INTEGRATED PROCESS-BASED SIMULATION OF SOIL CARBON DYNAMICS IN RIVER BASINS UNDER PRESENT, RECENT PAST AND FUTURE ENVIRONMENTAL CONDITIONS

Dissertation

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Abstract

Soils contain a large amount of carbon (C) that is a critical regulator of the global C budget. Already small changes in the processes governing soil C cycling have the potential to release considerable amounts of CO₂, a greenhouse gas (GHG), adding additional radiative forcing to the atmosphere and hence to changing climate. Increased temperatures will probably create a feedback, causing soils to release more GHGs. Furthermore changes in soil C balance impact soil fertility and soil quality, potentially degrading soils and reducing soils function as important resource.

Consequently the assessment of soil C dynamics under present, recent past and future environmental conditions is not only of scientific interest and requires an integrated consideration of main factors and processes governing soil C dynamics. To perform this assessment an eco-hydrological modelling tool was used and extended by a process-based description of coupled soil carbon and nitrogen turnover. The extended model aims at delivering sound information on soil C storage changes beside changes in water quality, quantity and vegetation growth under global change impacts in meso- to macro-scale river basins, exemplary demonstrated for a Central European river basin (the Elbe). As a result this study:

- Provides information on joint effects of land-use (land cover and land management) and climate changes on croplands soil C balance in the Elbe river basin (Central Europe) presently and in the future.
- Evaluates which processes, and at what level of process detail, have to be considered to perform an integrated simulation of soil C dynamics at the meso- to macro-scale and demonstrates the model's capability to simulate these processes compared to observations.
- Proposes a process description relating soil C pools and turnover properties to readily measurable quantities. This reduces the number of model parameters, enhances the comparability of model results to observations, and delivers same performance simulating long-term soil C dynamics as other models.
- Presents an extensive assessment of the parameter and input data uncertainty and their importance both temporally and spatially on modelling soil C dynamics.

For the basin scale assessments it is estimated that croplands in the Elbe basin currently act as a net source of carbon (net annual C flux of 11 g C m⁻² yr⁻¹, 1.57 10⁶ tons CO₂ yr⁻¹ entire croplands on average). Although this highly depends on the amount of harvest by-products remaining on the field. Future anticipated climate change and observed climate change in the basin already accelerates soil C loss and increases source strengths (additional 3.2 g C m⁻² yr⁻¹, 0.48 10⁶ tons CO₂ yr⁻¹ entire croplands). But anticipated changes of agro-economic conditions, translating to altered crop share distributions, display stronger effects on soil C storage than climate change. Depending on future use of land expected to fall out of agricultural use in the future (~ 30 % of croplands area as "surplus" land), the basin either considerably looses soil C and the net annual C flux to the atmosphere increases (surplus used as black fallow) or the basin converts to a net sink of C (sequestering 0.44 10⁶ tons CO₂ yr⁻¹ under extensified use as ley-arable) or reacts with decrease in source strength when using bioenergy crops. Bioenergy crops additionally offer a considerable potential for fossil fuel substitution (~37 PJ, 10¹⁵ J per year), whereas the basin wide use of harvest by-products for energy generation has to be seen critically although offering an annual energy potential of approximately 125 PJ. Harvest by-products play a central role in soil C reproduction and a percentage between 50 and 80 % should remain on the fields in order to maintain soil quality and fertility.

The established modelling tool allows quantifying climate, land use and major land management impacts on soil C balance. New is that the SOM turnover description is embedded in an eco-hydrological river basin model, allowing an integrated consideration of water quantity, water quality, vegetation growth, agricultural productivity and soil carbon changes under different environmental conditions.

The methodology and assessment presented here demonstrates the potential for integrated assessment of soil C dynamics alongside with other ecosystem services under global change impacts and provides information on the potentials of soils for climate change mitigation (soil C sequestration) and on their soil fertility status.

Zusammenfassung

Böden speichern große Mengen Kohlenstoff (C) und beeinflussen wesentlich den globalen C Haushalt. Schon geringe Änderungen der Steuergrößen des Bodenkohlenstoffs können dazu führen, dass beträchtliche Mengen CO₂, ein Treibhausgas, in die Atmosphäre gelangen und zur globalen Erwärmung und dem Klimawandel beitragen. Der globale Temperaturanstieg verursacht dabei höchstwahrscheinlich eine Rückwirkung auf den Bodenkohlenstoffhaushalt mit einem einhergehenden erhöhten CO₂ Fluss der Böden in die Atmosphäre. Weiterhin wirken sich Änderungen im Bodenkohlenstoffhaushalt auf die Bodenfruchtbarkeit und Bodenqualität aus, wobei eine Minderung der Bodenkohlenstoffvorräte wichtige Funtionen des Bodens beeinträchtigt und folglich den Boden als wichtige Ressource nachhaltig beinflusst.

Demzufolge ist die Quantifizierung der Bodenkohlenstoffdynamik unter heutigen und zukünftigen Bedingungen von hohem Interesse und erfordert eine integrierte Betrachtung der wesentlichen Faktoren und Prozesse. Zur Quantifizierung wurde ein ökohydrologisches Flusseinzugsgebietsmodell erweitert. Ziel des erweiterten Modells ist es fundierte Informationen zu Veränderungen des Bodenkohlenstoffhaushaltes, neben Veränderungen der Wasserqualität, der Wasserverfügbarkeit und des Vegetationswachstums unter Globalem Wandel in meso- bis makroskaligen Flusseinzugsgebieten bereitzustellen. Dies wird am Beispiel eines zentraleuropäischen Flusseinzugsgebietes (der Elbe) demonstriert. Zusammenfassend ergibt diese Arbeit:

- eine Quantifizierung der heutigen und zukünftigen Auswirkungen des Klimawandels sowie von Änderungen der Landnutzung (Bodenbedeckung und Bodenbearbeitung) auf den Bodenkohlenstoffhaushalt agrarisch genutzter Räume im Einzugsgebiet der Elbe.
- eine Beurteilung welche Prozesse, und zu welchem Prozessdetail, zur integrierten Simulation der Bodenkohlenstoffdynamik in der meso- bis makroskala zu berücksichtigen sind. Weiterhin wird die Eignung der Modellerweiterung zur Simulation dieser Prozesse unter der Zuhilfenahme von Messwerten dargelegt.
- darauf begründet wird eine Prozessbeschreibung vorgeschlagen, die die Eigenschaften der Bodenkohlenstoffspeicher und deren Umsetzungsrate mit in der betrachteten Skala zur Verfügung stehenden Messdaten und Geoinformationen verbindet. Die

vorgeschlagene Prozessbeschreibung kann als robust hinsichtlich der Parametrisierung angesehen werden, da sie mit vergleichsweise wenigen Modelparametern eine ähnliche Güte wie andere Bodenkohlenstoffmodelle ergibt.

• eine umfassende Betrachtung der Modell- und Eingangsdatenunsicherheiten von Modellergebnissen in ihrer räumlichen und zeitlichen Ausprägung.

Das in dieser Arbeit vorgestellte Modellsystem erlaubt eine Quantifizierung der Auswirkungen des Klima- und Landnutzungswandels auf den Bodenkohlenstoffhaushalt. Neu dabei ist, dass neben Auswirkungen auf den Bodenkohlenstoffhaushalt auch Auswirkungen auf Wasserverfügbarkeit, Wasserqualität, Vegetationswachstum und landwirtschaftlicher Produktivität erfasst werden können. Die im Rahmen dieser Arbeit dargelegten Ergebnisse erlauben eine integrierte Betrachtung der Auswirkungen des Globalen Wandels auf wichtige Ökosystemfunktionen in meso- bis makroskaligen Flusseinzugsgebieten. Weiterhin können hier gewonnene Informationen zur Potentialabschätzung der Böden zur Linderung des Klimawandels (durch C Festlegung) und zum Erhalt ihrer Fruchtbarkeit genutzt werden.

