Sink or source?

Uncertainties in large-scale model predictions of forest soil organic carbon dynamics

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Cover: Swedish coniferous forest from a soil perspective (photo: Carina Ortiz)

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Abstract

Soil organic carbon (SOC) is the largest terrestrial carbon pool and small changes in this pool may affect the global carbon balance, especially atmospheric concentration of CO2. Within the context of climate policy, the quantification of these changes is important, as pool changes may affect a country's national greenhouse gas budget.

The aim of this thesis was to assess and analyze uncertainty related to the up-scaling of modelled SOC stocks and change estimates to regional or national scale. Two process-based models Q and Yasso07, were used to estimate SOC stocks and changes at different regional scales in Swedish coniferous forests. The parameter uncertainty of the Q model was assessed and established with the Generalized Likelihood Uncertainty Estimation (GLUE) method through the Swedish Forest Soil Inventory (SFSI) data at county scale. The calibration resulted in a set of parameters that were used for further modeling at regional scale. The Q and Yasso07 models were used to assess the impact of different uncertainties in the SOC stocks and changes. The most important uncertainty source in the model estimates was litter production. Increased harvest residue extraction was analyzed with the Q model to study the effects on SOC accumulation. SOC accumulation decreased with increased harvest residue extraction, although there was temporal and geographical variation. However, increased emissions from changes in the SOC pool resulted in a net decrease in $CO₂$ emissions due to the substitution of coal combustion with biofuels.

The coherence of scales between large-scale inventory data and process-based simulation models was explored. Inventory data became more uncertain when going from national to regional scale, due to the smaller sample, whereas, model estimates became more uncertain when applied to larger areas, due to increased uncertainty in parameter determination at larger scales resulting from varying conditions. The magnitudes of the uncertainties for model and inventory estimates of SOC were comparable, but the origins of uncertainties differed and could not be compared. Both models and inventories can be used to estimate the carbon sink of Swedish forest soils at national level, but if the changes are small, a few $\%$ yr⁻¹ in the SOC pool, the uncertainty may prevent a definite answer, if there is a change in the SOC pool.

Keywords: SOC, GLUE, Swedish Forest Soil Inventory, models, uncertainty, GHG reporting, sensitivity analysis, coniferous forests

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Contents

List of Publications

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

- I Ortiz, C.A., Karltun, E., Stendahl, J., Gärdenäs, A.I., Ågren, G.I. (2011). Modelling soil carbon development in Swedish coniferous forest soils –An uncertainty analysis of parameters and model estimates using the GLUE method. *Ecological Modelling* 222 (2011), 3020-3032.
- II Ortiz, C.A., Liski, J., Gärdenäs, A.I., Lehtonen, A., Lundblad, M., Stendahl, J., Karltun, E. Soil organic carbon stock changes in Swedish forest soils – a comparison of uncertainties and their sources through a national inventory and two simulation models. (manuscript).
- III Ortiz, C-.A., Gärdenäs, A.I., Karltun, E., Ågren, G.I. Model predictions of soil carbon development over a stand age: What is most important sensitivity to climate or model parameter uncertainty? (manuscript).
- IV Ortiz, C.A., Lundblad, M., Lundström, A., Stendahl, J. The effect on soil organic carbon accumulation of increased extraction of forest harvest residuals for bioenergy use in Sweden. (manuscript).

7

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The contribution of Carina Ortiz to the papers included in this thesis was as follows:

- I Planned the modelling set-up together with the co-authors. Preformed the modelling work and the model result analyses. Preformed writing with the assistance from the co-authors.
- II Planned the modelling set-up together with the co-authors. Preformed the modelling work, the model result analyses and writing with the assistance from the co-authors.
- III Planned the modelling set-up together with the co-authors. Preformed the modelling work and the model result analyses, and the writing with the assistance from the co-authors.
- IV Planned the modelling set-up together with the co-authors. Preformed the modelling work, the model result analyses and writing with the assistance from the co-authors.

Abbreviations

1 Introduction

World soils contain a large quantity of soil organic matter (SOC) and forests are important carbon (C) sinks in the global C balance (Goodale *et al.*, 2002; Raich & Schlesinger, 1992). In the global carbon cycle, the soil C pool is both larger than the atmospheric (twice as large) and the terrestrial pools (2 to 3 times larger). Boreal forest soils (to 1 m depth) are estimated to contain 383±30 Pg C (Pan *et al.*, 2011), which is around half of global soil C (Lal, 2005). The main reason for this large soil carbon stock is a combination of relatively fast litter production and slow decomposition due to climatic conditions (Raich & Schlesinger, 1992). The SOC stock in Swedish forest soils is estimated at around 80 ton C ha⁻¹ (SLU, 2012b; Stendahl et al., 2010; Olsson *et al.*, 2009; Ågren *et al.*, 2007), which is equivalent to around 1600 Tg C, if the area of forests with a production capacity of $> 1m³$ per year is considered. The soil carbon pool in Swedish forests is 100 times larger than annual reported emissions in the national greenhouse inventory. Hence, the yearly SOC changes need to be monitored, as even a small change in this large pool will affect the national greenhouse balance. To be able to mitigate $CO₂$ emissions from land-use activities, the different pools within the carbon cycle and how these pools respond to management and climatic change needs to be understood.

There is considerable societal interest in the estimation of SOC stock changes at both regional and national level. The main driver for this interest is the need to develop climate change policies and to ensure Sweden will be able to report greenhouse gas (GHG) emissions to the United Nations Framework Convention on Climate Change (UNFCCC) and fulfill its commitment to The Kyoto Protocol. According to the Kyoto protocol, Annex I countries are obliged to report changes in forest SOC pools, unless they can prove the soils are not a source of $CO₂$ to the atmosphere (UNFCCC, 2006).

There are many ways of assessing SOC change (Smith, 2004; IPCC, 2003), including repeated measurements in soil inventories (Bellamy *et al.*, 2005),

CO2 flux measurements (Baldocchi *et al.*, 2001), empirical/statistical models (Martin *et al.*, 2011) with remote sensing, and process-based models (Liski *et al.*, 2006). According to the Intergovernmental Panel on Climate Change (IPCC) guidelines (IPCC, 2003), the most preferred methods for estimating SOC change (in Tier 3) are repeated measurements and process-based model estimates.

There is an increased interest in replacing fossil fuels with biofuels as a possible way of mitigating GHG emissions. The European Union (EU) has an emission target for reducing GHG emissions by 80-95%, compared to the values in 1990, excluding Land Use Change and Forestry (LULUCF) sector, by 2050 (European Council, 2009). Sweden is a country with large forested areas (around 23 Mha, according to the Swedish forest definition, which is based on the capacity of the forestland to produce). Currently, only 20% of all harvestable residues are used for bioenergy (Skogforsk, 2012; Swedish Energy Agency, 2012), thus, there is a large potential for increasing the extraction of harvest residues. However, intensive extraction of harvest residues means less litter input to the soil, which in turn has a negative impact on the carbon pools in forest soil (Repo *et al.*, 2011; Melillo *et al.*, 2009). This indirect effect of forest management needs to be considered when estimating the climate benefits of biofuels.

The measurement of soil carbon in forest soil inventories is normally associated with high cost and large spatial variability (Muukkonen *et al.*, 2009; Wilding *et al.*, 2001; Webster, 2000). Process-based models are subjected to uncertainties introduced through the model structure and in inputs or parameters (Verbeeck *et al.*, 2006; Walker *et al.*, 2003). The process-based models are developed and calibrated to describe a certain scale and the application of a model at larger scales introduces uncertainties in the estimates due to the processes described in the model not being adequate for a different scale (Heuvelink & Pebesma, 1999). Nevertheless, the models integrate the current knowledge on processes controlling decomposition of organic material, and as new data becomes available, these processes can be tested which improves the models and renders better estimations (Beven, 2010). However, there is a need for up-scaled estimates of SOC stock changes, and this raises the question whether process-based models can render accurate results at larger scales.

In this thesis I have analyzed and discussed uncertainties associated with the estimation of SOC stock changes through inventories and process-based models at both regional and national scale. The studies are based on processbased models applied at different scales and driven by input data from forest inventories: soil inventory data were used for calibration and evaluation.

¹²

2 Aim

The overall aim of this PhD project was to describe and quantify different sources of uncertainties affecting soil organic carbon change estimates in process-based models at regional and national scale.

The specific aims were to:

- \triangleright Calibrate the Q model and assess parameter uncertainties with soil inventory data at regional scale (Paper I).
- \triangleright Validate two different models (Q and Yasso07) with inventory data at regional scale and asses the uncertainty sources of estimates by sensitivity analysis (Paper II).
- \triangleright Investigate the comparability of model estimates (Q model) at plot level over stand age, including uncertainties from litter production due to site variability, with soil inventory data (Paper III)
- Estimate the long-term effects on national SOC accumulation for different levels of harvest residue extraction in a changed climate (scenario B2 from the IPCC), including parameter uncertainties (Paper IV).

