomposition, N will be mineralized or immobilized depending on the *Y*/*YN* ratio, the C/N ratio of the organism community (q_b), and its yield efficiency (e_Y). The amount of N entering *ON* is determined by the C/N ratio *O*/*ON* (q_h). In ICBM/2N, the *Y* and *YN* pools are divided into young, labile (Y_l, YN_l) and young, refractory (Y_r, YN_r) to handle inputs from crop residues separately from manure. A summary of the driving variables, parameters, and symbols used in the applications of the ICBM/2N model is presented in Table 1.

Table 1. *Parameters and symbols in ICBM/2N*

Parameter	Symbol
Initial C mass of the 'young and labile' pool (from crop residues)	Y_{0l}
Initial C mass of the 'young and refractory' pool (from organic amendments)	Y_{0r}
Initial C mass of the 'old' pool	O_0
Annual C input to soil, labile part (from crop residues)	i_l
Annual C input to soil, refractory part (from organic amendments)	i_r
Decomposition rate constant for the young pool	k_y
Decomposition rate constant for the old pool	k_o
Humification coefficient, fraction of 'young and labile' outflux to *O* (crop residues)	h_l
Humification coefficient, fraction of 'young and refractory' outflux to *O* (organic amendments)	h_r
External response factor that affects outflux from 'young' and 'old'	r_e
Initial N mass of the 'young and labile' pool	Y_{0Nl}
Initial N mass of the 'young and refractory' pool	Y_{0Nr}
Initial N mass of the 'old' pool	O_{0N}
Quality, C/N ratio of 'labile' input, i_l	q_{il}
Quality, C/N ratio of 'refractory' input, i_r	q_{ir}
C/N ratio of soil organism biomass	q_b
C/N ratio of the 'humification', the influx to *O*	q_h
Efficiency, the fraction of C flux from *Y* allocated to organism growth	e_y

The disadvantage of a simple model is that much detail falls outside the model's range. In many cases, this can be turned into an advantage, as a step-by-step approach to a complex problem is often the best approach because the generation of parameter values for a complex model can divert the focus away from the original research question. For example, the annual amount and quality of carbon input to the soil is difficult to estimate, however, best possible estimates, or even educated guesses, can be made from available data, – and these can be used as input to a simple and straightforward model. Alternatively, the soil carbon model can be used to calculate a probable input, in a sense, modeling the immeasurable (Magid *et al.*, 1997). Ideally, the input estimates are based on thorough investigations of annual surface and root litter input, including root exudates (Kätterer & Andrén, 2001).

4.1.1 External Climate Response Factor (r_e)

The effect of all external factors (soil moisture, temperature, soil type, soil tillage etc.) are condensed into the r_e factor. In the original parameter setting of ICBM, average r_e was set to 1, representing the annual mean conditions for a 35-year experiment with fertilized cereal crops on clay soils in south-central Sweden (the Ultuna frame experiment; Andrén and Kätterer, 1997). The default decomposition rate constants, k_y and k_o, refer to the original scaling of r_e. Thus, calculated r_e generates only relative response values, and these values must be scaled so the mean of all daily products over the year corresponds to r_e in ICBM.

In Paper III, r_e is one of the optimized parameters, since the model is fitted to measured data. In this case r_e represents an annual mean value averaged over the experimental periods (36 – 41 years).

In Papers I, II and IV, daily weather data and soil data are used to calculate daily r_e values used as driving variable for the model. The factor r_e is calculated from soil water content (θ; m^3 m^{-3}) and soil temperature (T; °C), and is the product of the daily outputs of the response functions r_θ and r_T: r_θ depends on θ and r_T depends on T. As T is assumed to affect decomposer activity according to a quadratic relationship (Ratkowsky *et al.*, 1982), it was normalized to 30°C, roughly the maximum soil temperature occurring at the site:

Equation 1

$$r_T = \max\left[0; \frac{(T - T_{\min})^2}{(30 - T_{\min})^2}\right]$$

where: activity is zero at T_{min}=-3.8 °C (Kätterer *et al.*, 1998), and r_T is approximately doubled by a 10°C increase in temperature.

The water store in soil was delimited by the field capacity (θ_{fc}) and a minimum water store corresponding to a certain fraction (α) at wilting point (θ_{wp}) (Papers I and II). The water response function used was:

Equation 2

$$r_\theta = \left\{ \left(\frac{\theta - \alpha\theta_{wp}}{\theta_{fc} - \alpha\theta_{wp}} \right)^{\beta} \right\}$$

where: the parameter β (=1.3) defines the shape of the function between $\alpha\theta_{wp}$ and θ_{fc}. In Paper IV, the water response function (r_θ) was assumed to depend on θ through:

Equation 3

$$r_\theta = \left\{ \begin{array}{ll} 0 & \theta < \alpha\theta_{wp} \\ \left(\dfrac{\theta - \gamma\theta_s}{\gamma\theta_s - \alpha\theta_{wp}} \right)^{\beta} & \alpha\theta_{wp} \le \theta \le \gamma\theta_s \\ 1 + (1 - r_s)\dfrac{\theta - \gamma\theta_s}{\gamma\theta_s - \theta_s} & \theta > \gamma\theta_s \end{array} \right\}$$

where: microbial activity increases from zero at a certain fraction (α; here set to 0.5) of θ_{wp} to a maximum at optimal water content ($\gamma\theta_s$), corresponding to a fraction γ of the saturated water content (θ_s). Above $\gamma\theta_s$, r_θ decreases to a minimum of r_s at θ_s (Figure 7). This water response function is similar to the functions implemented in other decomposition and ecosystem models such as NLEAP (Schaffer *et al.*, 2001), and is based on experimental work by Linn and Doran (1984) and Lomander *et al.* (1998). The values for θ_{wp} and θ_s were estimated from soil texture and carbon concentrations through pedotransfer functions (Kätterer *et al.*, 2006).