Contents

1	Intr	oductio	٦	1						
	1.1	Background		2						
	1.2	Object	ives and structure of the study	8						
	1.3	Approa	ach of the study and concepts for soil carbon turnover assessment	11						
2	Inte	Integrated eco-hydrological modelling of soil organic matter dynamics for the								
	asse	ssessment of environmental change impacts in meso- to macro-scale								
	rive	ver basins								
	2.1	Introduction								
	2.2	Conce	pts of soil organic matter models	20						
	2.3	Materials and methods								
		2.3.1	The Soil and Water Integrated Model SWIM	22						
		2.3.2	Soil organic matter module extension (SCN)	23						
		2.3.3	Model parametrisation and initialisation	28						
		2.3.4	Data sets and land management scenario	29						
		2.3.5	Statistical criteria for model evaluation	32						
	2.4	Results	3	33						
		2.4.1	Testing of soil organic matter processes	33						
		2.4.2	Effects of land management practices on long-term SOC trends	38						
	2.5	Discus	sion	43						
		2.5.1	Soil organic matter module	43						
		2.5.2	Testing of soil organic matter processes	45						
		2.5.3	Effects of land management practices on long-term SOC trends.	47						
	2.6	Conclusions		49						
	2.7	Acknowledgements		51						
3	Evaluation of water and nutrient dynamics in soil-crop systems using th									
	hyd	nydrological catchment model SWIM (Soil and Water Integrated Model) 53								
	3.1	Introdi	uction	54						

	3.2	Materi	als and Methods	56
		3.2.1	Experimental sites	56
		3.2.2	Model description	57
		3.2.3	Model parameterization and initialisation	62
		3.2.4	Statistical evaluation	63
	3.3	Results	s and discussion	65
		3.3.1	Soil temperature	65
		3.3.2	Soil water content	68
		3.3.3	Crop yields	74
		3.3.4	Soil nitrogen dynamics	77
		3.3.5	Soil carbon dynamics	81
	3.4	Conclu	sion	
	3.5	Acknow	wledgements	
4	Para soil	ameter a organic	nd input data uncertainty estimation for the assessment of lo carbon dynamics	ong-term 87
	4.1	Introd	luction	89
	4.2	Materi	als and methods	90
		4.2.1	The Soil and Water Integrated Model SWIM	90
		4.2.2	Model extension for SOM turnover	90
		4.2.3	Quantification of uncertainty and sensitivity	91
		4.2.4	Definition of model variables and selection of the Probability Distribution Functions	92
		4.2.5	Data sets and study area for uncertainty analysis	
	4.3	Results	and discussion	100
		4.3.1	Factors sensitivity and importance	100
		4.3.2	Assessment of uncertainty	
		4.3.3	Implications for long-term soil organic carbon dynamics	
	4.4	Conclu	ision	
	4.5	Acknow	wledgements	119
5	Inte	grated n	nodelling of soil carbon storage in croplands under climate a	nd agro-
	ecor	nomic cł	hange in a central European river basin	121
	5.1	Introdu	uction	

5.2	Methods		
	5.2.1	SWIM-SCN 126	5
	5.2.2	The Elbe river basin)
	5.2.3	Characterisation of climate)
	5.2.4	Characterisation of land use and crop share properties	3
	5.2.5	Characterisation of agricultural management	5
	5.2.6	Simulation set up, scenario assumptions and target results 140)
5.3	Results		1
	5.3.1	Regionalisation of agricultural land use	1
	5.3.2	Reference period (1951 – 2000) 146	5
	5.3.3	Scenario period (2001-2055) 152	2
5.4	Discuss	sion 168	3
	5.4.1	Reference period 170)
	5.4.2	Scenario period, combined land use and climate effects 173	3
5.5	Conclu	sion	3
5.6	Acknow	wledgement)
Sum	mary, c	onclusion and perspectives181	L
6.1	Model concept of SOM turnover and its integration in the eco-hydrological model SWIM		
6.2	Process	s interactions and key environmental drivers of soil C dynamics 185	5
6.3	Uncert	ainty and sensitivity	7
6.4	Region	alising external driving forces and regional impacts study)
6.5	Key ac	hievements and findings192	<u>)</u>
6.6	Perspe	ctives 194	1

References	
List of Figures	I
List of Tables	V
Curriculum vitae and Publications	IX
Erklärung	XII
0	

Chapter 1

Introduction

1.1 Background

The terrestrial carbon cycle is central to the Earth system and is tightly linked with climate, water cycles, nutrient cycles and the production of biomass through photosynthesis (see figure 1.1 for a simplified overview). The dynamics of soil Carbon (C) is governed by input of C (e.g. plant or animal derived) and turnover by soil organisms (figure 1.1). For stable systems equilibrium between input and release from soil prevails resulting in a characteristic soil C content depending on local environmental properties. Change in input or turnover properties result in increasing or decreasing soil C content.

Soil organic matter (SOM), with its major constituents soil organic Carbon (SOC) and Nitrogen (SON), is an essential component of ecosystems and their functioning. SOM is an important building block for soil structure and for the formation of stable aggregates, and influences soil water storage capacity and soil buffering capacity. It was already recognized at the beginning of the last century (King, 1907; Shutt, 1916) that "... organic matter is fuel for soils biological machinery". Decay of SOM releases nutrients necessary for plant growth, and consequently supply of SOM is a crucial factor for soil fertility and quality. Furthermore soils constitute an important resource for providing nutrients for humans.



Fig. 1.1: Illustration of the main stores and flows of C in a cropland, showing three pools of soil C for simplicity, though recognizing that soil C spans a continuum of forms. Adopted from (Janzen, 2006). SOC pools box schematically represents different turnover properties, thickness of arrows the approximate magnitude of fluxes.

SOM represents a major pool of carbon (C) in the Earth system. Soil C pool stores approximately twice as much as the atmospheric pool (\sim 770 Pg C, 1 petagram = 10¹⁵ g) and 2.5 times that of the biotic pool (\sim 610 Pg) on the global scale (Batjes, 1998; King et al., 2004). Anthropogenic interference of natural systems alters the storage of SOM along with other ecosystem functions. Alterations of the soil C pool consequently have a strong impact on global C cycling. Human intervention in the carbon cycle has been occurring for thousands of years, in Europe at least since the development of agriculture with the establishment of settlements and agriculture in Neolithic times. Although, only over the last two centuries has human interference in carbon cycle become comparable in magnitude to major natural fluxes (Field and Raupach, 2003), and it took until the last decades of the 20th century that humans recognised the threat of adverse consequences and begun to respond.

Major threats resulting from human interference in the carbon cycle are the rise in atmospheric Carbon dioxide (CO₂) which is an important greenhouse gas (GHG), and the depletion of soil C through land use with adverse effects on soil fertility and quality. An increase of atmospheric CO₂ can be attributed to two main sources, fossil fuel burning with related industrial activities and terrestrial carbon losses from land-use change which together cause a rise from ~280 ppmv (part per million volume) in pre-industrial times to approximately 370 ppmv in 2000 (Houghton, 1999; McGuire et al., 2001). Currently, atmospheric CO₂ concentration is increasing at the rate of 1.5 ppmv per year or 3.3 Pg C per year. In the 1990s emissions from fossil fuel combustion and cement production into the atmosphere accounted for ~6.3 (+/- 0.4) Pg C yr⁻¹ from which ~3.2 (+/- 0.1) Pg C yr⁻¹ remained in the atmosphere (Prentice et al., 2001). Approximately 2.1 (+/- 0.7) Pg C yr⁻¹ were taken up by the oceans (Bopp et al., 2002; Le Quere et al., 2003) with a remaining terrestrial uptake of 1.0 (+/- 0.8) Pg C yr⁻¹ estimated to close the balance (House et al., 2003). Land use change (cultivation, deforestation) released an additional 1.4 – 3.0 Pg C per year during this period (Houghton, 1996).



Fig. 1.2: The Vostok ice core record for atmospheric concentration (Petit et al., 1999) and the "business as usual" prediction used in the IPCC third assessment (IPCC, 2001). The current concentration of atmospheric carbon dioxide (CO₂) is also indicated. Adopted from (Global_Carbon_Project, 2003).