3 Background

3.1 Swedish forest carbon pool

The primary source of Swedish forest soil C is vegetation that through photosynthesis fixes C from the atmosphere. During the growth of the trees, above and below ground litter is produced when needles, branches and fine roots die. At harvest, stumps and tops are added to litter production. The litter production varies in amount, quality and vertical distribution. Decomposers in the soil use the litter as a source of C and energy for growth. The decomposition process is complex and involves different organisms, such as fragmenting soil animals, fungi, microbes and bacteria, and is controlled by environmental factors, such as temperature, moisture and soil properties. Most fresh litter falling to the forest floor decomposes quickly and the carbon is respired to the atmosphere. The remainder of the dead organic material decomposes at a slower rate due to the low quality of the organic matter or adsorption to soil mineral particles (Hassink, 1992; Allison *et al.*, 1949). Some organic material, a recalcitrant part, which decomposes at very slow rates can remain in the soil for thousands of years (Kleber, 2010).

3.2 Estimating SOC stock and changes

The measurement of SOC stock and SOC change in the soil has to consider the large spatial variability in the quantity of SOC. Although repeated sampling is the best method for assessing SOC change, it is associated with difficulties due to the large spatial variability and the destructive nature of sampling. Samples cannot be taken from the same pit, which renders measurements costly and time consuming, especially for forest soils (Muukkonen *et al.*, 2009). Flux measurements are an alternative method for indirectly detecting changes in the soil pool. This method estimates the short-term total fluxes of the ecosystem and requires additional assumptions for separating the changes in the soil from

other processes. Thus, these estimates are intensive, costly and site specific, and are difficult to scale up to a regional estimate (Baldocchi *et al.*, 2001). Due to the difficulties of directly measuring SOC stocks and changes, and the lack of inventory data, model approaches are commonly used, especially empirical and statistical models with functions where more easily detected variables can be used as independent variables to estimate SOC stocks and changes. These types of models require vast amounts of data for calibration, but are also associated with uncertainty (Martin *et al.*, 2011). As a Tier 1 method, the IPCC guidelines (IPCC, 2003) proposes an empirical model where SOC changes are related to a certain land use or land use change that is associated with a certain stock value (Smith, 2004). The applicability of this empirical approach is scale specific in the sense that it is limited to a specific region and time, thus: where and when the original data were collected. An alternative to empirical models is process-based models that describe the processes of the system through equations that depict how drivers (input variables) affect the state of the system (Bouma *et al.*, 1998; Hoosbeek & Bryant, 1992). The properties and response of the system is determined through a set of parameters in the model equations. If it is assumed the processes are correctly understand, the models can be applied, in both time and space, outside the data range for which they were developed. A discussion on the differences between model types and scales is presented by Bouma et al. (1998) and Hoosbeek and Bryant (1992). Although there are numerous process-based models describing how organic matter decomposes in soils, the models operate at different scales, ranging from plot to regional scale, and require different types of input (Peltoniemi *et al.*, 2007) and some models are only suitable for application at the scale they were developed for (Manzoni & Porporato, 2009). SOC decomposition models can be divided into two types: compartment models or continuous quality models. Compartment models describe the decomposition in each pool through a specific decomposition rate related to the different qualities of the organic matter: examples of compartment models are RothC (Coleman & Jenkinson, 1996), COUPModel (Jansson & Karlberg, 2004), DNDC (Li, 2000), Century (Parton *et al.*, 1992; Parton *et al.*, 1987) and Yasso07 (Tuomi *et al.*, 2011a; Tuomi *et al.*, 2011b; Tuomi *et al.*, 2009). Continuous models include a decomposition description of the whole spectra of different qualities of the organic material: the best known continuous model is the Q model (Ågren *et al.*, 2007; Rolff & Ågren, 1999). The number of compartments varies among the models.

3.3 Measurement uncertainty

Uncertainties in measurement are divided in random uncertainties, spatial variability and systematic errors. Random errors are not possible to reduce. The systematic errors are possible to reduce when the measurement technique is improved. Systematic errors in SOC measurement are either measurement errors or due to spatial variability. Measurement errors can arise during several stages in the measurement procedure. During fieldwork, errors can occur due to inconsistent identification of different soil horizons or inter-annual changes in sampling due to differences in weather. In the sample preparation step, errors can occur when preparation routines change and errors in the chemical analyzes occur when methodology and equipment change. During data handling, digitalization of handwritten raw data, decimal reduction on programming can introduce errors into the estimates. A change in staff introduces errors that affect the entire measurement process. Uncertainty due to spatial variability often involves small-scale variability, that is, over distances smaller than the shortest sampling interval, and depends on the size of the area investigated. Spatial variability in soil measurements normally becomes larger as the scale increases (Wilding *et al.*, 2001) and the uncertainty can be reduced through increasing the number of samples (Muukkonen *et al.*, 2009; Wilding *et al.*, 2001). In traditional (design based) statistics, the spatial variation in SOC measurements is treated as random because the sampling is *randomly* distributed. The uncertainty in a randomly distributed sampling includes random uncertainties, systematic errors and spatial variability. In geostatistics (model based statistics) the spatial variability is modelled separately and therefore it is possible to treat the spatial variability (and random uncertainty) separately from the systematic errors.

Many uncertainties in SOC stocks and changes are due to spatial variability and the increased costs associated with the larger sample size needed to decrease the uncertainty; although reported SOC stocks include measurement and random errors, they are difficult to separate from errors introduced due to spatial variability. Uncertainty estimates of small SOC stocks changes are subject to large uncertainties, which creates the ambiguity of non-significant sinks of C to the atmosphere (Ogle *et al.*, 2010; SEPA, 2009; Monni *et al.*, 2007). Sweden has large, managed forest areas with long rotation periods and the average SOC pool changes are expected to be small $(< 0.5\% \text{ yr}^{-1})$, thus, the estimates of SOC change require large sample sizes to determine statistical significant changes (SEPA, 2009; Peltoniemi *et al.*, 2004). To be able to detect any changes, there is a need to understand and reduce the uncertainties related to the SOC estimates. However, decreasing the uncertainties due to spatial variability will increase the uncertainties due to measurement errors, resulting

in higher precision (smaller uncertainty ranges) but lower accuracy (measuring the true value). Both low accuracy and low precision can affect the conclusions, especially when estimating small SOC changes, because low accuracy causes a bias in values whereas low precision leads to large uncertainties leading to non-significant estimates of sources or sinks.

3.4 Model estimate uncertainty

Model uncertainty of SOC stock changes has only recently been reported (Juston *et al.*, 2010; van Oijen *et al.*, 2005), and has three causes: location, level, and nature (Walker *et al.*, 2003). The *location* of the uncertainty describes where in the model the uncertainty is found, such as in the context (the boundaries of the model), the model itself (conceptually and computationally), the inputs, and the parameters (Verbeeck *et al.*, 2006; Walker *et al.*, 2003; Zak *et al.*, 1997). Often, the uncertainty in C pool model estimates is related to inputs and parameter uncertainties (Tuomi *et al.*, 2011a; Tuomi *et al.*, 2011b; Juston *et al.*, 2010; Mitchell *et al.*, 2009; Tuomi *et al.*, 2009; van Oijen *et al.*, 2005).

The *level* of uncertainty describes whether the uncertainty is due to deterministic knowledge or total ignorance. Deterministic knowledge means the uncertainty can be estimated statistically, as there are large amounts of supporting data and total ignorance means the uncertainty cannot be estimated, as there is little supporting data to base the estimation on. Scenario uncertainties are a *level* of uncertainty somewhere between deterministic knowledge and total ignorance, and scenario results are usually described with the range in a non-statistical way. Scenario uncertainties describe plausible descriptions of how a system might react when variables in the system are changed, such as in the IPCC scenarios of climate change.

The *nature* of uncertainty is due to imperfections of knowledge or to inherent variability (randomness). In the nature of uncertainty, epistemic uncertainty (random uncertainty) needs to be separated from the total contribution of uncertainties so the over-all uncertainties in the estimates can be reduced. The separation focuses on the factors that contribute the most uncertainty, and can be reduced through further empirical research.

There are two types of methods used for calibrating a model, which stem from two different ways of perceiving process-based models and represent different modelling philosophies. The models are either a true representation of the real world or not and this leads to different ways of treating the model residuals when calibrating the model. The calibration is either based on a formal or informal likelihood measure for estimating the fit of a model. A formal likelihood measure is based on the same type of likelihood measures used in formal statistics (minimizing model errors etc.). There are many informal likelihood functions, some of which are presented in Smith et al. (2008). In practice, both methods focus on determining the most likely parameterizations in the whole parameter space, and the parameter probability distribution functions (PDFs) are assessed through the calibration of the models. The two principal methods are the Bayesian calibration (including Markov Chain Monte Carlo (MCMC) and the Generalized Likelihood Uncertainty Estimation (GLUE) (GLUE: (Beven, 2009; Smith *et al.*, 2008). The application of Bayesian methods on process-based models has been criticized, because the true confidence limits cannot be estimated, as the residuals are often non-random. Thus, calibrating process based-models with a Bayesian method may be invalid, as model residuals are caused by errors that are not randomly distributed (Beven *et al.*, 2008; Beven *et al.*, 2007; Mantovan *et al.*, 2007; Mantovan & Todini, 2006) and leads to incorrect confidence limits, if the residuals are not transformed, as in Renard et al. (2010). Furthermore, the method might compensate values for correlated parameters that interact with each other and cause an incorrect distribution of parameters, as in Svensson et al. (2008a), where the calibrated values of some parameters in the CoupModel were correlated and compensated as the model fitted the data. This resulted in compensated parameter distributions rather than an estimation of the right distribution of those parameters. Although the model resulted in good simulations, with small residuals, it was for wrong reasons, as the new calibrated parameterization became a compensation to fit the data. The Bayesian method can be problematic if the calibration uses data of variable quality and quantity (daily: 1 data point, or monthly: 12 data points): the method favors quantity of data as the calibration method sums all residuals in the likelihood function and finds parameterizations according to this sum. If a model is calibrated against two variables, one with a small data set and the other with a large data set, the one with the large data set will have a larger impact on the likelihood because of more errors being summed. This results in a calibration that tunes the model against a certain data set and generates incorrect estimates of variables with small amount of data. The GLUE procedure has also been criticized, especially, by Bayesians (Mantovan *et al.*, 2007; Mantovan & Todini, 2006), because of the use of informal likelihood measure, which results in an objective sample of the models' parameters that perform well. The GLUE method uses informal likelihood measures for estimating the "goodness of fit" of a process model because the models are non-linear and can result in non-random residuals. Despite the non-random residuals of calibrated process-based models, the models might be useful for

quantifying and for improving knowledge of the processes. The GLUE methodology suits process-based models and the calibration procedure becomes straightforward and transparent.