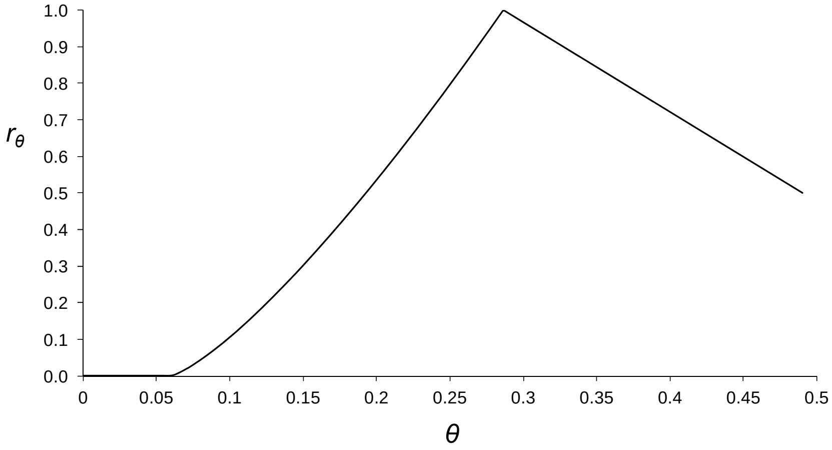

Figure 7. Example of the relation between θ (volumetric soil water content, m^3m^{-3}) and the value of r_θ (moisture response parameter) according to Equation 3.

The product $r_T r_\theta$ only provides relative response values as the default decomposition rate constants, k_Y and k_O, refer to annual mean r_e-values, which are set to unity in the climatic conditions of central Sweden (Uppsala region; Andrén and Kätterer, 1997). Thus, $r_T r_\theta$ must be scaled for the sum of all daily products over the year to correspond to r_e in ICBM:

Equation 4

$$r_{e\_day} = k_r r_T r_\theta$$

where: the scaling factor, k_r, is used as a free scaling parameter in the calculations (Paper IV).

A cultivation factor, r_c, was introduced to summarize daily r_e values as annual means, and k_r was calculated with data from the calibration site, Ultuna frame experiment (Papers I and II). The procedures and functions were applied to the 30 years of daily weather data (1970–1999) from the Ultuna weather station and the soil and crop data (clay loam, spring cereals, production region) corresponding to the treatment in the ‘frame’ experiment. This yielded an r_e of 0.11939. As r_e in the treatment at the calibration site was 1 by definition, all calculated r_e values were divided by this value. Thus, r_e at the calibration site became 1, and r_e for all other combinations of years, regions, crops and soil types were presented relative to the normalized calibration site. No further adjustments or ‘tunings’ were made in this study. The resulting daily r_e-values

(r_{e_day}) were summed over the experimental period. In applying the ICBM model to the data, and as with the use of temperature sums, time (t) as the independent variable could be replaced by r_e, the 'climate sum':

Equation 5

$$r_e = \sum_{t=1}^{t} r_{e\_day}$$

Thus, there was no need to run simulations, as the model was analytically solved and both t and r_e were quasi-continuous variables, and solutions can be determined through non-linear regression analysis (Kätterer & Andrén, 2001).

4.1.2 Soil Water Balance

The soil water balance calculations were based on FAO concepts (Allen *et al.*, 1998; Andrén *et al.*, 2007), with the inputs being daily weather station data, daily mean air temperature, precipitation, and reference evapotranspiration. For each day and unit studied, soil water store was calculated from present store + precipitation - evapotranspiration. The water store was then recalculated to relative water content, i.e., the fraction of the potential water store that is filled with water (Andrén *et al.*, 2004).

4.1.3 Pedotransfer Functions

For calculating soil water dynamics, soil water contents at wilting point (θ_{fp}) and at field capacity (θ_{fc}) are needed. As wilting point and field capacity are not generally measured, pedotransfer functions, can be used. Model 12, suggested by Kätterer *et al.* (2006), and developed from a database of arable soils in Sweden, was used to estimate the water content at θ_{fp} and θ_{fc} from texture and carbon concentration for each texture class.

4.1.4 Allometric Functions for Conversion of Yield to C Input

The allometric functions and the parameter values used to calculate annual carbon input from crop yield data were based on detailed investigations of carbon allocation in various crops, as described in Kuzyakov and Domanski (2000). The allometric functions were combined into:

Equation 6

$$C = a + sH$$

where: C denotes the carbon mass of straw, stubble or roots, and H is the observed crop yield (as kg carbon ha^{-1}). Parameters a and s are empirically based and differ between straw, stubble and roots and are different for different crop types (Table 2).

Table 2. *Parameter values used in the allometric function C=a+sH to calculate C input (C) from crop yield (H), kg ha^{-1}*

	Straw		Residues		Roots	
Crop	a	s	a	s	a	s
Spring cereals	140	0.83	500	0.15	570	0.20
Winter cereals	320	0.62	540	0.40	670	0.06
Spring oilseed	0	1.60	0	1.60	0	0.70
Winter oilseed	0	0.85	0	0.85	740	0.70
Root crops	0	0.00	0	0.42	0	0.20
Ley	0	0.00	330	0.20	0	0.40
Seed ley	2700	0.00	905	0.00	540	0.00
Green fallow	0	0.00	0	0.30	0	0.60
Fallow	0	0.00	0	0.30	0	0.60

4.2 Regional C Balances in Agricultural Soils (Papers I and II)

The calculations of annual Swedish arable soil C balances were based on four data sets:

(1) Regional yield data from nine crop types for 1989 to 2003.
(2) Daily data from 22 weather stations for 1990 to 2004 (temperature, precipitation and reference evapotranspiration – calculated from other meteorological variables).
(3) A nationwide sampling of agricultural soils (including soil type and C concentration etc.) (Eriksson *et al.*, 1997; Eriksson *et al.*, 1999)
(4) Pedotransfer functions for calculating bulk density that were developed from a another Swedish data base (Kätterer *et al.*, 2006).

ICBM in its original version was used for the calculations. In this application, a cultivation factor, r_c, was added, which accounted for the differences in decomposer activity between crops, due to variations in soil cultivation intensity and frequency, and was set to lowest in leys (0.87) and to highest in root crops (1.2) (Andrén & Kätterer, 1997; Kätterer *et al.*, 2008).

Swedish agricultural statistics are usually compiled for eight production regions (Figure 1 in Paper II), and annual yield statistics from SCB, Statistics Sweden, were used for calculating C inputs to the soil. For each year from 1989 onwards and for each production region, crop yields for 32 crops that were bulked into nine major crop types (Fallow, Green fallow, Ley, Root crops, Seed ley, Spring cereals, Spring oilseed, Winter cereals, Winter oilseed) were used. An allometric function (Equation 6) was used to calculate annual C input to soil for each region and crop type. Manure addition was calculated with annual regional data from SCB, and when data were available, manure was distributed between crop types accordingly. Crops left in the field (e.g., not harvested due to bad weather) were assumed to be input to soil.