This atmospheric CO₂ increase is expected, with high confidence, to continue at an accelerated rate in the future. Atmospheric CO₂ concentration is projected beyond 500 ppmv (Houghton et al., 2001) by 2100, depending on assumed future socio-economic development (Nakicenovic and Swart, 2000), with other GHGs (e.g. CH₄ and N₂O) increasing at comparable rates.

Compared to information on atmospheric CO₂ concentration derived from ice cores (Petit et al., 1999), the projected CO₂ concentrations are unprecedented within the last 420,000 years (figure 1.2a). There is no doubt that the increases in GHGs are due to human activities and are already having consequences on the earth system, mainly on the climate system. The contemporary climate system is already responding to changing GHG concentrations. The magnitude of human induced changes indicate that the earth system has moved well outside the range in which the carbon cycle operated over the past half million years (Field and Raupach, 2003).

Due to increasing GHG concentration the radiative forcing of the atmosphere is amplifying, resulting in an increase in global mean land surface temperature. Over the 20^{th} century the mean temperature increased by 0.6 K (+/- 0.2 K) globally, and the increase is anticipated to progress at accelerated rates to up to + 6 K relative to pre-industrial levels (Houghton et al., 2001) by the end of the 21^{th} century (figure 1.3).

One of the emerging threats to society resulting from increasing GHGs concentrations in the atmosphere is global climate change. Changes in precipitation and temperature regimes both in variability, quantity and intensity already can be attributed to climate change, but changes in climate manifest differently in different regions.

Climate change has various effects on terrestrial ecosystems beside impacts on society and economy. Concerning effects on SOC storage, Jenny et al. (1949) and Jenny (1980) already stated a strong inter-dependence between climate and soil C. Climate change and increased atmospheric CO₂ concentration alter Net Primary Productivity. Changing climate affects decomposition and mineralisation patterns of SOM. Hence, the main determinants of SOC cycle are influenced: amount and quality of organic matter input to soils and its turnover properties. Here modified soil temperature and soil moisture regimes are known to possess the highest impacts, as both are the primary rate determinant of microbial processes. Depending on local properties, higher soil temperature and / or higher soil moisture will exacerbate the rate of decomposition and mineralisation leading to a decrease of the SOC pool (Lal, 2004a). Climate change and particularly land use change led to a depletion of SOC (figure 1.3). Recent studies indicate to large soil carbon losses in temperate regions most probable due to climate change. For example measured losses of topsoil C in England and Wales during the period 1978 to 2003, equal reduced CO₂ emissions achieved between 1990 and 2002 in the United Kingdom (Bellamy et al., 2005; Schulze and Freibauer, 2005).



Fig. 1.3: Northern hemisphere temperature anomaly relative to 1961-1990, based on proxy-data (1600-1980) and thermometer records (1900-2000) taken from (Mann et al., 1999), as well as projections of global annual air temperature for 2000-2100 derived from several IPCC climate change scenarios, based on (Houghton et al., 2001).

The role of SOC dynamics on the historic increase of atmospheric CO₂, and its strategic importance in decreasing the future rate of atmospheric CO₂ is not widely recognized yet. Considerable potential of C sequestration in world soils is estimated at 0.4 - 1.2 Pg C per year, which corresponds to a substitution effect of 5 - 15 % of current global fossil-fuel

emissions (Lal, 2004a). The potential of adapted land management practices and adapted land use have been proven to offer options for soil C sequestration (e.g. West and Marland, 2003; Freibauer et al., 2004; Lal, 2004b; Smith, 2004). These possibilities, which are both beneficial in terms of climate change mitigation and enhancing soil quality, are meanwhile issues in international (e.g. Umweltbundesamt, 2003; UNFCCC, 2005) and national regulations (e.g. Bundesbodenschutzgesetz BBodSchG (UmwR, 2005). Land use or land management changes increasing soil C storage may be accounted for emission reduction targets in the frame of the Kyoto protocol (Article 3.3 and 3.4). Recommended management practices offer the potential to increase or stabilize SOC content, at least to the cumulative historical C loss due to land use change (Lal, 2004a, figure 1.4). Soil C sequestration through transferring atmospheric CO₂ into SOC offers the prospective for climate change mitigation and enhancing or maintaining soil fertility. Hence sequestration of C in soils constitutes a noteworthy instrument, aside the key instruments of reducing fossil fuel usage and the decarbonisation of energy generation.



Fig. 1.4: A Schematic of the soil C dynamics upon conversion from a natural to agricultural ecosystem, and subsequent adoption of recommended management practices (RMPs), adopted from (Lal, 2004a).

SOM dynamics are driven by various environmental processes, mainly soil physical, chemical and biological processes, such as soil microbial activity, soil water retention, nutrient cycling, gas flux, and plant growth (Fang et al., 2006b; Rees et al., 2005; Zhang et al., 2002; Wang et al., 2004; Al-Kaisi et al., 2005). Furthermore, the rates of decomposition and mineralization are controlled and altered by the processes of soil formation, which are dependent on climate, topographic position, parent material, potential biota, time, and human activity (Amundson, 2001). Anthropogenic climate change and land use change are influencing these major drivers of SOM dynamics.

Climate change leads to the alteration of turnover rates of SOM due to changes in soil moisture and soil temperature. Elevated atmospheric CO₂ content leads to effects on plant growth and reduced of plant stomatal conductance, and therefore an increase in water use efficiency (Drake and Gonzàlez-Meler, 1997; Olesen et al., 2004). Alterations in turnover properties of SOM as well as in organic matter quality and quantity are the consequence (Jenny et al., 1949; Lieth, 1973; Davidson et al., 2000; Kirschbaum, 2000; Wang et al., 2000). Land use change can affect C inputs, residue composition, organic matter decomposition and mineralization, soil physical properties, nutrient availability, and soil fauna (Guo and Gifford, 2002; Murty et al., 2002; Aaron et al., 2004; DeGryze et al., 2004; Miller et al., 2004; Smith, 2004).

As described schematically in figure 1.5, the SOC pool and its dynamic play an important role in all components of soil quality and biodiversity (like soil structure, soil hydrology, soil biodiversity and soil fertility) with consequences on different ecosystem services, for instance soil quality, agronomic/forest productivity, food security, water quality and soil biodiversity (Lal, 2004a).

Concerning the emergent problems related to climate change, the depletion, and important functions of soil C, it is of paramount interest to estimate soil C changes due to global change impacts, both for the recent past and for the future. In addition, tools allowing to quantify impacts of e.g. adapted land management and land use on soil C storage are needed. So here integrated and spatially explicit considerations are required to take into account soil processes like soil temperature, soil water, organic matter and nutrients dynamics together with vegetation and hydrologic processes, and its driving forces climate and land use.



Fig. 1.5: The SOC pool and its dynamic play an important role in all components of soil quality and biodiversity. Adopted from (Lal, 2002).

1.2 Objectives and structure of the study

Global environmental changes such as climate and land use change develop differently at the regional scale. Together with regional environmental settings such as climatic, land use and soil properties, these external environmental driving forces have to be characterized at the regional scale.

The external driving forces impact ecosystem functions such as water quality, water quantity, soil quality and soil fertility as well as vegetation productivity. These ecosystem functions provide goods and services central to the human system such as food production, water availability and water quality. Therefore it is desirable to quantify the present day situation of ecosystem services and to estimate their trajectory of change at local, regional and global scales, under anticipated global environmental change. As described in chapter 1.1, soils and soil C play a central role for various ecosystem functions and for soil-plant-atmosphere interactions, which is addressed within this study for regional scale settings.