The GLUE method takes the *equifinality* problem into consideration, which means different parameter sets within a model structure might predict equally well (Beven, 2009). GLUE is based on a large number of Monte Carlo simulations, each with randomly generated parameter set-ups sampled from prior parameter distributions. The results of each simulation are compared with available observed data. A quantitative measure of performance ("likelihood") is needed to assess the acceptability of the model parameterization based on the model residuals. This quantitative measure of performance increases monotonically with increasing goodness-of-fit; thus, each simulation or model can be evaluated and scored to form a distribution of acceptable simulations. Unacceptable simulations should have a likelihood of zero, meaning these simulations will not form part of the total simulation distribution. For predictions, all the simulations with a likelihood measure greater than zero contribute to the distribution of the predictions (Beven, 1992). Model uncertainty analysis in process-based model applications is implemented mainly through calibration and sensitivity analysis, however, there is potential for model uncertainties to be used in hypothesis testing and to develop models that perform better (Beven, 2010). During calibration, the models might be rejected or accepted for the wrong reasons: a poor model can be accepted or a good model can be rejected, when it should have been accepted. Wrongly accepted or rejected model estimates occur when the uncertainty in input data and observations is so large that the performance of the model only results in vague indicators of good or poor estimates. To avoid wrong conclusions on calibration and evaluation of process-based models, a limits-of-acceptability approach is used in the evaluation of the model's performance (Beven, 2006), this includes the different type of errors in input data and observations that might affect the evaluation of model estimates.

A sensitivity analysis is a suitable way of testing how a model reacts to different changes in input or parameters. A sensitivity analysis examines which parameters contribute most and least to the model output, whether parameters interact, and determines the initial parameter intervals for use in calibration (Janssen and Heuberger 1995): this is also valid for driving variables. Sensitivity refers to how much a quantity within the system will change due to changes in another quantity or due to external consequences. The sensitivity methods are normally estimated locally or globally (Ratto *et al.*, 2001; Saltelli *et al.*, 2000; Saltelli *et al.*, 1999). Local sensitivity mainly examines sensitivity through changing one parameter or variable at a time, and is a popular

application in process-based models. As process-based models include many parameters that might interact, the sensitivity of a certain parameter needs to be assessed for all possible values of a parameter. Global sensitivity takes into account the various combinations of parameterizations, and calculates the contribution of each parameter or input factor of interest. Monte Carlo-based methods are increasingly used to assess the uncertainty of environmental models, and soil and forest models that have been analyzed by these methods include ICBM (Juston *et al.*, 2010) and Century (Ogle *et al.*, 2010) for agricultural SOC changes and BASFOR for forest carbon balances (van Oijen *et al.*, 2005). Simulations are run with a randomly selected set of parameters or input values that result in the estimation of distribution functions and the variance for the output variables (Saltelli et al. 2000). Scenario uncertainties are normally described non-statistically through a range of different scenarios and present possible descriptions of how a system might react when variables change within the system. Uncertainty in scenario analyses are represented by a range in the output due to different underlying assumptions, uncertainty about which changes and developments are relevant for the output (e.g. sensitivity analysis of certain parameters), or as uncertainty about the levels of the relevant changes (Walker *et al.*, 2003).

3.5 Process-based models and scaling issues

There are three reasons why process-based models are scale specific. First, the dominant process differs between scales, secondly, the availability of data might differ between scales and thirdly, the scale of the variables used in the model (the specific scale of the model: Heuvelink and Pebesma (1999). There is an increasing knowledge gap between model scales, with a general increase in scale, the knowledge gap regarding C and nitrogen (N) interactions increases (Gärdenäs *et al.*, 2011). The most familiar scale is the ecosystem scale, which highlights the necessity of further regional studies, and up-scaling processbased models results in averaged model inputs and outputs. SOC stocks and change estimates can be up-scaled through aggregating or averaging observation data from a smaller scale (S1) to a larger scale (S2), averaging model inputs to a model rendering average outputs at the larger scale (S2), and by summing the results of model estimates at a smaller scale (S1) to a larger scale (S2) (Figure 1). Another way is through up-scaling the process-based model itself by developing lumped and averaged models, i.e. meta-modelling (Bierkens *et al.*, 2000). The results from the second and the third method should render the same results, unless the model is non-linear in its variables and parameters, even so, non-linearity is normal within environmental models.

However, the questions of whether some process-based SOC models might be used to estimate SOC stocks and changes at larger scales and what the uncertainties related to these estimates are still remain.

Figure 1. A schematic illustration of the different steps in the procedure of up-scaling measurements and model estimates from the scale S1 to S2. In a) up-scaling by averaging the observations, b) up-scaling model input variables or parameters, and c) up-scaling model output variables (modified from Bierkens et al. (2000).

4 Materials and Methods

4.1 The Swedish Forests

More than half of the land area of Sweden is covered with forest, most of which is located in the northern parts, with agricultural land being predominant in the south. The total land area of Sweden is 41 Mha of which 22.5 Mha is productive forestland with a production capacity of $> 1 \text{m}^3$ wood yr⁻¹, with a further 4.2 Mha being protected areas within national parks or nature reserves. The standing volume is 3 billion $m³$, mostly consisting of coniferous species, i.e. 42% Norway spruce (*Picea abies Karst*) and 39% Scots pine (*Pinus sylvestris L.*), and 12% birch (*Betula pubescens L.* and *Betula pendula R.*) (Swedish Forest Agency 2011): the average annual productivity of these forests is $111 \text{ m}^{-3} \text{ yr}^{-1}$. The total standing volume of Swedish forests has increased by over 80% since the 1920s, although the areal extent of forested land has remained about the same at national level (Swedish Forest Agency, 2011).

The most common forest soils in Sweden are Podzols (45% land cover), Arenosols (20%), Leptosols (11%), Cambisols (10%), Histosols (8%) and Regosols (6%). Podzols are mostly located in the northern parts of the country, Arenosols are evenly distributed over the country, and Leptosols, Cambisols, Histosols and Regosols are more frequent in the south of Sweden (SLU, 2012a).

4.2 Study area

Sweden was divided regionally into governmental administrative counties (Paper I) and climatic regions (Papers II, III and IV: Figure 2). The reason for division into county level was that long term litter input production data, estimated from 1926 to 2000 and originating from the Swedish National Forest Inventory (SNFI), could only be calculated at the county level. The climatic regions were defined by both temperature and precipitation (SMHI, 2002; Raab & Vedin, 1995) and were considered as representative units for describing the climatic gradient in Sweden.

Figure 2. Division of Sweden into county and climatic regions. In (a), the counties are divided into two groups for calibration (hatched) and validation (uniform). The division of the climatic regions in (b) is represented by the different shades.

4.3 SOC measurements and the Swedish forest soil inventory

The Swedish Forest Soil Inventory (SFSI) is a long-term national inventory that is integrated with the Swedish National Forest Inventory's (SNFI) permanent plots (SLU, 2012a). Clusters of eight plots (four plots in the

southwest) are distributed systematically and objectively over the country. The inventory is continuous with 1/10 of the plots being sampled each year, with the complete country as the sample frame: a complete inventory takes 10 years. Thus, each year's data can be considered an unbiased sample of Swedish forestland (Figure 3). The inventory includes site descriptions of the plot and landscape properties, basic soil properties, soil type classification, and chemical properties of both organic and mineral soil horizons for a subset of plots. The first inventory was carried out during 1983-1987, the second inventory was carried out during 1993-2002, and the third inventory is ongoing and ends in 2012. Due to changes in sampling design and sampling methods, it is difficult to compare the first and the second inventories, which is the reason why data from the first inventory was not used in these studies.

Figure 3. A schematic figure of the Swedish Forest soil Inventory (SFSI) at different scales. The complete 10-year inventory period covers around 11 000 sampling plots on forestland or grassland. Out of these, samples of mineral soil are collected from 4500 plots. Each dot in (a) and (b) represents a cluster (c) comprising 8 samples points. The yearly sampling is objective and systematic according to the scheme in (b). The years with open circles in (b) are not included in the SOC estimates of Paper II.