Daily climate data from 22 weather stations managed by SMHI, the Swedish Meteorological and Hydrological Institute, were used. Each region was represented by 2–4 stations, and the daily variables used in the model calculations were air temperature (°C), precipitation (mm), and reference evapotranspiration (mm). Reference evapotranspiration was not available in the weather dataset and was calculated from wind speed ($m\ s^{-1}$), relative humidity (%), cloudiness (%) and daily mean temperature (°C) (Allen *et al.*, 1998; Andrén *et al.*, 2007). Air temperature was converted to topsoil temperature according to a semi-empirical equation proposed by Kätterer and Andrén (2008).

Datasets from a Swedish agricultural soil survey (Eriksson *et al.*, 1997; Eriksson *et al.*, 1999) were used to calculate areas of each 14 soil types and recent topsoil carbon mass for each region. The 12 mineral soil texture classes used were clay, silty clay, silty clay loam, clay loam, sandy clay loam, loam, silt loam, sandy loam, loamy sand, and sand (Eriksson *et al.*, 1999). High C (organic) soils were divided into high C (>7% C, <11.6% C) and very high C (>11.6% C). The pedotransfer functions used and the water balance calculations are described in Section 4.1.

This conceptual model, using national agricultural crop yield statistics and allometric functions to calculate C input to the soil together with ICBM are called ICBMregion.

4.3 Long-term Arable Field N Balances (Paper III)

ICBM/2N was used to calculate changes in soil organic N pools over a 30-year period and to compare system N balances with and without SON dynamics. ICBM/2N assumes two pools of young C and N, and one pool of humus C and N, and data from two Swedish long-term experiments were used, Ultuna and Fjärdingslöv.

The Ultuna experiment is located in Central Sweden close to Uppsala (59°48' N, 17°38' E) and began in 1956 to investigate the long-term effects of regular application of various types of organic material. The soil is a clay loam and the crops are cereals, oil seed, and in some years, root crops (Kirchmann *et al.*, 1994). The climate is cold temperate and semi-humid. The mean annual precipitation in nearby Uppsala during 1961 – 1990 was 544 mm and the mean annual air temperature was 5.7˚C (SMHI, 2000). The Ultuna experiment was included as it is well designed and probably the most investigated field experiment in Sweden regarding changes in soil C and N, and the original ICBM model was preliminarily calibrated with results from this experiment, and other models have been tested there (Parton *et al.*, 1983; Paustian *et al.*, 1992; Hyvönen *et al.*, 1996; Andrén & Kätterer, 1997; Barre *et al.*, 2010).

The Fjärdingslöv experiment is located near Trelleborg, Skåne county in southern Sweden (55°24′ N, 13°14′ E) on a sandy loam soil (Kirchmann *et al.*, 1999), where one rotation including ley and manure and one without are compared at different levels of N fertilizer application. The yearly precipitation during 1961 – 1990 in the area (data from nearest meteorological station) was 590 mm and the mean temperature during the same period was +8.1ºC (Carlgren & Mattsson, 2001).

4.4 Site-specific Annual N Mineralization (Paper IV)

N mineralization dynamics was simulated for 34 unfertilized plots in a 15 hectare large field in south-west Sweden (58° 06´N, 12° 51´ E, Figure 8).

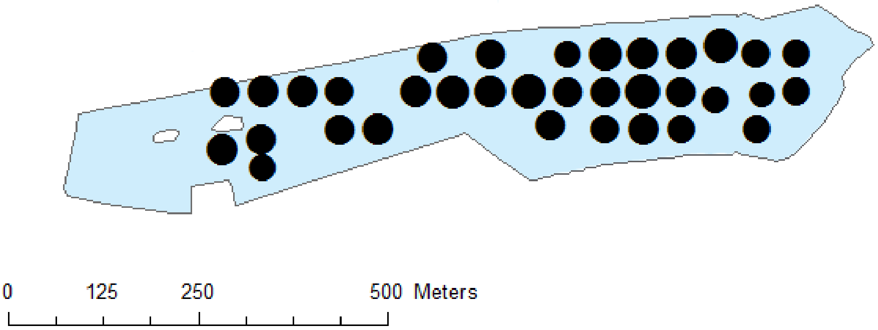

Figure 8. The size of the dots are proportional to SOC concentration (2.65 – 4.55%), 0 – 0.20 m soil depth.

The data from the experiment have been analyzed in a static model which did not explain the variation in mineralization between years (Delin & Lindén, 2002). Samples from topsoil (0-0.20 m depth) were analyzed for total C, total N, and texture: the soil varies in texture from sandy loam to silt loam.

Crop in experimental plots were sampled for aboveground biomass and C and N concentration. C and N inputs from crop residues were calculated from the allometric relationship from the previous crop's grain yield, as described in Section 4.1. A detailed description of the sampling and analysis can be found in Delin & Lindén (2002) and Paper IV. Daily mean values from weather variables recorded hourly at one location in the field (Delin & Berglund, 2005) were used in the calculations. Dry bulk density, soil water saturation point (θ_s), field capacity (θ_{fc}), and wilting point (θ_{wp}) were estimated from soil texture and SOC concentrations by pedotransfer functions (Kätterer *et al.*, 2006).

The amounts of SOC and SON in the topsoil were calculated from the C and N concentrations and bulk density. Soil samples were taken from the plots early in spring and after harvest, and analyzed for mineral N. Apparent net N mineralization (*Nm*) was calculated according to Delin and Lindén (2002), that is, as the sum of N in harvested crop (N_c) and the change in soil mineral N stored in topsoil ($\Delta Nmin$) during the growing season. Thus:

Equation 7

$$Nm = Nc - \Delta Nmin$$

The model parameters γ (fraction of water-filled porosity at maximum heterotrophic soil activity), k_r (scaling factor for r_e) and e_y (microbial growth efficiency) were simultaneously optimized by a modified Gauss-Newton method (non-linear regression analysis, Proc NLIN, (SAS Institute Inc., 2004)) to obtain the best model fit for the apparent mineralization in all small plots and for both years. These parameters were selected for optimization, as values cannot easily be estimated from the literature or measured and the parameters are critical for model performance.