As a consequence of the apparent need to establish tools for integrated assessment of global change impacts at the regional scale, this study aims for proposing an approach for an integrated process-based simulation of soil organic matter dynamics (coupled soil C and N turnover) under present, recent past and expected future environmental conditions, defined by a time frame from 1951 to 2055, and within the structure of an eco-hydrological modelling tool. The study therefore addresses following objectives:

- I. Integrating present day understanding of soil organic matter dynamics into an eco-hydrological modelling system, which should be able to assess global change impacts on soil organic matter dynamics at the regional scale / river basin scale. Additionally, the constraints of data availability for parameterisation and testing at the regional scale have to be considered. (chapters 2 and 3)
- II. Developing a robust modelling system, which integrates soil temperature, soil water, vegetation and soil nutrient dynamics (coupled soil C and N processes), and which is driven by climate, land use and land management in lateral and vertical domains for river basins. (chapters 2 and 3)
- III. Elaborating and describing mathematically physical, chemical and biological soil processes and feedbacks, which affect the storage of organic compounds and their release to the atmosphere (chapters 2 and 3)
- IV. Integrating an algorithm for the generation of spatial crop cover patterns on arable land and apply it for assessing impacts of land use and climate change (chapter 5 and Wechsung et al., 2006)
- V. Quantifying impacts of major land management practices on long-term soil carbon storage (chapters 2 and 5)

- VI. Evaluating the effects of crop rotations and crop shares and their importance for water, nutrients and soil organic matter dynamics (chapter 5 and Hattermann et al., 2005a)
- VII. Assessing uncertainty related to model parameters and input data in long-term soil carbon assessments and evaluating the input factor's importance, and rating the consequences thereof for present day C storage and for C storage under changing environmental conditions (chapter 4)
- VIII. Estimating combined and particular impacts of changing land use and climate on soil carbon storage in large river basins for croplands (chapter 5)

These objectives are specifically addressed within chapters 2 to 5. Chapter 2 provides the definition and test of a model extension to assess soil organic matter dynamics (coupled soil N and C dynamics) within an eco-hydrological modelling system. Furthermore the ability to simulate impacts of recommended management practices on soil organic matter dynamics and for soil carbon sequestration assessments is demonstrated. Chapter 3 evaluates process dynamics in soil-crop systems at the plot scale, which form a pre-condition for spatio-temporal distributed eco-hydrological modelling of environmental change issues in agro-ecosystems. The ability to simulate agro-ecosystem process interactions and feedbacks for biomass growth (crop yield), soil processes (soil temperature, soil water dynamics) and soil nitrogen and carbon dynamics under different edaphic, climatic and management conditions is testified and the importance of integrated consideration of these processes is given. Chapter 4 provides a quantification of model parameters and input data uncertainty for long-term soil carbon assessments (model parameters and input factors as soil, climate, and agricultural management). Further on, a ranking and sensitivity assessment of all input factors and their interrelations is done. Integrated views of main factors influencing simulation results, which are base for interpretation of regional landscape response / ecosystem behaviour, are provided. Chapter 5 gives a first assessment on soil carbon dynamics in croplands in the recent past, present and future regionalized socio-economic and climate conditions for croplands in the Elbe river basin (Central Europe). Chapter 5 provides a quantification of relative contributions of agro-economic and climate impacts on soil C storage.

In adopting the stated objectives the study aims to provide sound information and an extended simulation tool to address the following questions:

- What are the joint effects of land-use (land cover and land management) and climate changes on the soil carbon balance in the Elbe river basin (Central Europe) in the present and in the future?
- Which processes, and at what level of process detail, are necessary for an integrated simulation of soil organic matter dynamics at the meso- to macro-scale?
- How can the global external driving forces climate and land use be regionalized for regional scale impact studies?
- What is the effect of parameter and input data uncertainty both temporally and spatially on modelling soil carbon dynamics, and which model factors contribute most to the model uncertainty?

1.3 Approach of the study and concepts for soil carbon turnover assessment

Changes in soil C storage can be assessed in different ways. One obvious and important method is by establishing long-term observations for different land cover, land uses and environmental settings. For agro-ecosystems for example the Global Change and Terrestrial Ecosystems (GCTE) programme of the International Geosphere-Biosphere Programme (IGBP) established the soil organic matter research network (SOMNET) where data from long-term experiments are collected and provided for analysis (Powlson et al., 1998). Data from these experiments on soil organic matter dynamics can be used to derive relationships between e.g. agricultural practices or climate and changes in soil organic carbon content. Relationships between certain driving forces and soil organic carbon content can be derived through regression techniques and can be used for extrapolation either temporally (e.g. extrapolate the relationships derived through linear regression in the future) or spatially (e.g.

assume same relationships for areas with similar environmental settings). This was successfully demonstrated by Smith et al. (1997b) for deriving carbon sequestration potentials in European soils.

Relationships derived from long-term experiments on soil organic matter dynamics can be used by bookkeeping models. They keep track of changes in e.g. soil carbon stocks (Dixon, 1994; Houghton, 1999) due to land-use change based on historic records. Most often these relationships are up-scaled to global or regional scales. Examples using this method are numerous (e.g. Ogle et al., 2003; Sleutel et al., 2003; VandenBygaart et al., 2004; Neufeldt, 2005; Singh and Lal, 2005).

Furthermore relationships and accounting factors gained from long-term soil organic matter experiments are being proposed in the meantime by the IPCC Guidelines for National Greenhouse Gas Inventories reference manual (IPCC, 1997) or the German humus accounting scheme ("Humusbilanzierung", Körschens et al., 2004 and 2005) and are used for soil organic matter assessments to provide information for liability verification under national regulations.

Meanwhile, information and relationships derived from long-term experiments have become indispensable in global change impact research on soil organic matter. But as such, they do not consider the effect of environmental changes on soil carbon storage. Extrapolation of relationships derived from long-term experiments delivers highly uncertain information. Only process based modelling tools are capable of reproducing observed trends to changes in soil C storage and provide the capability to allow scenario based assessments of possible future trajectories of the soil C balance under environmental change.

This method is represented by simulation models that encode environmental process understanding by numerical or analytical equations, but has to be used in combination with information gained from long-term experiments, but also with information gained from remote sensed data or laboratory investigations. The process descriptions have to be evaluated against ecosystem measurements for some (representative) regions. In terms of soil organic matter processes early mathematical formulations have been published by (Jenny et al., 1949). In this publication, the change in the amount of total C in the soil over time was characterized by the difference between inputs from plants and losses in form of CO₂, based on a first-order decay model. The decay of soil C is thereby controlled by a factor determining the fraction of C lost as CO₂ each year. This concept refers to a simple singlepool C model, and they are rigorously applicable if the entire SOM pool is dynamically homogeneous. Categorically this basic concept is still widely and successfully used in a strongly modified form. Introducing of reduction functions to mirror the influences of environmental conditions (e.g. soil moisture, soil temperature, soil acidity status) and discriminating different soil carbon pools with intrinsic residence times and turnover properties (see figure 1.1) are the main modifications of this concepts.

Developments of the basic concept led to so called multi-compartment, process-based models, whereas each soil compartment or pool is characterised by its position in the model's structure and its decay rate (expressed by first-order rate kinetics with respect to the concentration of the pool). Since the results of ¹⁴C measurements, indicating that different constituents of SOC have different residence times, most models discriminate between (a) an active pool, including fresh plant material and root exudates with residence times of $^{\sim}$ 1 year, (b) a slow pool, including SOC that is decomposed at intermediate rates, with residence times of $(10^{\circ} - 10^{2} \text{ years}, \text{ and (c)} a passive pool, including SOC that, for physical reasons, has a residence time of <math>\geq 10^{2} - 10^{3}$ years (Amundson, 2001; see SOC pools box in figure 1.1). Good summaries for the process-oriented, multi-compartment SOM model types can be found in e.g. (Paustian, 1994; McGill, 1996; Molina and Smith, 1997; Smith et al., 1997a; Brussaard, 1998; Smith et al., 1998; Smith, 2005). Main representatives of this type are CANDY (Franko et al., 1997b), DAISY (Jensen et al., 1997), CENTURY (Parton et al., 1987) or Roth-C (Coleman et al., 1997).