Soil samples for soil organic carbon (SOC) estimates were taken from the O horizon, B horizon, B/C horizon (45 cm below the surface) and C horizon (55-65 cm from the top of the mineral soil surface) (Figure 4). The soil samples were analyzed for carbon (C) by dry combustion. For the O horizon, C stocks were calculated from the determinations of the total amount of soil material in the organic layer (O horizon), <2 mm per sampled area, and the C concentration of the sample. The amount of C in the mineral soil for each horizon was calculated with the C concentration, thickness of the sampled

26

horizon, and empirical relationships for bulk density and stoniness with Equations 1 and 2 (SEPA, 2009).

$$
SOC_i = [C]_i \times W_{fei} \qquad \qquad \text{Eq. 1}
$$

where: *SOC_i* is the soil organic carbon in a certain layer in Mg ha⁻¹. *[C]_i* is the concentration of carbon in the fine earth (2 mm) in %. *W_{fei}* is the amount of fine earth in soil layer i in Mg ha⁻¹, and depends on the bulk density (BD) and the stoniness. The bulk density is estimated with a pedotransfer function based on empirical relationships and with Equation 2 (Gundersen *et al.*, 2006).

 $BD = 1.5463 \times e^{-0.3130 \times \sqrt{[C]} \mathbf{i}} + 0.00207 \times AD$ Eq. 2

where: AD is the average depth of the soil layer (cm). The stoniness is calculated with the stoniness correction coefficients estimated for different parent material classes, as presented in Stendahl et al. (2009).

Total mineral soil C, down to 50 cm depth, was calculated by the measured concentrations of carbon in the sampled horizons and linear interpolation, and in a few cases, linear extrapolation for the part of the profile where no samples were taken.

Figure 4. The soil organic carbon estimation method down to 50 cm depth for the sample plots (Photo: Åke Nilsson).

The method for estimating the amount of soil carbon is identical to the Swedish method for calculating the amounts of soil carbon reported to the UNFCCC (SEPA, 2009). The SOC stocks were estimated on two restricted subsets of data. The first dataset contained data from 2064 plots sampled between 1994 and 2000 (Paper II) and 2002 (Paper I), the second dataset was 371 plots sampled between 1993 and 2002 (Paper III). The reason for restricting the data sets was to meet the input data requirements for the models. Sample plots selection criterion was that at least 70% of the basal area of a plot was either Norway spruce or Scots pine on mineral soil. The inventory started in 1993, but due to temporary changes in the sampling, only the southern part of the country was inventoried, and in 1994, only the northern part of the country was measured; therefore, both of these years are reported as 1994. The annual SOC changes were estimated as the difference between the estimates for one year and the subsequent year. The SOC change was estimated with 748 plots from plots re-measured between 2003 and 2007. The change was calculated as the stock change between inventories divided by the time between the inventories.

4.4 Process-based models

The process-based models used were the Q model (Rolff & Ågren, 1999) and the Yasso07 (Tuomi *et al.*, 2011a; Tuomi *et al.*, 2011b; Tuomi *et al.*, 2009). The Yasso07 is a typical multi-pool model and the Q model describes decomposition continuously and follows each fraction of a certain quality in time. Both Q and Yasso07 require annual input of litter production and annual climate data.

4.4.1 The Q model

The theory behind the Q model is based on the assumption that microorganisms are carbon limited and their growth rate is dependent on available carbon sources. The carbon used by the microorganisms originates from litter that varies in initial quality. With a higher quality of the litter, the more rapidly microbes can grow on this particular litter. A convenient way of describing the different qualities of litter is through a continuous variable (*q*), which allows the whole distribution of litter quality to be included in the total amount of carbon from each litter component. Thus, a component of litter with a certain quality will be followed in time, as the quality of litter will change: this is described by the x-axis in Figure 5. The quality of litter declines as the material decomposes, which is described by the y-axis in Figure 5. The decomposition is described by the production-to-assimilation efficiency, the rate of the decomposer biomass growth per unit of carbon used, and the

dispersion of carbon after the assimilation by the decomposers. The production-to-assimilation efficiency determines the fraction of carbon going into new decomposer biomass per unit of carbon used. The rate of the decomposer growth per unit of carbon is dependent on the carbon quality that is used. The transformation of the quality of the litter after the decomposers have assimilated the carbon they need has a large range, but on average, the quality decreases. The mass of organic material remaining after assimilation in a fraction (needles, fine roots, understorey vegetation, branches, stumps, coarse roots and stem) and the depletion in the quality of the fraction as the microbes assimilate the carbon are described by the curves in Figure 5. The decomposition of the woody fractions is initially delayed due to the time decomposers need to invade the organic material totally: this is seen in the lag phase of the functions in Figure 5, and is longer for stump, coarse roots and stems than for branches. The decomposition function for needle litter and fine roots, *g*(t), is given by Equation 3, as an example of how the parameters appear in the model.

$$
g(t) = (1 + f_c \beta \eta_{11} u_0 q_0^{\beta} t)^{-(\frac{1 - e_0}{\beta \eta_{11} e_0})}
$$
 Eq. 3

where: f_C is the carbon concentration in decomposer biomass, q_0 is either the initial litter quality in needles (q_{0n}) or the initial litter quality in woody components(q_{0w}). The parameter e_0 is microbial decomposer growth efficiency and describes the fraction of carbon incorporated into new decomposer biomass per unit of used carbon. The rate of decrease in quality is described by η_{11} , and β is the shape of decomposer quality response and describes how fast the decomposition rate changes with quality. The decomposer growth rate $(u_0 = u_{00} + u_{01} * T)$ is related to the average air temperature (*T*) at the site. For woody litter, Equation 2 has to be modified to include the parameters *maxb* (yr) and *maxs* (yr) to describe the time required for microorganisms to invade branches and stems completely. The model parameters can be combined into three lumped parameters: z , α_n (needles and other finer material) and α_w (woody material) (Eq. 2), which are combinations of the decomposer and substrate parameters f_c , q_{0n} , q_{0w} , e_0 , η_{11} , β , and u_0 . The lumped parameters simplify the decomposition function to Equation 4.

$$
g(t) = (1 - \alpha_n t)^{-z} \qquad \text{Eq. 4}
$$

where: *n* in α_n represents the decomposition of needle litter. For the lumped parameters, *z* is related to the shape of the decomposition curves in Figure 2, and α_n (needle litter decomposition) and α_w (woody litter decomposition) are more strongly related to the rate of movement along the curves.

The mathematical description of the model and applications is explained in several publications (Ågren *et al.*, 2007; Ågren & Hyvönen, 2003; Hyvönen & Ågren, 2001; Hyvönen *et al.*, 1998).

Figure 5. A schematic illustration of the Q model. The curves describe the mass of different litter fractions remaining as a function of time (from Paper I).

4.4.2 Yasso07

The Yasso07 model is a development of the old Yasso model (Liski *et al.*, 2005) which was based on five assumptions about decomposition of organic material. These assumptions are

1. Litter and soil organic matter consist of different chemically defined fractions, which decompose at their own typical rates regardless of their origin (foliage, fine roots, branches, coarse roots, stems and stumps in Figure 6)

- 2. Decomposition of woody litter is delayed as not all woody litter is immediately exposed to microbial decomposition.
- 3. Decomposition fractions lose a certain proportion of their mass per unit of time (fluxes of carbon, arrows in Figure 6)
- 4. A part of the decomposed mass is lost from the soil as heterotrophic respiration or leaching, and the remainder is transformed to more recalcitrant compounds (arrows, carbon fluxes out of the box in Figure 6)
- 5. Microbial activity, and thus decomposition rates, and exposure rate of decomposition depend on temperature and moisture conditions.

Figure 6. Flow chart of Yasso07. The boxes represent different soil organic carbon compartments and the arrows carbon fluxes between the compartments (Sol. refers to soluble).

A more detailed mathematical description of the Yasso model is presented by Liski et al. (2005) and of the Yasso07 model by Tuomi et al. (2011a; 2011b; 2009). The Yasso model has been improved to include more measurement data for calibration and more advanced mathematical algorithms. Yasso07 has been calibrated to a global dataset with the Markov Chain Monte Carlo (MCMC) method, which presents possibilities for the user to extract uncertainty bounds for the model results. The most important applications of the Yasso and Yasso07 models for this thesis are outlined in Liski et al. (2006), Monni et al. (2007) and Peltoniemi et al. (2006).

4.5 Calibration (Paper I)

The GLUE "Limits of Acceptability" approach, described in (Beven, 2006) (Paper I), was chosen as the calibration method due to the non-linearity of the Q model (Wetterstedt & Ågren, 2011) and the availability of uncertainty estimates of the data. Twelve counties were used in the calibration (shaded areas in Figure 1) and the remaining eleven counties (colored areas in Figure 1) were used in the validation of the model. The calibration and validation counties were selected so each climatic region was represented in both the calibration and validation datasets. Both the calibration and validation was done for the same period that SFSI data were available (1994-2002). The total number of sampling plots per county varied between 2 and 85 for individual years: the lowest number of sampling was found in counties 10 and 12.