5 Results and Discussion

In this thesis, the soil organic matter dynamics model ICBM was applied at different spatial and time scales.

5.1 Regional C Balances in Agricultural Soils (Papers I and II)

In a European context, carbon concentrations in Swedish arable soils were high, even when high C soils were excluded. The proportion of high C soils differed considerably between regions, with the highest proportions in plain districts in Svealand, forest districts in Götaland and upper parts of Norrland.

The average inputs for each region decreased from South to North, depending on climate, crop choice, crop yield, crop residue handling, and manure application. However, the differences in input were smaller than might be expected from crop yield differences (Table 1 in Paper II), as the proportion of grass leys, which generally generates higher C inputs than other crops, was higher in the North. In terms of regional differences (Table 3), region 1 in the Southwest had the highest climatic factor (r_e) for most years, and regions 7–8 in the North had the lowest, this was mainly due to temperature differences (Table 3 in Paper II).

Region 1 had the lowest C mass per hectare, regions 2, 3, 4 and 6 had intermediate C mass per hectare, and the forest districts in Götaland (5) and the two northernmost regions (7, 8) had the highest topsoil C mass (Table 3). Carbon input increased by a factor of 1.3 from North to South and the corresponding factor for r_e was 1.8. Thus, a higher steady state C mass would be expected in the North, which was reflected in the calculated long-term balance (C_{ss}) and the measured value (C_m) (Table 3 in Paper II). Region 5 had a high ley proportion and manure input (which rendered a high humification coefficient, h), which supported the high C mass.

Due to the stability of most soil organic C and the lack of dramatic changes in i or r_e, the annual changes were small. The soil was generally close to steady state, that is, the annual inputs were equivalent to the decomposition of organic matter.

Table 3. *Average values for 1990-2004 for each region, organic soils excluded. Annual C input from crop and manure (i,t ha^{-1}), climate factor (r_e), projected total topsoil C (TotC, t ha^{-1}). Trend indicates projected increase or decrease in topsoil C in the region.*

Region	i	r_e	TotC	Trend
1. Plain districts in southern Götaland	3.29	1.30	69.8	→
2. Central districts in Götaland	3.07	1.05	79.3	↗
3. Plain districts in northern Götaland	3.08	1.04	81.5	↘
4. Plain districts in Svealand	2.68	1.04	80.0	↘
5. Forest districts in Götaland	3.01	0.99	91.5	↘
6. Forest districts in central Sweden	2.63	0.88	83.2	↘
7. Lower parts of Norrland	2.59	0.69	92.4	↗
8. Upper parts of Norrland	2.57	0.67	93.4	↗

According to these projections, central Swedish regions (3–6) appeared to be losing topsoil C mass, as C_m and calculated present C mass were higher than the calculated long-term balance (Css). Northern regions 7–8 and region 2 appeared to gain C in their mineral soils. Region 1 appeared close to balance. However, the use of twelve years of data extrapolated to eternity is questionable, as ICBM was originally designed for simulating C dynamics over a 30-year period, and the steady-state values are directly proportional to parameter values.

The proportion of high C soils varied between regions, from 1.8% in region 1 to 11.2% in region 8 (Table 2 in Paper II). If these soils were included in mean C mass calculations, the average C mass became substantially higher in certain regions, for example, over 110 t ha^{-1} in region 8. Although the soil carbon appeared in balance, there was considerable subsidence in organic soils, that is sinking of the soil surface in cultivated organic soils, – which is partly due to compaction and partly due to decomposition of SOM in situations with a lowered water table and soil cultivation. If soil is cultivated to the same depth every year, subsidence results in subsoil matter being transferred into the topsoil. Due to this input, the organic topsoils are close to steady state, as the inputs from subsidence are lost as CO_2 each year. For high and very high C soils, the annual input and consequential loss as CO_2–C can be 7 t ha^{-1}.

The total C mass in Swedish agricultural topsoils decreased from 269 Mt in 1990 to 251 Mt in 2003, partly due to a slight reduction in the area of arable land between 1990 (2.84 Mha) and 2003 (2.67 Mha). No dramatic changes or trends were detected.

The estimates for 1994–1995 C mass, based on more than 3100 soil samples, provided a baseline estimate of C mass, and effort was made to retain high precision and avoid bias (Eriksson *et al.*, 1997; Eriksson *et al.*, 1999). Although this sampling has been repeated (Eriksson *et al.*, 2010), no significant change in C stock has been detected. However, due to the low rate of change expected, only clear trends can be detected and only after considerable time (10–20 years): this type of monitoring is a long-term commitment.

The findings indicated mineral soils were near steady state and the simple model approach performed satisfactorily. However, to sufficiently test and possibly reject the model hypotheses, long-term, high precision and unbiased data sets are needed, and these are rare in soil biology (Andrén *et al.*, 2008).

The calculations of the climate factor, r_e, were based on three components: the effects of soil temperature, soil water content, and degree of cultivation. The effects of soil temperature and soil water content were general and based on experimental data, but the effects of soil cultivation *per se* were less investigated and probably have less effect in general. Although the cultivation factors used, e.g., 1.0 for cereals and 0.87 for grass leys, were rough estimates, the same principle has been applied in a study on changes in soil C stocks in fields with varying cultivation over time (Kätterer *et al.*, 2008). Intense soil cultivation increases decomposer activity through increased aeration and comminution of litter and soil aggregates. However, the development of a general function to describe this effect and identifying parameter values for different cultivation measures and soils is not an easy task. However, this factor is important, as the decomposition rate appears to depend on the availability of SOM to the microorganisms (Schmidt *et al.*, 2011). There is limited information about if and how the intensity of soil cultivation and other important cultivation conditions are changing in agriculture. For example, in Belgium, the amount of SOC has increased in grasslands in some areas and decreased in others (van Wesemael *et al.* (2010). This inconsistent result can be explained in one region, in that grasslands are largely old arable land converted to grassland, therefore, the amount of carbon increases, whereas, in another region, drainage intensity has increased, which increases decomposition and reduces SOC stocks.

Due to the limitations of the data available, the distribution of crops was assumed the same on all soil types within a region, although this is never true, for example, a higher frequency of potato crops would be expected on light soils. This bias might cause SOC stock to change differently to the simulated projections for specific soil types, and highlighted the necessity of continuing and improving national surveys and obtaining more data to avoid discrepancies.