The above mentioned type of process description (first order reaction kinetics) and derivates from them (e.g. second order reaction kinetics), however, do not describe the process itself. Macro- and micro-organisms in soils consuming organic matter and changing the chemical state of organic matter and its quantity are responsible for turnover of organic matter in soils. Hence the suggested and commonly used terminology of a process-based soil organic matter model is a bit misleading in this context. Models attempting to reflect soils organism consumption and alteration of organic matter already exist and are known as e.g. food web models or organism-oriented models. But as noted by Smith et al. (1998), processoriented models (first order reaction concept) are simpler to calibrate and easier to parameterise than organism-oriented models, at least for meso- to macroscale applications. Additionally food webs in soils and process understanding of organic matter transformation are not yet completely understood. This makes meso- to macro-scale applications of this type of model difficult as does the lack of spatially distributed data on food-web structures.

Accordingly this study adopted a simplified but robust process-based approach reflecting the facts of process testability using observed data and relating them to commonly measured soil carbon pools. The adopted description is a module of the forest growth model 4C describing soil organic matter dynamics for forest ecosystems (Grote et al., 1999; Lasch et al., 2002) and is similar to the CANDY model developed by Franko et al. (1995). Hence for forest ecosystems this description is proved to be applicable. A discussion on the used modelling approach is given in chapter 2 and 3.

Since soil organic matter dynamics are influenced by various soil processes, but mainly by soil temperature and soil moisture, a representation of soil hydrology and temperature dynamics is crucial. These main factors influencing soil C storage need to be mirrored accordingly, especially in terms of climate and land use change impact on soil C storage. Beside adequately representing these soil processes, soil C dynamics are coupled and interrelated with soil N dynamics, not only through nutrition (mainly the inorganic nitrogen forms nitrate, ammonia, and phosphorous) effects on plant growth. Coupled soil carbon and nitrogen processes in this context are important due to carbon turnover providing energy for soil nitrogen processes, and the absence of sufficient inorganic nitrogen will inhibit the carbon turnover. Explicitly considering N dynamics together with soil carbon dynamics is important for correctly representing long-term soil C trends.

Therefore, the approach proposed here aims at considering and integrating the relevant processes with a level of complexity feasible at the scale it should operate on. So soil C and N dynamics, soil hydrology and soil temperature are considered. They are linked with plant growth and basin hydrology, as described in chapters 2 and 3. The model should be used for

regional scale applications of global change impacts on ecosystem functions with a focus on soil C dynamics. The regional scales referred to here are meso- $(100 - 10\ 000\ \text{km}^2)$ to macroscales (> 10 000 km²) according to the definition provided by (Becker and Braun, 1999). A well tested method to describe matter fluxes (as soil C and N, soil water etc.) is the consideration of semi-closed systems defined by river basins. Here, the flow and transformation of water and nutrients within the basin environment can be simulated using hydrological models. The model used in this study is the Soil and Water Integrated Model (SWIM, Krysanova et al., 1998), which can be assigned as an eco-hydrological river basin model of intermediate complexity, and is distributed spatially based on hydrological response units (see chapter 2 to 5 for details). SWIM integrates hydrology, vegetation, erosion, nutrients (nitrogen, N and phosphorus, P), and sediment fluxes at the river basin scale. The model is connected to meteorological, land use, soil and agricultural management data and is designed for integrated assessments of global change impacts on water quality, water quantity and plant growth in river basins. The model setting of SWIM therefore offers the potential to integrate a process description of soil organic matter (soil C and N) turnover to perform integrated assessments of soil C and N dynamics in relation to other ecosystem functions.

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Chapter 2

Integrated eco-hydrological modelling of soil organic matter dynamics for the assessment of environmental change impacts in meso- to macroscale river basins

Keywords: *Eco-hydrological modelling, soil carbon, soil nitrogen, soil organic matter turnover, land use change, land management, carbon sequestration*

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Abstract: An extension of the eco-hydrological river basin model SWIM (Soil and Water Integrated Model) is proposed to simulate soil organic matter (SOM) dynamics for environmental conditions in Central European river basins. The novel aspect and main advantage of the extended model is an integrated consideration of hydrological processes, vegetation dynamics and biogeochemical cycles (soil carbon, phosphorus, and nitrogen) in semi closed systems (river basins). The extension used is a process-based multi-compartment SOM model that describes the linked processes of decay of soil carbon (C) and nitrogen (N) pools by first order rate kinetics.

The aim of the extended model is the assessment of soil organic matter dynamics under present, recent past and future environmental conditions in relation to other relevant ecosystem services (e.g. water quality and quantity issues, crop productivity) in meso- to macro-scale river basins.

The model extension was tested for the main processes describing and influencing SOM dynamics using observed data sets considering primary organic matter (plant biomass) decomposition, heterotrophic soil respiration and long-term soil organic carbon development. The new SOM model adequately represents these processes when compared to observed data on three experimental field sites and literature studies.

Application of the extended model to assess impacts of land management practices (different organic and inorganic fertilisation schemes, different crop rotations, inclusion of cover crops and crop residue returns) on long-term soil organic (SOC) carbon dynamics used data from two experimental field sites in the eastern part of Germany. The simulated quantification of different fertilisation regimes led to changes from -0.13 to +0.1 t C ha⁻¹ yr⁻¹ in SOC, different types of crop rotations and cover crop impacts changed SOC between -0.13 and +0.07 t C ha⁻¹ yr⁻¹ and incorporation of grain straw residuals led to changes between -0.1 and + 0.027 t C ha⁻¹ yr⁻¹ in SOC at the two sites. The modelled results are in general agreement with experimental studies reported in literature. The extended model is hence able to quantify the impacts of selected land management practices on long-term SOM dynamics and allows land management practices and their impacts on water availability, water quality, carbon storage in soils, and vegetation growth to be assessed in integrated an way.

2.1 Introduction

Quantification of soil organic matter (SOM) dynamics at global and regional scales plays a crucial role in sustaining environmental quality, soil productivity, food and timber production and soil carbon sequestration to offset fossil fuel emission (Schlesinger, 1999; Post and Kwon, 2000; Lal, 2004b; Smith, 2004). Changes in SOM status affect soil fertility and nutrient availability, soil water holding capacity and soil aggregation, which are important ecosystem functions (Tilman et al., 2002; Lal, 2004a; Robertson and Swinton, 2005). In addition, soil organic carbon (SOC) dynamics also have a strong impact on the global (and regional) Carbon (C) cycle, as C stored in world soils (2500 Gt, Gigatons, 1 GT = 10^{15} g) is about 3.3 times the size of the atmospheric pool (760 Gt) and about 4.5 times the size of the biotic pool (560 Gt, Lal, 2004a). Therefore even small changes in the SOC pool will change the global C cycle (Johnston et al., 2004).

SOM dynamics are primarily affected by the input of organic matter compounds and their release to the atmosphere (as CO₂ or other greenhouse gases), and the quantity of SOM is hence dependent on the balance between primary productivity and the rate of decomposition of plant biomass and mineralization of SOM in soils (Kuzyakov and Domanski, 2000). The rates of decomposition and mineralization are controlled by climate, topographic position, parent material, potential biota, and human activity (Amundson, 2001). The storage and release of soil organic matter compounds is mainly driven by soil texture and structure, soil moisture, soil temperature, soil nutrient availability, soil pH status, soil microbial activity, land cover and land management practices (Amundson, 2001; Johnston et al., 2004; Lal, 2004b).

All of the mentioned factors governing SOM dynamics are perturbed by human activities. Two main categories causing variations in SOM can be distinguished and are intensively discussed in scientific literature in the last decades (Houghton, 1996; Post and Kwon, 2000; Guo and Gifford, 2002; Janssens et al., 2003; Freibauer et al., 2004), namely variations in SOM due to climate and due to land use change (change in land cover and in land management).

In the context of climate change mitigation, soil C sequestration can be considered as a substantial opportunity. Aim of soil C sequestration is to transfer atmospheric CO₂ into long-living soil pools and storing it securely so it is not immediately reemitted (Lal, 2004a).