The 95% confidence intervals of the measured soil carbon data for each individual year were used as "limits of acceptability" in each county. The modelled SOC output for Norway spruce and Scots pine/Lodgepole pine were pooled to be comparable with the soil inventory data. The simulation results lying within these limits were considered acceptable simulations. For the detailed methodology on the specific GLUE procedure, see Paper I.

The Q model was run with the long-term estimated county-based litter input from Swedish forest statistics on standing volume that was contained in the Swedish National Forest Inventory from 1926 to 2002. The model was initialized with a steady state assumption, which implied annual litter production was in steady state with decomposition. This assumption was made to reach the values of soil carbon in 1926. The years between 1926 and 1994 (when the comparison with data started) were considered as a spin-up period to reduce instability of the initialization of the model estimates at the beginning of the simulation.

4.6 Uncertainty Sources (Sensitivity Analysis) (Paper II)

The sensitivity analysis on the uncertainty sources (Paper II) was run with the same set of parameterizations in the already calibrated models Q and Yasso07. Thus, the possibility that parameter interactions would affect the sensitivity of the model was discarded.

To assess which of the uncertainty sources had the greatest effect on the model estimates, a sensitivity analysis that introduced additional uncertainty into the different input variables of the models was run (Paper II). In the Yasso07 model simulations, the uncertainty of chemical composition was included through a deviation between measurements and average values of coefficients of variation (CV) calculated from a plant specific-dataset (Liski et al. 2006). In both the Q and Yasso07 simulations, the error in the quantity of litter input was accounted for by coefficients of variation calculated from a national study in Finland (Peltoniemi et al. 2006). The climate uncertainty was represented by annual climate variability, with data from Swedish Meteorological Hydrological Institute (SMHI) (Johansson 2000; Johansson and Chen 2003). This procedure assumed the uncertainty sources from quality and quantity of litter, and climate variability and parameter uncertainty could be added, as there was no interaction between these uncertainties. In each climatic region, one hundred (n=100) Monte Carlo (MC) simulations were made with the Yasso07 model, and between 92 and 326 MC simulations (all accepted parameterizations from the calibration) were made with the Q model. The uncertainty results are presented as the 95% confidence limits (CL) for the Yasso07 estimates and $95th$ and $5th$ percentiles for the O model estimates.

4.7 Up-scaling process-based models and uncertainty (Paper III)

The study on the comparability of model estimated SOC stocks with inventory data over stand age was done by simulating the Q model at site level in region 3 (Figure 2).

The litter input to the Q model was estimated with the biomass growth functions based on the number of trees, basal areas and height development of Pine and Spruce, as described in Ågren and Hyvönen (2003). The annual biomass for each tree fraction was estimated with the biomass functions for pine and spruce trees developed by Marklund (1988; 1987). The understorey biomass was estimated with the biomass functions from Muukkonen and Mäkipää (2006). The annual litter production was then estimated with turnover rates for the specific fractions of the biomass needles, fine roots, braches and

the understorey. A normal forest management strategy for the site productivity indices in the region was applied.

The annual litter input was estimated for each plot with information on site productivity index, latitude and longitude obtained from the SFSI. The temperature was taken from a weather station in the centre of the region (Malmslätt; Lat 58.4N, Long 15.5E).

In the site level simulations, the model was run with the most likely parameterization of that region, which was assessed in the study in Paper I. Thus, the model uncertainty reflected the variability of litter input due to different productivity levels at the different sites. The Q model was initialized with the steady state assumption that litter input was in steady state with the decomposition of organic material in the soil.

4.8 Scenario Analysis (Paper IV)

The effects of different forest residue extraction procedures on SOC accumulation was assessed by scenario analysis and the results are presented as a range in the output. The calibrated Q model from Paper 1 was used to include the interaction between parameters and their uncertainty. The sensitivity analysis assessed how the SOC accumulation in the Swedish forest soils was affected by management procedures. The scenarios that deviated from a base scenario were simulated with the model. Three scenarios were for increasing levels of residue extraction and one scenario was for increased forest harvest intensity, a production scenario (Figure 7).

Figure 7. Schematic illustration of the scenarios, illustrated as energy production in TWh for all Sweden.

The base scenario was based on current forest management strategies and environmental policies decided to 2010 (Swedish Forest Agency, 2008). The magnitude of harvest residue extraction in this scenario was around 8 TWh yr ¹. The production scenario was based on the assumption of different silvicultural actions, such as improvements in management strategies and new measures such as improved rejuvenation methods, increased conventional fertilization of clear-cut areas, optimized fertilization, and afforestation on former agricultural land, which increased forest production.

Litter input for modelling the scenario analysis was estimated with the HUGIN system, which simulates regional forest development (Lundström & Söderberg, 1996) at county level for the years 2010 to 2110. The counties were aggregated to the same climatic regions as in Paper II (Figure 2). The HUGIN system has been applied in the latest national forest impact analysis (Swedish Forest Agency, 2008) and uses current data on standing tree level from the SNFI to predict long-term regional forest harvest levels. All scenarios were run with the climate change scenario B2 (IPCC, 2000).

The harvest level for the extraction scenarios was assumed the same as in the reference scenario. Thus, the extraction scenarios were based on the same simulations as the reference scenario. The increased extraction of harvest residues and stump was based on the assumption forest fuel utilization will increase to meet the demand for bioenergy to replace fossil fuel energy. This demand is estimated to increase the use of bioenergy from the current level of 8 TWh to 15 TWh, 25 TWh and 25 TWh + stump extraction (Swedish Forest Agency, 2008). The 25 TWh scenarios were further estimated as the largest potential increase in harvest residue extraction. Residue extraction was assumed to increase during the first 20 years and then remain constant. The extraction potential varied regionally in the country because current harvest residue extraction is greater in the south than in the north, which means there is lower potential in the south and larger potential in the northern parts of the country. The amounts of harvest residue extraction were calculated as the amount of branches and tops corresponding to an energy amount of 15 and 25 TWh. The stump extraction scenario was calculated as a gradual increase in stump harvesting to a gradual increase in stump harvesting up to 30% stump removal a year (or 50% of the stumps from clear-cut areas) by 2030, after which harvesting continued at the same level.

5 Results and Discussion

5.1 Calibration of the Q model for regional SOC stocks and changes

The parameters of the Q model were calibrated with data from the SFSI for obtaining parameters at county level for large scale conditions. The GLUE calibration resulted in county specific parameter distributions. While the original distributions of each parameter were uniform, the posterior countyspecific distributions were triangular for some of the parameters of the model ($q\theta_{\rm n}$, $q\theta_{\rm w}$, β , $t_{\rm max}$, *z* and $\alpha_{\rm n}$) (Figure 8). Before the calibration, the parameters were assigned uniform distributions with all values within a range being given the same probability because of a lack of knowledge. Thus, the uncertainty bounds of simulations before the calibration reflected large uncertainty bounds due to limited knowledge about the probability of the values of the parameters. After the calibration, new probable values for each parameter were determined for Swedish county-level conditions. The new parameter distributions reduced the parameterizations that did not describe the decomposition of organic material at the county scale. Thus, after the calibration, the parameterizations kept were those best describing the decomposition; therefore, parameter uncertainty was reduced after the GLUE calibration. The up-dated parameter distributions represented an improvement in the model estimates of SOC stocks and changes because the parameter uncertainty due to incorrect parameterization was reduced when going from a uniform distribution to a triangular (Figure 8 and Table 1 in Paper I). The distributions with the most variations were in southern counties 19 and 23 (Figure 8) for the parameters *q*0n, *q*0w, *β*, *tmaxs,* and *z*: detailed values of the parameters and the distributions are presented in Paper I. The variation in parameters, especially for β in these counties, was due to variation in calcium carbonate $(CaCO₃)$ or clay content (SLU, 2012a). An increase in liming increases the SOC stock (Ågren &

Bosatta, 1996; Persson *et al.*, 1990) and the presence of $CaCO₃$ has a preserving effect on SOC (Duchaufour, 1982). Increased clay content also increases SOC stocks through binding organic material to clay mineral surfaces (Hassink, 1992; Allison *et al.*, 1949). The distribution of the lumped parameter *z* narrowed due to the calibration, thus, at the county level, SOC stocks could only be described with a more limited combination of that parameter (for parameter value ranges see Paper I). The two optima for the lumped *z* parameter reflected two types of ecosystems: *z*>1 steady state was possible and *z*<1 steady state was not possible. The system describing a steady state needed decomposers that were sufficiently effective in decomposing the organic material. In the model, this was described by three parameters: carbon efficiency use (e_0) , the rate conversion to low quality carbon (η_{II}) , and the sensitivity of carbon use to the quality (β) . With efficient decomposers (high e_0), less carbon is lost and the accumulation of SOC increases. If there is a high rate of conversion to low quality of carbon (e_0) , the SOC rapidly becomes less accessible to the decomposers and SOC accumulates faster. If the sensitivity of carbon use is high (*β*), the quality of carbon and the access of quality of the decomposers decreases, which results in an increase of SOC. The parameter densities from the calibration could be used for estimating uncertainty bounds (percentiles) of future large-scale simulations with the Q model.