The ICBMregion approach has been applied to national datasets from Norway (Borgen *et al.*, 2012) and the USA (Lokupitiya *et al.*, 2012), with comparable results to other studies. ICBMregion increases insight into inter-annual variability, as actual crop areas and outputs are considered in the model. Although other simulations of regional SOC balances has been conducted (Ogle *et al.*, 2007; Smith *et al.*, 2007; Kirk & Bellamy, 2010; Ungaro *et al.*, 2010; Meersmans *et al.*, 2011), the surveys of SOC stocks at national level have not clearly demonstrated whether it is land use, management and/or climatic changes that cause the observed changes in SOC stocks. However, model-based estimates based on detailed land use data and weather have not been verified by national surveys (Saby *et al.*, 2008; van Wesemael *et al.*, 2010).

As in many other national C stock simulations, no formal estimates of uncertainty were included in Papers I – II. However, methods for including uncertainty estimates of ICBM projections are being established (Juston *et al.*, 2010). In conclusion, ICBMregion appears a cost-effective method for calculating and explaining changes in SOC stocks in arable land.

5.2 Long-term Arable Field N Balances (Paper III)

The optimized r_e factor differed between treatments in the Ultuna experiment, and was probably due to the influence of the crop on the soil environment (Table 3 in Paper III). For example, the r_e factor for the unfertilized crop treatment was 1.2 and the treatment with mineral fertilizers had an r_e of 0.8. The transpiration from a well-developed crop with a high leaf area index is higher than from a poor crop, and is much higher than the amount of water evaporated from bare soil. At Fjärdingslöv, the differences in r_e between treatments were not as apparent, although r_e was slightly lower for treatments with ley (average for all fertilizing levels 1.0) than for rotations without ley (1.1 – 1.6).

The inclusion of changes in soil N altered the balances for the treatments at Ultuna (Table 4). The balance increased (higher N surplus) in treatments with bare fallow, unfertilized, and calcium nitrate, and decreased for treatments receiving organic amendments (straw, green manure, farmyard manure and straw + calcium nitrate).

Table 4. *N balances for Ultuna long-term experiment, 1956-1991, calculated without and with changes in soil organic N*

	No N, no crop	No N	Calcium nitrate	Straw	Green manure	Farmyard manure	Straw + calcium nitrate
A. Fertilizer	0	0	78	0	0	0	78
B. Organic amendments	0	0	0	27	104	86	27
C. Deposition	3	3	3	3	3	3	3
D. Removed plant parts	0	43	88	44	83	65	90
E. Balance, applied – removed (A+B+C-D)	3	-39	-7	-14	24	24	17
F. Simulated change in soil N	-36	-23	-11	9	23	46	21
G. Balance including changes in soil N (E-F)	39	-16	4	-23	1	-22	-4

Persson and Kirchmann (1994) have used a linear function to describe the changes in soil C at Ultuna, and the fit was similar to that for ICBM, but this may be due to a lack of precision in the measurements. However, a linear function cannot be extrapolated outside the period of measurements, as it would result in an infinite increase in soil N. A model such as ICBM will achieve steady state, where input equals output: this is theoretically more realistic and can be supported by empirical evidence (Johnston *et al.*, 2009).

Fjärdingslöv was similar to Ultuna, the inclusion of changes in soil N reduced the deficiency for low N fertilization and reduced the surplus in the rotation with high N fertilization. However, in a comparison of individual crops in a crop rotation, the balance can change greatly if mineralization from SOM and residues from preceding crop and N returned to soil in crop residues are considered. If only in-output balance is considered, barley appears the most N-efficient crop (proportion of N input recovered in harvested crop): 92% of N was recovered (Table 5). However, barley had low efficiency when N content in total crop (including aboveground residues and roots) was divided by available N from fertilization and mineralization of SOM and the large amount of residues from the preceding crop (sugar beet). In this instance, sugar beet was most efficient. When considering the risk of N losses from the different crops, in-output balances, mineralized N and N remaining in crop residues, need to be included.

Table 5. *N balances for crops in a soil fertility experiment at Fjärdingslöv, mean for a 35-year period, kg N ha^{-1}*

	Crop			
	Winter wheat	Sugar beet	Spring barley	Spring oil seed
A. Fertilizer	100	140	60	100
B. Deposition	6	6	6	6
C. N removed in harvest	72	84	61	60
D. N balance (A+B-C)	34	62	5	46
E. Relative N uptake (C/(A+B)*100 (%)	68	58	92	57
F. Simulated net mineralisation from SON and previous crop residues	76	55	102	89
G. Total crop N uptake	132	198	109	123
H. N balance (A+B+F-G)	50	3	59	72
I. Relative N uptake (G/(A+B+F)*100 (%)	73	99	65	63

Two sets of sub-samples randomly taken from the same homogenized soil sample from the Ultuna long-term experiment carefully analyzed with two methods produced different results (Table 7 in Paper III). The overall means for C concentration for each set were more similar than individual measurements from each sample, this indicated a random factor was involved, such as differences due to subsample preparation (Kätterer *et al.*, 2011). When the values for C concentrations are obtained, they have to be converted to mass, and this requires additional knowledge about the bulk density of the soil and cultivation depth (top soil depth): this information is often lacking, but the effects of these errors are sometimes clear. A comparison of the C amounts for 1974 and 1975 in the Ultuna experiment (Figure 1 in Paper III) revealed the C amounts for some treatments appeared to decrease drastically during one year. The treatment with green manure apparently lost 1.7 t C ha^{-1} over the year and the treatments with bare fallow and calcium nitrate lost more than 1 t C ha^{-1} over the year. As these values were more than a model would indicate, this highlighted the difficulty of simulating exact predictions for the amounts of C mineralized in a single year, even with a good model. However, an increase in C can never be larger than the input, and providing all inputs have been considered, there will always be some mineralization of existing SOM. Between 1987 and 1989, the C amount in the farmyard manure treatment appeared to increase by 5.9 t C ha^{-1}, whereas, the input was calculated to 5.6 t C ha^{-1} during the same period. Although estimations are always subject to uncertainty, measurements such as weighing the manure rate and measuring its water content can be precise in a well-managed field experiment. Even so, the mineralization has still not been accounted for and even carefully selected data can be wrong or at least inexact, and can be revealed through a model approach.