Opportunities for soil C sequestration are land cover conversions (agriculture to grassland or forest) or judicious land use and management practices (Smith et al., 2000; Freibauer et al., 2004; Lal, 2004b; West et al., 2004). It is hence of paramount importance to assess SOM dynamics and soil C sequestration potential at the landscape level.

The aim of the paper is to describe and test an extension of the integrated process-based eco-hydrological river basin model SWIM (Soil and Water Integrated Model, Krysanova et al., 1998) for SOM dynamics and demonstrate its ability to investigate land management effects on long-term SOC dynamics. The novel aspect and main advantage of the extended model is an integrated consideration of hydrological processes, vegetation dynamics and biogeochemical cycles in semi closed systems (river basins).

2.2 Concepts of soil organic matter models

A large number of computer models to describe SOM dynamics in different spatial resolutions and timeframes have been developed in the past decades, e.g. ICBM (Andren et al., 2004), CENTURY (Parton et al., 1988), RothC (Jenkinson, 1990), DNDC (Li et al., 1994), CANDY (Franko et al., 1995).

Generally, model concepts for the description of SOM dynamics can be divided into (1) process-oriented, (multi)-compartment models, (2) organism-oriented models (food-web models), (3) cohort models describing decomposition as a continuum and (4) a combination of (1) and (2) (Paustian, 1994; McGill, 1996; Brussaard, 1998; Smith et al., 1998).

As noted by Smith et al. (1998) process-oriented models seem to be simpler to calibrate and easier to parameterise for meso- to macro-scale applications, they are less sensitive to soil community structure, and the predictive use of organism-oriented models may still be some way off. But the main advantage of organism-oriented models is the explicit description of soil biota, which of course is the main driver for SOM processes, (McGill, 1996; Brussaard, 1998; Smith et al., 1998). The understanding of changes in soil biota under global change impacts will improve scientists capability to investigate global change impacts. Currently however, there is no evidence that soil biota abundance limits process rates at the ecosystem level (Paustian, 1994). This is one precondition for the use of process-oriented models (using firstorder rate kinetics).

Since the results of ¹⁴C measurements, indicating that different constituents of SOC have different residence times, most models discriminate between (a) an active pool, including fresh plant material and root exudates with residence times of 1 year, (b) a slow pool, including SOC that is decomposed at intermediate rates, with residence times of between 10° and 10^{2} years, and (c) a passive pool, including SOC that, for physical reasons, has a residence time of more than $10^{2} - 10^{3}$ years (Amundson, 2001). Good summaries for the process-oriented, multicompartment SOM model types can be found in e.g. (Paustian, 1994; McGill, 1996; Smith et al., 1998; Smith, 2001).

One problem related to multi-compartment SOM models is the comparison of assigned compartments with measurable SOM fractions, and therefore the testing might be limited (Elliott et al., 1996). Additional parameterisation might be problematic for the same reason and an assignment of e.g. a passive pool size and a rate might be difficult due to a small amount of measured data sets to derive these relationships.

The model extension used here can be assigned to the first group of process-oriented models. This type of SOM model focuses on the processes mediating the movement and transformations of matter and energy and assumes first-order rate kinetics.

The model extension of SOM dynamics has to fulfil the following requirements: (a) it has to fit into the overall process description complexity of SWIM and has to cover relevant processes, (b) it has to consider the coupled C and N processes, (c) the model parameterisation has to relate to measurable quantities (through field or laboratory experiments) and required data has to be available, and (d) it has to be implemented as spatially distributed module and has to operate at time steps appropriate for the natural processes described. In our case, we adopted a fairly simple structured process-oriented model of SOM turnover, considering two SOM pools (compartments (a) and (b) for soil C and N, see text above), one inorganic soil C pool (CO₂) and three inorganic soil N pools (NH₄-N, NO₃-N and volatilised N). Thereby soil C and N processes are interlinked. The extension should be able to describe SOM dynamics for meso ($100 - 10\ 000\ \text{km}^2$) to macro scale (> 10 000 km²) river basins (Becker and Braun, 1999). It should also offer an ability to perform integrated assessments of climate change impacts and land use change (land cover change and recommended management practices, RMPs) impacts on SOM dynamics at the river basin scale.

2.3 Materials and methods

2.3.1 The Soil and Water Integrated Model SWIM

SWIM (Soil and Water Integrated Model, Krysanova et al., 1998) is a continuous-time, spatially distributed model. SWIM works on a daily time-step and integrates hydrology, vegetation, erosion and nutrients (Nitrogen, N and Phosphorus, P) at the river basin scale. The spatial aggregation units are sub-basins, which are delineated from digital elevation data. The sub-basins are further disaggregated into so called hydrotopes, hydrologically homogenous areas. The hydrotopes are defined by uniform combinations of sub-basin, land use and soil type (Krysanova and Wechsung, 2000). The model is connected to meteorological, land use, soil and agricultural management data. For detailed process descriptions and data requirements it is referred to publications by (Krysanova et al., 1998; Krysanova and Becker, 1999; Hattermann et al., 2005a).

The original nitrogen module includes the pools nitrate nitrogen (N-NO₃), active and stable organic nitrogen, and the processes, mineralisation, nitrification, denitrification, plant uptake, input by precipitation, wash-off with surface and subsurface flows, and leaching to groundwater. The nitrogen mineralisation model is a modification of the PAPRAN model (Seligman and Keulen van, 1991).

SWIM has recently been extended for better representation of groundwater dynamics and processes in riparian zones (Hattermann et al., 2004) and forest growth and management impacts on hydrology (Wattenbach et al., 2005). SWIM has been validated for hydrology, vegetation growth, erosion and nitrogen dynamics for river basins according to a multi-scale, multi-site and multi-criteria approach. Verification results for soil temperature, soil water dynamics, comparison of modelled and simulated crop yields and nitrogen dynamics at the plot scale and different site conditions in Germany are summarized in (Post et al., 2005a).

2.3.2 Soil organic matter module extension (SCN)

The soil carbon and nitrogen module (SCN) is based on the tight relationship between soil and vegetation. An input to the soil exists from the accumulation of organic material through above and below ground plant residuals and input of organic fertilizer, which is derived from SWIM. Beside this, there is a withdrawal from the soil of water and nitrogen by vegetation, release of CO₂ into the atmosphere and export of inorganic nitrogen by soil water flows (e.g. leaching into groundwater, lateral flow processes, figure 2.1). Denitrification, plant uptake of N and water, leaching and lateral transport of N and water are calculated within the SWIM model. The carbon and nitrogen turnover are coupled to each other in order to properly describe feedbacks and interactions between them, which highly influence the process of SOM turnover. Thereby soil C turnover provides energy for N turnover and immobilisation of N can slow down C turnover (Franko, 1990). The SCN module considers ammonification and nitrification processes.



Fig. 2.1: Schematic representation of the SOM model extension (SWIM –SCN)

To describe the carbon and nitrogen budget organic matter is differentiated into Active Organic Matter (AOM) and Primary Organic Matter (POM). The latter is separated in to five fractions for each vegetation and crop type. For forest types, for example, the dead plant materials are allocated into stems, twigs and branches, foliage, fine roots and coarse roots. The POM entering soil is calculated for crop types using the crop yield estimates according to an empirical relation for main crop types (Franko, 1990; Franko et al., 1997a), and is then allocated based on literature surveys on harvest residues (above and below ground, (Klimanek, 1987, 1997). For perennial vegetation (forest and grassland types) allocation values from literature are used, which derive POM amounts from biomass growth. Further on standard literature values for C content and C/N ratios in POM fractions, vegetation types and organic fertiliser determine the C and N quantities in the POM fractions (Franko et al., 1997a; Klimanek and Schulz, 1997; Nicolardot, 2001). The fine and coarse roots are further distributed into the soil layers (z) according to rooting depth and a root mass allocation scheme (Jackson et al., 1996).