Figure 8. The posterior probability density functions of some parameters in the Q model after the GLUE calibration. The values of the different parameters are presented on the x-axis and the distribution is presented on the y-axis. Each density in each figure describes the density function of the parameter in each county (colored lines in each figure).

5.2 Evaluation of model estimates

5.2.1 SOC Stocks

The calibrated Q model (Paper I) and the Yasso07 model were evaluated with independent observations from the SFSI to ensure the models parameterizations were applicable at regional scale under Swedish conditions. The agreement between the modeled and the observed SOC stocks at county scale in 2002 is illustrated in Figure 9 for both the calibration and the validation simulations (Paper I). In most cases, the agreement of the validation simulations was comparable to the agreement of the calibration simulations, except for counties 11 and 13 where SOC estimates deviated considerably from the observations. Both the range of the validation simulations and the confidence intervals of the observations crossed the 1:1 line for six of 10 validation counties. The over-estimated SOC stocks were mostly for small counties with few observations points, indicating data uncertainty. There was a high correlation $(r=0.82)$ between the observed and calibrated values but a lack of correlation between the observations and the validated values (r=0.03) due to a few deviating counties that reduced the correlation. One reason for the lack of correlation in the validation simulations was the adjustments of the administrative borders since 1923; this affected stock estimates because the area used in each county remained constant. At national scale, this assumption was valid because the total area had not changed during the 75 years, but the county scale areas had changed considerably. For example, in county 11 where the SOC stock was overestimated by 50%, the area had decreased by 35% between 1951 and 2000 (Swedish Forest Agency, 2011; Eriksson & Janz, 1975). The removal of these outliers rendered a correlation of $r=0.53$. Thus, area changes could be corrected through implying functions of area development for each county.

Figure 9. The SOC stocks in t ha⁻¹ estimated by the Q model (y-axis) and the Swedish Forest Soil Inventory (x-axis). The calibrated counties are represented by the dots and the validation counties by triangles. The inset figure is the same figure without the error bars.

The agreements between the SOC stocks simulated with both the Yasso07 and the Q models for 2000 and the observations from the Swedish Forest Soil Inventory at regional scale are presented in Figure 10. The precision of both models varied among the regions, with the largest errors being in regions 1 and 2 (southwest Sweden) in both models. The Q model estimates deviated from observations in region 6 (northeast Sweden). The under-estimated results for southern Sweden (regions 1 and 2) were possibly due to the N deposition effects on decomposition not being included in the models. The effects of increased N deposition on SOC decomposition are unclear, but there is indication excess N hampers decomposition, resulting in increased SOC accumulation (Knorr *et al.*, 2008; Arnebrant *et al.*, 1996; Nohrstedt *et al.*,

1989). In the observations, the SOC stocks in southern Sweden increased and the most probable explanation is increased N deposition in these areas (Olsson *et al.*, 2009; Kleja *et al.*, 2008; Svensson *et al.*, 2008b). In region 6, the Q model over-estimated the SOC stock by 80%, which was explained by the parameterization used from the calibration. The calibration of the model was at county scale and used half of both regions 6 and 7 (Figure 2). These two regions differed in annual litter production and precipitation and illustrated the implications of applying a calibrated model from one region to another region (Manzoni & Porporato, 2009; Rykiel, 1996; Oreskes *et al.*, 1994). There are two possible ways of improving the simulated estimates: first, through calibrating at the same scale at which the simulations will be run and second, by including the processes that affects the increase in SOC accumulation.

Figure 10. Simulated SOC stocks in t C ha⁻¹ for Yasso07 (left) and Q (right) (on y-axis) and the observed values from the Swedish Forest Soil Inventory (SFSI) (on x-axis). The different points represent the stock values from the different climatic regions (R1-R7) in Sweden.

The inventory-based SOC stocks (Paper I) were lower in the north (low county numbers), 60 t C ha⁻¹ for the most northern county, than in the south (high county numbers), 140 t C ha^{-1} in the most southern county (Figure 11). Likewise, the range in confidence limits varied between the counties: county 12 had a range of 100 t C ha⁻¹ and county 1 had a range of 20 t C ha⁻¹. The number of samples for the calibration also varied between the countries, with inter-annual variations within some counties and more samples per county in the north than in the south. The SOC stocks of the calibrated model simulated (solid lines) within the confidence intervals of the inventory data (dashed lines)

Figure 11. The calibrated, modeled, and measured SOC stocks in t ha⁻¹ (y-axis) during the whole calibration period 1994 to 2002. The simulations with the Q model are mean values with the $5th$ and 95th percentiles (lines) and the observations are presented as dashed lines. The bars represent the number of samples from the Swedish Forest Soil Inventory (SFSI) in each county (1-23) per year, and the numbers represent the identity of the county.

in all counties and all years, except for county 16, where the observation were extremely low in year 1994, are presented in Figure 11. The large inter-annual variability in the observations of small counties (e.g. county 16) revealed the

importance of scale difference between the inventory and the model. Simulated estimates do not vary between years as much as observations do, and can therefore supplement data at county scale when needed. As the SFSI was designed for national estimates, downscaling of the inventory data to county scale rendered greater uncertainty in the observations.

The SOC stocks in the south east of Sweden (estimated in Paper III) were compared to observed SOC stocks at stand level. The SOC stocks were comparable in magnitude at regional level simulations and inventory data resulted in approximately 75 t C ha⁻¹ (Figure 12). The simulations had larger variability over stand age than the inventory data. In the simulations, SOC accumulation declined at the beginning of stand development, then, stabilized over time, with some peaks due to thinning, and finally, increased due to final felling. One reason the model simulations varied in stand age more than the observations was that the SOC in the simulations included organic carbon originating from woody litter, such as coarse roots, branches, tops and stumps. When the woody fractions are produced as litter, they enter the SOC pool in the model. In the inventory, these woody fractions are not measured as SOC. This is illustrated in in a separate simulation with the Q model without the woody litter in Paper III. The inventory data represents the mean and 95% confidence limits of between 113 and 43 samples (depending on age class), with age classes of 10 years. Variability in thinning, harvesting and site productivity index could have mitigated some of the variability in SOC development over stand age. A decline in SOC stocks after harvest is found in the O horizon (Georgiadis, 2011; Johnson & Curtis, 2001; Olsson *et al.*, 1996; Covington, 1981), and in south-eastern Sweden, the site productivity index increases with stand age at the beginning of the stand development, implying increased SOC stocks (Ågren & Hyvönen, 2003). Any further division into site productivity classes was difficult due to the small sample size. The uncertainty bounds of the simulated regional estimates reflected inter-annual variability in litter production, as the uncertainty bounds increase when the harvest regimes start. The discrepancies in the comparison of the regional simulations with regional inventory data were associated with the different operating scales of the methods. An improved comparison could be made by assessing the SOC stocks with the model at plot level and starting simulation at the current age of the stand. This approach requires information on the age of the trees at each site and would result in constant regional stocks over time, similar to the stocks estimated in Papers I, II and IV.

SOC Stocks

Figure 12. Mean (dark line) and 95th and 5th percentiles (dashed lines) plot level simulations, with the Q model, at stand level with the present climate and data from the Swedish forest Soil Inventory for southeast Sweden. The uncertainties in the simulations are due to litter production variation in each plot and are presented as $5th$ and $95th$ percentiles: the uncertainty bars for the data are the 95% confidence limits.

5.2.2 SOC Changes

The SOC changes at regional scale during the period of 1994 to 2000 varied between the three methods (Paper II), but were within the same magnitude (Figure 13). The mean values for the SOC changes during the seven-year period were 1.7 (\pm 8.8) T g C yr⁻¹ for Yasso07, -3.2 ($+10$;-17) T g C yr⁻¹ for Q and 6.6 (\pm 7) T g C yr⁻¹ for observations from the SFSI. None of the methods resulted in a significant change in C stock, except for the Yasso07 model during 1996. The differences in the simulated uncertainty of the models are partly dependent on the calibration data used and the calibration technique. The Q model was calibrated at the county scale with uncertain data for some years

and counties. The Yasso07 model was calibrated to a large global data set (Tuomi *et al.*, 2009). A small data set increases the uncertainty bounds, as fewer simulations best fit the data. Fewer well-fitting simulations render less definable distributions of the models parameters and result in larger uncertainty bounds (see Figure 12, counties 1 and 3 versus 10). Thus, a large data set decreases the uncertainty bounds and renders a more robust model.

SOC Changes

Figure 13. SOC changes in T g C yr⁻¹. Average values for 1994 to 2000 together with the uncertainty bound for the modeled change (95% confidence limits for Yasso07 and $5th$ and $95th$ percentiles for Q) and the 95% confidence interval for the repeated measurements in a, and the annual change in SOC in T g C for 1994 to 2000 in b.

The calibrated Q model was used to assess the impact of forest management on SOC accumulation in a scenario application (Paper IV). The yearly litter production and the SOC stock development for the different management scenarios compared with the reference scenario under present forest conditions and management are presented in Figure 14 (Paper IV). The stump extraction scenario had the lowest litter production. The production scenario (reflecting an increase in harvest intensity of 10%) resulted in slightly higher litter production than the reference scenario. In all scenarios, SOC stock accumulation was lower than the reference scenario, except for the production scenario (10% increase of harvest intensity).