Although results from long-term experiments are necessary for developing soil C and N models, the precision of the data was insufficient for enabling model calibration or validation. This problem presents the greatest obstacle to developing better models and increasing the understanding of processes in the soil. Thus, soil C and N modeling requires more resources to be dedicated to high-quality long-term experiments (Andrén *et al.*, 2008).

With a model, N mineralization can be distributed over different years, and mean soil N changes do not need to be used for every year. In the model, inputs were changed every year according to crop type and yield, and although it would have been useful to include the effects of weather during a specific year, the average climate for each year was used to keep the model simple.

In conclusion, without considering changes in soil N, N balances are underestimated in treatments with organic amendments and N surpluses are overestimated in treatments without organic amendments. The calculated surplus for different crops in a rotation can also change significantly.

5.3 Site-specific Annual N Mineralization (Paper IV)

ICBM/N was applied to plots in a single field and with daily time-steps (Paper IV). The optimized value for γ was 0.5, which was the lower boundary set in the optimization procedure, and corresponded to θ values between 0.24 and 0.28 m^3 m^{-3} in the plots. The estimated value for k_r (10.5) implied the annual r_e was 1.72 for 1999 and 1.73 for 2000. The optimized value for e_y was 0.21. Both a relative high r_e and a low e_y drove the simulation to high heterotrophic respiration; consequently, less C was transferred and stored in the *O*-pool.

The optimized value for γ was low, but was within the range of values presented in other studies (De Neve & Hofman, 2002; Whalen *et al.*, 2009). This might be due to N losses at high water content, such as through denitrification and N leaching (not measured), as discussed by Delin and Berglund (2005), as both seasons were wet, with parts of the field periodically waterlogged.

The yearly mean of estimated N mineralization (*Nm_sim*) values matched the measured mean *Nm* values exactly: 44 kg N ha^{-1} during the growing season of 1999 and 71 kg N ha^{-1} during the growing season of 2000. The observed *Nm* values during 1999 were similar to previous measurements in this area, whereas, those for 2000 were generally higher (Lindén *et al.*, 1992). The model underestimated the measured variation of *Nm* in the field, although this is a common feature in model simulations (Kersebaum *et al.*, 2005; Pringle *et al.*, 2008), and may be due to some important field level processes, such as leaching or denitrification, not being included in the model. For 1999, the standard deviation of the estimated mean values was 7.1 and 15 kg N ha^{-1} for the measurements. In 2000, the standard deviation of the estimated mean values was 5.4 and 16 kg N ha^{-1} for the measurements. For both years together, the model accounted for 56% of the total variation (Figure 5 in Paper IV).

Soil water content θ was not measured, but was estimated from a pedotransfer function and a soil water model, and measurements of N leaching and denitrification were not included in this on-farm experiment. Hydrological models can estimate N losses through leaching and denitrification, but need careful site-specific calibrations to be useful, even so, the results from complex hydrologic models are sometimes ambiguous (Schmidt & Persson, 2003).

In addition to soil water content θ, several soil properties were estimated by pedotransfer functions, which considered soil texture and C concentration. The values for θ_{fc} and θ_{wp} were critical for the model's performance. Although the overall performance of the pedotransfer functions used to estimate these parameters is sufficiently good, the accuracy for the prediction of individual values is low (Kätterer *et al.*, 2006).

In the regression including data from both years simultaneously, the estimated climate factor r_e accounted for both the mean differences in Nm between the two growing seasons and for 36% of the variation. Thereafter, only the regression between Nm and total soil N at the beginning of experiment (N_0) was significant. For single growing seasons, N_0 was the most significant variable. In 1999, N_0 accounted for 14% of the variation and *silt* for another 8%. In 2000, N_0 accounted for 34% of the variation and r_e for 8%.

Although the ICBM simulation explained much of the difference between the years, it did not fully explain the interaction between year and location within the field. The possible explanations for this were crucial processes, such as leaching and denitrification, were not included in the model or there was low precision and bias in the measurements.

5.4 Variability, Uncertainty and Bias

A model requires reliable input data to provide accurate output and to be verifiable. The natural variation in all soil variables and the problems in measuring these variables affect the prospect of accurately modeling soil processes. Therefore, assessment of the impact of variation and uncertainty on the model are essential.

There is spatial variation at all scales for all soil properties, for example, a field can have a CV of 35% or more for C concentrations (Goidts *et al.*, 2009).

For most soil properties, there is temporal variation and long-term dynamics (Schrumpf *et al.*, 2011), therefore, sampling must have a proper design with a sufficient number of samples to achieve acceptable accuracy, and that ensure the intended segments, both horizontally and vertically, are sampled (Western & Blöschl, 1999). In the subsequent laboratory analyses, additional errors and uncertainties can be introduced (Goidts *et al.*, 2009). As specific processes are dominant at different scales, accurate information about the governing processes for a particular scale is important, and during modeling, these critical processes must be included in the model to produce reliable results (Manzoni & Porporato, 2009). In the various applications presented here, different versions of ICBM were used, thus, ICBM has proven to be a model that can be adapted for use at different scales.

5.4.1 Variation in Soils

SOC and Mineral N

Although relatively small changes in the amount of SOM under certain conditions can be detected, such as, with repeated sampling and several replications under homogeneous conditions (Brock *et al.*, 2011), major changes in the amount of SOM or extensive sampling operations are required to detect the occurrence of a significant change (Post *et al.*, 2001; Smith, 2004; VandenBygaart & Angers, 2006). There were no large changes in soil C in mineral soils between 1990 and 2004 (Paper II), and these findings were in accordance with a recent soil survey (Eriksson *et al.*, 2010).

Mineral N concentrations often have high variation, and a high proportion of small-scale variation. Giebel *et al.* (2006) and Baxter *et al.* (2003) found spatial correlation limits between 40 and 90 m, whereas, other studies found correlations over much shorter distances (Bogaert *et al.*, 2000) or no spatial pattern (Ilsemann *et al.*, 2001; Haberle *et al.*, 2004). The CV for mineral N concentration in the studied field was not large, 12 – 37% (Paper IV). The plots were sampled in early spring and at harvest, and the measured change in soil mineral N during the growing season was small, generally less than 1 kg ha^{-1}, thus N mineral N measurements did not indicate large variation in N mineralization.