The carbon and nitrogen turnover into the different pools follows the concept of first order reaction kinetics (Parton et al., 1988; Jenkinson, 1990; Franko et al., 1997b) as shown in figure 2.1. The processes are controlled by substrate specific reaction coefficients.

The dominant process is the carbon mineralization from $C^{i}_{POM}(z,t)$, which provides the energy for the whole turnover of the organic matter. The decomposition of each POM fraction (*i*) is controlled by the fraction specific reaction coefficient $k^{i}_{POM} = k^{i}_{1} + k^{i}_{2}$ (see Figure 2.1) and is described as (with t = time, z = soil layers, i = plant fraction):

$$\frac{\partial}{\partial t} C^{i}_{POM}(z,t) = -k^{i}_{POM} \cdot R_{min}(z,t) \cdot C^{i}_{POM}(z,t)$$

(eq.2.1)

The reduction function R_{min} represents the influence of soil water content, soil temperature and pH-value of each soil layer on the mineralization process (Franko, 1990; Kartschall et al., 1990).

The transformation of primary organic matter $C^{i}_{POM}(z,t)$ to active organic matter $C_{AOM}(z,t)$ is controlled by the synthesis coefficient k^{i}_{SYN} , which is specific to the litter type (plant type and plant fraction) whereas $k^{i}_{I} = k^{i}_{SYN} \cdot k^{i}_{POM}$. The turnover of carbon in active organic matter is made up from the synthesised portion minus the carbon used in the process of mineralization:

$$\frac{\partial}{\partial t} C_{AOM} (z, t) = k^{i}_{SYN} \cdot k^{i}_{POM} \cdot R_{min} (z, t) \cdot C^{i}_{POM} (z, t) - k^{i}_{AOM} (z, t) \cdot R_{min} (z, t) \cdot C_{AOM} (z, t)$$
(eq. 2.2)

How much nitrogen is absorbed into the active organic matter and what proportion is mineralised depends on the C/N ratio of both organic fractions and on the carbon used in the synthesis of the active organic matter. The net mineralization of nitrogen in the primary organic matter is described analogous to eq. 2.1. The change in nitrogen in the active organic matter takes place in a similar way to the turnover of carbon, whereas the C/N ratios of both
organic fractions Q_{pom}^{i} and Q_{aom} modify the synthesis coefficient k^{i}_{SYN} to $k^{''}_{SYN}$ (Franko, 1990; Kartschall et al., 1990).

$$k_{SYN}^{*i} = k_{SYN}^{i} \cdot \frac{Q_{pom}^{i}}{Q_{aom}}$$
(eq. 2.3)

In addition, changes of nitrogen in the reserves of ammonia N_{NH4} and nitrate N_{NO3} are considered. Thus, the net turnover of nitrogen is described by the following system of differential equations (Klöcking, 1991; Grote et al., 1999) for each soil layer:

$$\frac{\partial}{\partial t} N^{i}_{POM}(z,t) = -k^{i}_{POM} \cdot R_{min}(z,t) \cdot N^{i}_{POM}(z,t)$$
(eq. 2.4)

$$\frac{\partial}{\partial t} N_{AOM}(z,t) = k_{SYN}^{*i} \cdot k_{POM}^{i} \cdot R_{min}(z,t) \cdot N_{POM}^{i}(z,t) - k_{AOM}(z,t) \cdot R_{min}(z,t) \cdot N_{AOM}(z,t)$$
(eq. 2.5)

$$\frac{\partial}{\partial t} N_{\text{NH4}}(z,t) = (1 - k_{\text{SYN}}^{*i}) \cdot k^{i}_{\text{POM}} \cdot R_{\text{min}}(z,t) \cdot N^{i}_{\text{POM}}(z,t) + k_{\text{AOM}}(z,t) \cdot R_{\text{min}}(z,t) \cdot N_{\text{AOM}}(z,t) - k_{\text{NIT}} \cdot R_{\text{nit}}(z,t) \cdot N_{\text{NH4}}(z,t)$$
(eq. 2.6)

$$\frac{\partial}{\partial t} N_{NO3}(z,t) = k_{NIT} \cdot R_{nit}(z,t) \cdot N_{NH4}(z,t)$$
(eq. 2.7)

Heterotrophic (substrate induced) soil respiration is calculated through the decay of $C^{i}_{POM}(z,t)$ and $C_{AOM}(z,t)$ pools per day. Root respiration therefore is not considered.

The reduction functions for mineralisation and nitrification r_{min} and r_{nit}, respectively, show the effect of soil water content and soil temperature on these processes (Franko, 1990; Kartschall et al., 1990). Each component is figured in a single function and the product of all three functions forms the following reduction function:

$$\boldsymbol{R}_{i}=\boldsymbol{R}_{i_{W}}\cdot\boldsymbol{R}_{i_{T}}\cdot\boldsymbol{R}_{i_{P}}$$
 , $i=min,$ nit

(eq. 2.8)

The mineralisation is inhibited, if the water content Ws (z,t) decreases below half of the saturated water content W_s^{sat} (z,t).

$$R_{\min_{W}}(W_{S}) = \begin{cases} 4 \cdot \frac{W_{S}}{W_{S}^{sat}} \cdot \left(1 - \frac{W_{S}}{W_{S}^{sat}}\right) &, W_{S} \le 0.5 \cdot W_{S}^{sat} \\ 1 &, W_{S} > 0.5 \cdot W_{S}^{sat} \end{cases}$$
(eq. 2.9)

The influence of soil temperature T_s (t) on the mineralisation is described by van't Hoffs rule (Van't Hoff, 1884):

$$R_{min_{T}} = Q_{10min}^{0.1 \cdot (T_{S} - T_{min}^{opt})}$$

with $Q_{10_{min}} = 2$ and $T_{min}^{opt} = 35^{\circ}C$ (eq. 2.10)

The reduction of nitrification by drought is similar to the reduction of mineralisation, despite the decrease in nitrification under conditions of a very high water content, which results from the deficiency of oxygen.

$$\mathsf{R}_{\mathsf{nit}_{\mathsf{W}}}(\mathsf{W}_{\mathsf{S}}) = 4 \cdot \frac{\mathsf{W}_{\mathsf{S}}}{\mathsf{W}_{\mathsf{S}}^{\mathsf{sat}}} \cdot \left(1 - \frac{\mathsf{W}_{\mathsf{S}}}{\mathsf{W}_{\mathsf{S}}^{\mathsf{sat}}}\right)$$
(eq. 2.11)

The temperature depending reduction function for nitrification is analogous to that for mineralization (see eq. 2.10, 2.11) with optimal temperature value $T^{opt} = 25^{\circ}C$.

2.3.3 Model parametrisation and initialisation

A detailed description of parameterisation and initialisation for processes in SWIM related to hydrology and vegetation growth can be found elsewhere (Krysanova et al., 1998; Krysanova and Wechsung, 2000; Hattermann et al., 2005b; Wattenbach et al., 2005).

Initial organic carbon and nitrogen contents and initial nitrate content have to be provided alongside with land management practices (crop rotation, crop management, and fertilisation). The model was initialised using data for the experimental field sites obtained from the data holder (see table 2.1). For each plot at the Bad Lauchstädt site, initial SOC content was set by simply using the value from 1951 derived from the linear trend of the measured data (1901 – 2002, dotted lines in figure 2.3). At the Müncheberg site, SOC initialisation was done with the first measured value.

The reaction coefficients kⁱPOM and kⁱSYN have to be determined for each plant species (forest types, crop types, grassland types) and primary organic matter fraction (fine roots, coarse roots, twigs and branches, foliage and stems). Determination of these coefficients is mainly done either by field experiments (litter bag experiments) or under laboratory conditions (incubation experiments). The parameters gained through experiments can directly be assigned to the pools and coefficients used in our approach. C/N ratios and C content in plant fresh matter for primary organic matter fractions are derived through literature studies (Franko et al., 1997a; Klimanek and Schulz, 1997; Nicolardot, 2001) and initial soil C/N ratios are derived from soil data.