The difference in SOC accumulation varied among the scenarios: SOC accumulation decreased in the stump extraction scenario with a rate of change of -0.088 t C ha⁻¹ yr⁻¹, and in the 15 TWh energy production scenario with a rate of change of -0.037 t C ha⁻¹ yr⁻¹, compared to the reference. The effect on SOC accumulation varied between the different scenarios, and between regions and the time perspective considered (Figure 15). All scenarios decreased SOC accumulation both short-term (20 years) and long-term (100 years), except for the production scenario (equivalent to 10% increase in harvest intensity). At national scale, the short-term (20 year) decrease in SOC change, relative to the reference, was 26% (15 TWh), 39% (25 TWh), 48% (Stump) and 0% (Production) (Figure 16). The long-term (100 years) effects on SOC changes were smaller than the short-term effects because the changes were spread over a longer period.

Short-term SOC accumulation was faster in the northern regions than in the southern regions, but long-term SOC accumulation was slower in the north than in the south. The regional differences in SOC change between the scenarios were mainly due to climatic differences and that the potential for increasing harvest residue extraction is higher in the northern than in the southern regions. Another explanation for the larger accumulation in the southern regions is the parameterization used in these regions (taken from the calibrated Q model from Paper I.). The parameters for southern Sweden reflect increasing SOC accumulation, based on the SFSI data (Paper I). The most likely reason for SOC accumulation in the southern regions of Sweden is the increase in N deposition: the increase in SOC accumulation is a combination of an increased litter production and an increased decomposition. Recent global climate models indicate global warming will affect the carbon cycle through both increased biomass and increased decomposition (de Vries, 2009; Jansson *et al.*, 2008; Kellomaki & Vaisanen, 1997). However, how this increase in temperature will affect decomposition over longer periods is an on-going debate (Karhu *et al.*, 2010; Wetterstedt *et al.*, 2010; Ågren, 2010; Vanhala *et*

al., 2008; Liski *et al.*, 1999). The reason for the larger, long- term effects on SOC accumulation in the northern regions was a due to a combination of increased litter input production resulting from an increase in temperatures, increased fertilization, and conversion from pine to lodgepole pine (Swedish Forest Agency, 2008).

Yearly Litter Production

time

Figure 14. The yearly litter production and the SOC stock development (in t C ha⁻¹ yr⁻¹) in the different harvest-residue extraction scenarios, relative to the reference. The scenarios are equivalent to an energy production of 15 or 25 TWh and a production scenario if harvest intensity increases 10%. The solid line represents 15 TWh, long dashes represent 25 TWh, small dashes represent 25 TWh and stump extractions, and the dashed-dot line is the production scenario.

None of the scenarios resulted in completely positive uncertainty bounds. As the uncertainties only included parameter uncertainties, the uncertainty bounds were under-estimated: the reason for not including input uncertainty was to facilitate the comparison between the scenarios. As the simulations presented were not predictions, but scenarios, this meant the results illustrated the potential impact forest management has on SOC accumulation, therefore, the values should be interpreted with caution.

The SOC changes estimated for the 15 TWh scenario were 0.014 t C ha⁻¹ (20 years) and 0.34 t C ha⁻¹ (100 years). These results were comparable to the studies of Palosuo et al. (2008), who estimated SOC changes of 0.05-0.23 t C ha⁻¹ yr⁻¹ over a rotation period with the two models Yasso and ROMUL. Eriksson et al. (2007) estimate a decrease in SOC of 0.05 t C ha⁻¹ yr⁻¹ and Peckham and Gower (2011) estimate a decrease by 0.012 t C ha⁻¹ yr⁻¹ in the annual rate of change over a 500-year period (after extracting more harvest residues for bioenergy use). The results in this thesis include additional uncertainties associated with the processes of carbon accumulation of disturbed forests. Although little is known about how stump extraction affects SOC accumulation in forest soils, an increase in harvest residues and stump extraction can change nutrient and water availability (Egnell, 2011; Akselsson *et al.*, 2007; Vanhook *et al.*, 1982) and understorey cover, and cause soil disturbance (Strömgren *et al.*, 2011; Walmsley & Godbold, 2010; Vanhook *et al.*, 1982): these affect SOC accumulation. However, the type of sensitivity analysis, as presented in this thesis, is useful for both policy development and for identifying aspects of the system that require further study (Oreskes *et al.*, 1994).

Figure 15. The national SOC changes in $t C$ ha⁻¹ yr⁻¹ estimated in different harvest-residue extraction scenarios. The changes are estimated as 20 and 100 year means with parameter uncertainties for the different harvest residue extraction scenarios (a and b) and for seven climatic regions in Sweden for the reference scenarios (c and d).

5.2.3 Input Uncertainty

Input to the model is crucial: if input is low in quality, the output will reflect the low quality and render uncertain simulations. As good quality data is not always available for running the models, uncertainty is introduced. The use of observations as input is associated with natural variation and this causes variability of the estimates and affects uncertainty bounds. For the simulation period 1926 to 2000, the effect of parameter uncertainty, climate variability and litter input uncertainty on the total uncertainty estimates in the modeled SOC stock changes is presented in Figure 16 a-d. Q simulations gave slightly wider uncertainty bounds than the Yasso07 model, but in general, the magnitude of the uncertainty was comparable (Figure 16). The parameters contributed least to the uncertainty levels of the models in terms of amount and inter-annual variability of SOC changes (Figure 16d), but the climate variability introduced inter-annual variability into the SOC stock changes (Figure 16c). Litter input was the largest uncertainty source in the SOC change estimates (Figure 16b). According to Peltoniemi et al. (2006) and Monni et al. (2007), fine root and understorey litter production are the litter fractions contributing the most to the uncertainty. The uncertainty in understorey litter was introduced into the models in different ways. First, the estimates were made with Finnish biomass functions (Muukkonen & Mäkipää, 2006) that have not tested in southern Sweden but which could be associated with larger uncertainties than the ones used in the study for Paper II. Second, as there was lack of long-term data, the understorey litter was assumed constant during the entire simulation period. This might have under-estimated the contribution of the understorey litter to SOC accumulation because the forest were less dense at the beginning of the simulation period (Swedish Forest Agency, 2011). Third, the understorey biomass varied in stand age.

Figure 16. The contribution of parameters uncertainties, climate variability and litter input uncertainties to the uncertainty in simulated SOC changes (in $t C$ ha⁻¹). a) displays all the uncertainties, b) the parameter and input uncertainties, c) the parameters and variable climate, and d) the parameter uncertainty. The 95% confidence limits for the mean Yasso07 simulations are presented as lines, and the $5th$ and $95th$ percentiles of the mean Q simulations as dashed lines.

The choice of model affected the SOC stock and change estimates and there were differences in SOC stock estimates between Q and (Papers II and III). The model comparisons reflected different views of the system, and these could reveal whether some processes need to be included or not in the description of the system (Paper III). The exclusion of processes generates model uncertainty (Walker *et al.*, 2003), which introduces systematic errors in simulations. Both Yasso07 and the Q model underestimated SOC stocks in southern regions (Paper II), probably due to the exclusion of increased N deposition. In turn, the choice of model was related to the research questions, data availability, and scale specificity. Small-scale models often require more information and represent more detailed process descriptions than simpler, larger scale models (Palosuo *et al.*, 2012; Peltoniemi *et al.*, 2007). One way of assessing systematic errors in models due to excluding processes is through the simultaneous comparison of several models, as in the IPCC climate change model scenarios (IPCC, 2007).

The quality and availability of the data are important for evaluating SOC estimates with process-based models and increased quantity and quality of data are needed for improving the calibration and evaluation of models. Observational data of high quantity and quality can be used to tune the model in accordance to the uncertainty of the observations (Beven, 2006), so that the model uncertainty will reflect observational uncertainty. A calibrated model with uncertainty bounds is useful for complementing observational data associated with large inter-annual variability. In the calibrated county 19 (Figure 11), the observations indicate large inter-annual variability, which leads to increasing SOC accumulation. However, the calibrated model simulated within these uncertainty ranges and rendered more stable simulations reflecting a slower trend. Process-based models simplify the real world, and several processes can be excluded intentionally, or unintentionally. This creates difficulties in the validation of a model, as in the strict sense the model verifies the truth (Oreskes *et al.*, 1994). In addition, there is always the possibility the model fits the data for the wrong reasons due to the simplification of the real world. Therefore, validation of a model should be a process that highlights how a model agrees with known facts at a given time (Rykiel, 1996), which in turn, can question a models' predictive value.

5.2.4 Comparability of simulated and observed uncertainties

The level of uncertainty associated with the SOC stock and change estimates and both models and observations were comparable in terms of magnitude (Papers I, II and III); however, the sources of the uncertainties differed. The uncertainty of the observations was caused by spatial variability and random

measurement errors. The uncertainty in the simulations was due to parameter uncertainty and uncertainty in input data and climate inter annual variation and model structure errors. Therefore, when studying the inter-annual variation of the SOC stock with the two approaches, the reason for the variation will differ and require different strategies for reducing the errors.