Bulk Density

The spatial variability of dry bulk density is typically less than for SOC and SON concentrations, but can still be sufficiently large to conceal the effects of experimental treatments (Lee *et al.*, 2009). A CV of 1-9% is reported for bulk density, with lower variation across scales than for SOC concentration (Don *et* *al.*, 2007; Goidts *et al.*, 2009). SOC concentration and bulk density are often negatively correlated, i.e., a higher C concentration typically entails lower density; consequently, C content and bulk density partially cancel each other out, even though bulk density has a large effect on the calculations of the amount of carbon in soil.

As no density measurements were available, they were estimated from pedotransfer functions (Papers I, II and IV). Pedotransfer functions render good estimates and should provide reliable values for regional and national estimates. For individual samples, precision is lower, depending on soil tillage (De Vos *et al.*, 2005; Kätterer *et al.*, 2006; Suuster *et al.*, 2011), thus, locally calibrated pedotransfer functions have better performance (De Vos *et al.*, 2005; Pringle *et al.*, 2007).

Bulk density is one of the most important soil factors affecting soil model precision (Post *et al.* (2008). This rendered the situation more problematic in the study for Paper IV, as there were only estimates for 34 locations in the field, and if some of these were not correctly estimated, the simulation results would be affected.

5.4.2 Sampling in the Field

In addition to the natural variation in C concentrations, other factors, such as sampling depth and dry bulk density measurements, contribute to the uncertainty in the estimation of SOM stocks. In the monitoring of SOM stock changes over time, the distance between the sampling location and re-sampling are other sources of uncertainty to be considered (Kulmatiski & Beard, 2004; Goidts *et al.*, 2009), although this is seldom investigated. As SOM concentration is usually higher in the upper soil layers, there is always a risk of contamination of samples from deeper soil layers with lower SOM concentrations. Therefore, the depth of the soil layer investigated needs to be measured precisely. The variation in sampling depth is usually about 0.01 m, but the variation can be higher when different landscape elements are sampled and on re-sampling, (Goidts et al., 2009).

Dry bulk density measurements require care for avoiding compaction of the samples, as the difference between measurements among different sampling people can be up to 8.2% (Kulmatiski & Beard, 2004), which can mask any treatment differences or lead to misinterpretation of the actual dynamics. During the monitoring of changes in C storage over time, it is important to return to the same plot and as close as possible to previous sampling points because of the spatial variation in C concentration.

During experiments, several different measurements are of interest and these measurements can be excluding, if one or several measurements require destructive sampling, if it is impossible to measure all variables from the same sample or if the same analyses need to be repeated at different times. In these cases, it is common practice to use abutting samples, assuming close proximity means the soil characteristics and processes are or are almost the same. However, the mean differences between abutting samples can be up to 12% of the mean value for SOM concentration (Amador *et al.* (2000).

The scale at which data are collected is often different from the scale at which the predictions are needed. If the proportion sampled is large compared with the process scale, most variability is smoothed out and the apparent variance will be smaller than the true variance (Western & Blöschl, 1999). In this thesis, sampling was properly conducted according to standard procedures, but improvements can always be made and sampling variance can be reduced through careful consideration of sampling design and implementation (Raczkowski *et al.* (2012).

5.4.3 Subsampling and Laboratory Analysis

By sending the same sample twice to the same laboratory, Goidts *et al.* (2009) determined a CV of 6.8% for the analysis of SOC. If SOM concentrations are estimated from loss on ignition, it is necessary to convert SOM concentrations to SOC. Conventionally, it is assumed SOM contains 58% C, which gives a conversion factor of 1.724 (Van Bemmelen, 1890). This “van Bemmelen factor” was proposed in unpublished data (Schulze, 1849), and is still proposed in modern textbooks. However, theoretical considerations and empirical observations indicate a conversion factor of 2 (50% C) is more relevant (Pribyl, 2010). There is a wide range in observed values due to organic material consisting of mixtures of materials with varying degrees of decomposition.

Two sets of analyzes from the same soil sample is uncommon, but in the Ultuna long-term soil fertility experiment (Paper III), soil samples were analyzed twice. However, individual analytical values can vary, probably due to variation in the selection of the subsamples. In a comparison of different batches of analyses, Kätterer *et al.* (2011) did not find any consistent bias, although individual analyses were different, i.e., 2.38 or 3.15% C.

5.4.4 From Yield Estimates to C and N in Crop

The parameter values used to calculate C input from reported yield (Table 2) probably differ among crop species and varieties, climate, and fertilizer dose, and will change over time with the introduction of new varieties with different harvest indices. The C input from roots and extra-root is especially difficult to estimate (Andrén *et al.*, 1990; Campbell & de Jong, 2001; Kätterer *et al.*, 2011).

The amount of crop residues for each crop category (Papers I-II) consisted of inputs from many different crops and varieties grown under a variety of conditions, so the estimates are probably the best available if actual measurements are not made.

Precision in the estimates of N taken up into the crop and in crop residues is crucial when estimating mineralization by crop uptake (Equation 6). Only the amounts of N in stubble and roots were estimated with allometric functions (Paper III), since N in harvested products and straw was measured. It is possible that during particular years, growth conditions affected the normal proportion of roots, although over a longer period, the estimates should be reasonable.

In the experiment described in Paper IV, the quantity and concentration of N in crop residues was measured and it was possible to calculate crop uptake of N. As the mean of change in mineral N in soil during the growing season was close to zero, the amount of N found in crop residues was important.

5.4.5 Precision and Uncertainties in Models

Uncertainty in the model results arise from uncertainties in model structure and input parameters. Model functions should describe the most important processes for the scale of interest and have an appropriate level of simplification of reality (Manzoni & Porporato, 2009). There could be errors in the measurements of parameter values, uncertainty in scaling up from point values to model scale, and in the estimation of parameters and initial conditions via indirect measurements or from values that cannot be directly measured (Post *et al.*, 2008).

Model Structure and Spatial Scales

Models are commonly best suited to specific scales (Pringle *et al.*, 2008), and C and N dynamics at larger spatial and temporal scales can be described by relatively few variables (Manzoni and Porporato (2009) Franko *et al.* (2011). As complexity increases when processes need to be described at a smaller scale, the model needs appropriate complexity for the scale it is intended to describe or should be sufficiently flexible to allow the addition or removal of modules as required (Manzoni & Porporato, 2009).