The observation data was associated with larger inter-annual variations (Paper I) that can be caused by sample variation and differences in sampling conditions (e.g. wet or dry years) or staff changes. The only way to decrease the spatial variability of the SOC change estimates is through increasing the size of the sample (Muukkonen *et al.*, 2009; Ellert *et al.*, 2001; Wilding *et al.*, 2001). The presence of systematic errors in combination with large sample size results in lower precision, but high accuracy. Low precision in combination with high accuracy can generate erroneous conclusions, which are problematic, especially when SOC changes are small.

Calibration and analysis of the uncertainty sources is crucial for reducing uncertainties in modeled SOC estimates. The comparison with observations also highlighted discrepancies between the observations and simulations and indicated the system described in the model was too simple or there were processes that needed to be included. When the model simulations were comparable with the observations of stocks and changes, the model was appropriate. One problem of quantifying SOC changes is associated with the determination of small changes in large pools, which creates non-significant changes, even with moderate uncertainty.

According to the Kyoto protocol, all Annex I countries, including Sweden, need to report changes in forest SOC pools, unless the country can prove evidence the soils are not a source of $CO₂$ (UNFCCC, 2006). In the reporting guidelines (IPCC, 2003), the inventory and model-based estimates are classified as the most sophisticated methods (Tier 3) for estimating SOC changes in forest soils. These changes should be reported along with uncertainty estimates, from either error propagation or Monte Carlo simulations. However, the sources of uncertainty, and the way it can be described and assessed, differ between methods. Thus, the choice of reporting method becomes important for reflecting uncertainties.

The ambition to decrease uncertainties in SOC change estimates of both simulations and observations goes beyond scientific interest and has implications on emission reporting and the fulfillment of international agreements. Therefore, continued critical discussion on the uncertainty in the different methods is pertinent.

6 Conclusions

I studied the description and quantification of different sources of uncertainties affecting soil organic carbon change estimates in process-based models at both regional and national scales. The main conclusions are:

- \triangleright The use of data from the Swedish Forest Soil Inventory in the calibration of the Q model improves SOC estimates at regional scale. As parameter uncertainty decreased, the uncertainties were found to be scale specific. This needs to be considered in future simulations at regional scale.
- Yasso07, Q model and the current GHG reporting method, based on inventory data, are comparable in estimating SOC stock levels, and the magnitude of uncertainties and inter-annual variability at the national level are similar. Given the expected rate of change, the large uncertainties render it difficult to draw definite and reliable conclusions on the rate and direction of short-term changes (<10-20 yrs).
- \triangleright The sources of uncertainty in model and inventory data differ. The uncertainties in model estimates are due to model input uncertainty and variability, whereas, the inventory data uncertainties are due to spatial variability and measurement error.
- \triangleright There is a balance between the minimum operating scale of inventory data and the maximum scale of the process-based models. The comparability of ecosystem models to national data sets is scientifically challenging, and a 'trade-off' between dataset quality and model input specificity needs to be identified. Aggregated county level, i.e at least 2 to 3 counties, is the minimum limit for down-scaling the Swedish Forest Soil Inventory data, and county-scale simulations are the limit for up-scaling process-based models.
- \triangleright Models are complementary methods for estimating SOC estimates, especially when observations have large spatial variability. Conversely, data for evaluation and model development are necessary: with new data,

the processes in the models and the model estimates can be tested and improved.

- \triangleright A comparison of the soil inventory with regional model simulations at stand level is difficult because of differences in the pool definitions. Woody material such as stumps, branches and tops have a large impact on the variation of SOC stocks over stand age.
- \triangleright Changes in forest management, such as harvest extraction, have little effect on SOC accumulation at national scale, but may vary regionally depending on climate and the intensity of the extraction.
- \triangleright Both models and inventories can be used to estimate SOC sing at national level, but if the changes are small, a few ‰ of the SOC pool, the uncertainties may prevent definitive answers of the question if there is a change in the SOC pool. Therefore, continued discussions on uncertainties in the methods used for reporting SOC changes to UNFCC and the Kyoto protocol is necessary for determine when definite conclusions on whether soils are sources or sinks of $CO₂$ to atmosphere can be drawn.

7 Future Perspectives

The focus of this thesis was on the decomposition of organic material of coniferous forest at larger scales. Even if broad leaved forests have a small contribution to the national biomass volume, the areas involved can be substantial in some regions. Thus, to be able to include these forested areas in a full cover national estimate, suitable functions for the decomposition and parameterization for broad-leaved organic matter need to developed.

As this thesis highlighted the SOC changes on forestland, future research should focus on the applicability of process-based models for estimating SOC changes due to change in land use, and for evaluating the impact these changes have on carbon sequestration. This is also important to improve the nation's SOC change estimates to the Kyoto protocol.

The inter-annual variability of models and observations were not comparable because they arise from different sources. To be able to compare the variability of model results with observations and to improve the models, further study on the inter-annual variability of SOC due to climate is needed. The full extent of different sources of uncertainty in model estimates should be targeted in the future modelling of SOC stock and changes.

As the parameter uncertainties are estimated at regional scale, information on litter input uncertainties at regional scale, under Swedish conditions, need to be included in the uncertainty: litter production makes a large contribution to uncertainties in the model estimates. To improve the model simulations and the quantification of SOC changes, there is a need for enhancing litter production estimates, with a focus on fine root litter, branches, and understorey production. The improvement of understorey litter production estimates should include both the time development of litter production and estimates of litter production under Swedish conditions at the larger scale (regional and national).

8 Sammanfattning (Swedish Summary)

Det största lagret av aktivt kol i landekosystemen finns i marken. Det är viktigt att studera markens stora förråd av kol eftersom små förändringar där leder till stora förändringar i den globala kolbalansen. Framförallt är det koncentrationen av koldioxid i atmosfären som påverkas. För att kunna förutsäga vilken roll skogen och dess skötsel spelar för växthusgasbalansen och för att vi ska kunna rapportera Sveriges utsläpp av växthusgaser till Klimatkonventionen och Kyoto-protokollet, behöver vi veta hur stora förändringarna i markens kollager är. Det är också viktigt att känna till hur osäker beräkningen är, för att veta med vilken säkerhet man kan dra slutsatser om det sker förändringar i markens kolförråd och hur stora de förändringarna är.

I denna avhandling studerades de osäkerheter som uppkommer när skattningar av kollagrets storlek och förändring skalas upp från en lägre nivå till att gälla hela Sverige. Exempel på en sådan uppskalning är när man går från ett skogsbestånd till region. De regionala skalorna i denna avhandling var län eller regioner som består av sammanslagna län.

Två modeller: Q och Yasso07 användes för att uppskatta storleken på och förändringarna i markens kollager i gran- och tallskogar på olika regionala skalor i Sverige. Q-modellen kalibrerades genom att data från Markinventeringen, en landsomfattande kartläggning av markförhållanden och markkemi på länsnivå, jämfördes med modellens beräkningar. Då kunde osäkerheten fastställas hos de parametrar som modellen använder för att uppskatta kollagret. Exempel på en sådan parameter är mikroorganismernas effektivitet. Kalibreringen resulterade i en optimerad uppsättning parametrar som användes i andra studier på regional skala.

Modellerna Q och Yasso07 användes vidare för att bedöma hur olika säkerhetskällor påverkar uppskattningen av förändringar i markens kollager.

Värdet på den årliga förnaproduktionen var den viktigaste källan till osäkerhet för de skattade förändringarna i markens kollager.

Skattningar av markens kollager över ett skogsbestånd utfördes med Qmodellen. Detta genomfördes för att bedöma jämförbarheten mellan modell och data. Simuleringar utfördes på den minsta skala som var möjlig (varje provyta i inventeringen). Modellen och data visade sig svåra att jämföra på beståndsnivå. Anledningen till olikheterna var att kolförrådet i marken i modellen och inventeringens data definieras olika. I modellen ingår grövre fraktioner som grenar, toppar och stubbar i markens kolförråd, vilket påverkar kolmarkens dynamik över ett bestånd till en stor grad.

Olika scenarier med ökat uttag av skörderester och stubbrytning analyserades med Q-modellen. Detta för att studera effekterna på markens kolinlagring när avverkningsrester används som biobränsle och ersätter kol i fossilt bränsle. Minskningen i markens inlagring av kol var större på ett 20 års perspektiv än på 100 år. Inlagringen av kol påverkades mer negativt i norra Sverige. Den minskade inlagringen kompenserades dock av klimatnyttan genom minskade koldioxidutsläpp med ersättning av fossila bränslen.

Denna avhandling undersökte samstämmigheten mellan markinventerings data och modellers skalor. Modellerna är ofta avsedda att beskriva processer som pågår på ekosystemnivå medan inventeringens data främst är avsedd för nationella uppskattningar. Avhandlingen visar att osäkerheten ökar när data från inventeringen skalas ner och modellernas uppskattningar skalas upp. Därför bör man välja metod beroende på vilken skala man vill studera.

Skattning av osäkerheterna i modeller och inventering är ofta i samma storleksordning men orsakerna till osäkerheterna är olika. Det krävs således olika angrepssätt för att minska osäkerheterna.

Både modeller och inventeringsdata kan användas för att uppskatta storleken på kolsänkorna i svensk skogsmark på nationell nivå, men när de förväntade förändringarna i markens kolförråd är små, några få promille per år, är det svårt att säkert skatta förändringens storlek med både inventeringar och modeller.

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