ICBM is a flexible model where different functions can be added as modules, and the model was adapted to the situations in different applications. At the regional scale with changes over several years (Papers I - II), the basic version of the model was appropriate, but in order to study N mineralization over longer periods and with the addition of organic materials of different qualities, ICBM/2N was more appropriate (Paper III). To follow the N mineralization during the growing season (Paper IV), ICBM/N was used.

Estimation of Critical Parameters

In the mineralization dynamics of SOM, carbon use efficiency (e_y) and parameters regulating the influence of temperature are among the most crucial model parameters (Post *et al.* (2008). Other crucial factors are initial SOC content and bulk density, which affect the estimates of many soil properties, and input of C from crop residues.

In Papers I-III, the e_y-value from the original ICBM/N calibration was used as it is well adapted to average arable conditions (Kätterer & Andrén, 2001). In Paper IV, the optimization of e_y rendered a value of 0.21, which was considerable less than the default value (0.4).

The same temperature response functions were used in Papers I,II and IV, with reasonable outputs: in Paper III, an average r_e was used for all years.

In all experiments, the soil carbon content was measured as precisely as possible; however, for the regional estimation (Papers I-II), point estimates had to be scaled to a regional scale. The bulk density was estimated with pedotransfer functions, which added uncertainty to the model outputs.

Inputs of organic matter have different resistance to decomposition, for example, sewage sludge and manure, which already are partially decomposed in earlier processes, decompose slower than green manure from clover. Roots *in situ* decompose 2.3-2.4 times slower than above-ground crop residues (Rasse *et al.*, 2005; Kätterer *et al.*, 2011), possibly due to chemical recalcitrance, physico-chemical protection, and physical protection (Rasse *et al.* (2005). Based on these findings, a higher *h* for roots should not affect the results from Papers III and IV, but might have an impact on regional C balance calculations (Papers I-II). The distribution of different crops varies within the regions and the proportion of C allocated to roots is specific for each crop: this warrants further investigation.

Among the parameters and initial conditions, the estimation of dry bulk soil density and input of C from crop residues are areas with the greatest uncertainty, and should receive more attention in the future.

Soil Hydrology

Modeling soil hydrology is complex. Topography is considered the dominant influencing factor on small scale (<100 m) variation in soil water dynamics. However, attempts to create topographic wetness indices to predict soil water content have not been successful (Schmidt & Persson, 2003). Preferred flow pathways can create small-scale variation (<10 m) and it is difficult to predict characteristics for a given site without detailed studies (Western *et al.*, 2004; McMillan *et al.*, 2011). Reliable methods for estimating and explaining the mechanisms behind soil water dynamics over larger areas would provide useful information (Herbst *et al.*, 2010): the development of different field-based sensors for proximal soil sensing has provided alternative methods for measuring soil moisture, such as γ-ray spectometers, near infrared reflectance spectroscopy (NIR) and time domain reflectometry (TDR) (Viscarra Rossel *et al.*, 2011).

Soil Type

The water balance model used for calculating the daily soil water balances was crude, but perhaps sufficient. However, the only effect of soil type on soil C balances, included in ICBM so far, is that different soil types have different wilting points and field capacities, and the difference between these factors determines the water storage capacity. This capacity defines how long a saturated soil can retain sufficient soil water under a drought period to maintain decomposer activity, this differs by a factor of three between the lowest (sand) to the highest (silt loam). However, under normal Swedish weather conditions, usually wet conditions during the growing season, the difference in mean annual activity between soils due to differences in water storage capacity were small. The influence of soil type on soil organic matter stability, e.g., clay ‘stabilization’ should possibly also be considered.

6 Conclusions

6.1 Summarizing Conclusions

ICBM proved to be useful for modeling SOM turnover at different scales. The structure of ICBM is flexible and it can be adapted for requirements at different scales, and add insight into control factors and relationships. Crop yields and climate affect the total SOM content in soils in different regions of Sweden (Papers I – II). The necessity of including changes in SON for nitrogen budgets was demonstrated (Paper III) and the weather impact on nitrogen mineralization under different growing seasons was modeled (Paper IV).

With a model, various what-if scenarios can be tested. For example, at the regional scale, how much higher temperatures increase mineralization and the yield increases needed for counteracting the mineralisation can be studied. At the small scale, the influence of harvest residues on SOM can be followed.

When there are discrepancies between modeled results and measurements, new insights can be gained. Reanalysis of samples indicate that major variation is due to the selection of subsamples for analysis and / or in the chemical analysis itself. In additon, the estimates of the theoretically possible changes in amount of SOM indicate some measured values are unrealistic (Paper III). However, differences between modeled results and measured data are difficult to explain with certainty (Paper IV). There is uncertainty in the measurements and there is spatial variation, and there are limitations in the model for simulating an actual situation, especially in the simulation of water balances. Certain modules, such as pedotransfer functions, could have been better calibrated to the current situation.

For an appropriate test of how well the model can simulate SOM mineralization at field level, field experiments with more extensive measurements than were available are required (Paper IV). Alternatively, an experiment within a controlled environment, such as a lysimeter experiment could be performed.

The simulation of mineralization over short periods on a small spatial scale needs to include relevant processes, and hydrological processes have a key role in agricultural fields. Water and transportation of substances affect the rate of turnover of SOM, and to be able to relate the simulated mineralization to measurements, the model has to simulate both the environment for mineralization and for transportation and losses. These processes can be measured, but it is a resource intensive task.

From a decision support perspective, commonly available field data are usually sufficient for models such as ICBM/N for predicting the long-term effects of agricultural management on C and N stocks at field or regional scale. However, more detailed information and probably more complex models are needed for short-term applications at small spatial scales, for example, for decision support in a precision farming context.

6.2 Lessons Learnt and Future Research

ICBM is a flexible model that can be adapted with several modules for use at different scales. However, it is necessary to be aware of the uncertainties and errors involved, and some measure of uncertainty should be included. The inclusion of replications in all steps in the data collection would enable the calculation of a measure of the variation. These error and uncertainty estimates can be compiled to a total variance and uncertainty of the projections.

As water content is crucial for the prediction of SOM mineralization and possible N losses, reliable water balance models are needed at plot scale. Other improvements would be a cheap and reliable direct measurement of water content and a refinement of the estimation of C and N input from crop residues.

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