The reaction coefficient values for agricultural plants (kⁱPOM and kⁱSYN) are deduced from previous studies (Franko, 1990; Franko et al., 1995; Klimanek, 1997; Lettau and Kuzyakov, 1999; Kuzyakov and Domanski, 2000; Nicolardot, 2001). Forest types studies from (Berg and Staaf, 1980a, 1980b; Bergmann et al., 1999) and for grassland ecosystems (Riedo et al., 1998; Riedo et al., 2000) were used. The coefficients kAOM and kNIT are soil and land cover specific and can be found e.g. in different sources (Franko, 1990; Franko et al., 1995; Bergmann et al., 1999).

2.3.4 Data sets and land management scenario

For the testing of the extended model three experimental field sites have been chosen. Sites used for testing decomposition of POM, soil heterotrophic respiration, soil N dynamics and long-term soil C dynamics are described in table 2.1.

To test decomposition of POM, field experiments using mesh bags of Scots Pine (*Pinus sylvestris* L.) needle litter, spring barley and winter wheat straw have been used. Soil heterotrophic respiration has been tested with data obtained from the agricultural experimental field site for cultivation of energy crops (Hellebrand et al., 2003). For the comparison of measured soil respiration with simulated soil heterotrophic respiration, the root/rhizosphere contribution has been subtracted. The value of root/rhizosphere contribution of total soil respiration measurements is based on literature studies and on data analysis of the soil respiration measurements (Hanson et al., 2000; Schlesinger and Andrews, 2000; Raich and Mora, 2005). Using soil respiration measurements during fallow periods or on set-aside field plots allows deriving root/rhizosphere contribution, because root/rhizosphere contribution is limited to the growing season in temperate-zone annual croplands (Raich and Mora, 2005). A value of 75 % contribution of root/rhizosphere respiration for this site was assumed on a yearly basis, not accounting for intra-annual variations.

10cauon (simulation period)	data provider (Reference)	description	fertilisation r <i>eg</i> ine	input data for model simulation
Apelsvoll Research Centre, Division Kise, Norway (800 days)	(Henriksen and Breland, 1999)	Field incubation of Spring barley and Winter Wheat straw, loamy soil		Climate data: Station Nesbyen, approx. 150 km west of the experimental field site (derived from PIK* database), Soil data: (Henriksen and Breland, 1999)
Neu Giobsow, State of Brandenburg, Germany (800 days)	(Bergmann et al., 1999)	Field incubation of <i>Scots Pine</i> needles, loamy-sand soil		Climate data: Station Neuglobsow (derived from PIK* database), Soil data: (Bergmann et al., 1999)
Potsdam - Bornim, State of Brandenburg, Germany (1999 - 2001)	ATB* (Hellebrand et al., 2003)	Soil respiration measurements, sandy soil	150 kg M ha ^{ʻl} yr ^{ʻl}	Climate, soil, management data provided by data holder, Crop rotation: rye – triticale - rye
Bad Lauchstädt, Plot 1 (1951 – 2002)			30 t ha ⁻¹ fresh matter farmyard manure every two years and varying rates of inorganic fertiliser (NPR, amounts	
Bad Lauchstädt, Plot 6 (1951 – 2002)	UFZ* (Körschens and	long-term static fertilizer experiment, soil organic	between 80 and 170 kg N ha ⁻¹ yr ⁻¹) 30 t ha ⁻¹ fresh matter farmyard manure every two years	Climate, soil, management data provided by
Bad Lauchstådt, Plot 13 (1951 – 2002)	Müller, 1996; Franko et al., 2005)	carbon measurements m U-2U cm soil depth, loess soil (chernozem)	received varying rates of inorganic fertiliser (NPK, amounts between 80 and 170 kg N ha ⁻¹ yr ⁻¹)	data holder. Urop rotation: spining battey / potatoes / winter wheat / sugar beet
Bad Lauchstädt, Plot 18 (1951 – 2002)			no fertilisation	
Müncheberg, unfertilised plot (1963 – 2000)	ZALF/FAL* ~~~~	long-term field experiment	no fertilisation	Climate, soil, management data provided by
Müncheberg, fertilised plot (1963 – 2000)	(rogasik and Schroutter, 1999; Rogasik et al., 2004)	v 140, sou organic carbon measurements in 0-25 cm soil depth, sandy soil	 2 (t ha⁻¹ yr⁻¹) or ganic dry matter of farmyard manure to root and tuber crops and various amounts of inorganic fertilisation (162 kg N ha⁻¹ yr⁻¹ on average) 	data noter. Crop rotaton: winter iye, potatoes, winter wheat, sugar beet, spring barley

Table 2.1: Description of experimental sites used for testing SOM model extension

2.3 Material and methods

Table 2.2: Description of crop rotation types, fertilisation regimes and crop residue management practices considered in the

nario label 1: criginal rotation Müncheberg W 2: original rotation Bad Lauchstädt S 3: grain - maize S 3: grain - maize S 5: grain - maize S 6: grain - maize S 7: 4 yrs grain - cover crop P 7: 4 yrs grain - 2 yrs grass F 7: 4 yrs grain - 4 yrs grass F 7: 4 yrs grain - 2 yrs grass F 7: 4 yrs grain - 2 yrs grass F 9: rape - winter wheat C 10: rape - winter wheat N 11: winter wheat - spring barley - cov C 11: winter wheat - spring barley - cov C 11: winter wheat - spring barley - cov C 11: winter wheat - spring barley - cov C 11: winter wheat - spring barley - cov C 11: winter wheat - spring barley - cov C 11: winter wheat - spring barley - cov C 11: winter wheat - spring barley - cov C 11: winter wheat - spring barley - cov C 12: winter wheat S
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Testing of long-term SOC dynamics and main recommended management practices (RMP) impacts on SOC dynamics have been done at the plot scale for Bad Lauchstädt and Müncheberg experimental field sites (see table 2.1). The simulation setup is described in table 2.2. The long-term influence of diverse crop rotations and cover crops, fertiliser management (organic and inorganic) and addition of harvest surplus on SOC dynamics on the two sites (Müncheberg and Bad Lauchstädt) were chosen from the set of RMPs.

For crop rotations and cover crop impacts ten typical crop rotations have been created. Impact of fertilisation regimes is demonstrated with the different fertilisation regimes in place at the experimental field sites (see table 2.1). For the harvest surplus simulation the original crop rotations have been considered, whereas the amounts of residuals for the grain crops have been manipulated (see table 2.2). At the Bad Lauchstädt site, every two years a grain crop was present, and hence every two years the respective amounts of straw residues were added. At the Müncheberg site on average every three years (since 1975 every two years) a grain crop was present. Average management practices at the field sites involved a more or less total export of grain straw residuals together with the harvested corn.

2.3.5 Statistical criteria for model evaluation

For a quantitative assessment of simulation results with observed data, detailed frameworks have been proposed (Addiscott and Whitmore, 1987; Loague and Green, 1991; Smith et al., 1996; Smith et al., 1997b). Here we use the root mean squared error, *RMSE*, (Loague and Green, 1991), the sample correlation coefficient, r, (Draper and Smith, 1966) and the relative error, E, (Addiscott and Whitmore, 1987) for a statistical assessment, all of which are described in Smith et al. (1997b). The *RMSE* is a measure of coincidence between measured and simulated values and indicates how closely the simulated values match the measured ones. To assess consistency of errors, the relative error (E) can be used to assess if the model is biased to either over or underestimation (Smith et al., 1997b). The sample correlation coefficient r gives information whether the shape of plotted simulated values is similar to the measured one (Smith et al., 1996).

2.4 Results

2.4.1 Testing of soil organic matter processes

In respect to SOM dynamics testing of decomposition of primary organic matter, soil heterotrophic respiration, soil N and long-term soil organic C dynamics is given here.

Decomposition

Decomposition of Scots Pine (*Pinus sylvestris* L.) needles as representative of forest type decomposition and decomposition of spring barley straw and winter wheat straw residues for agricultural species is shown in figure 2.2.



Fig. 2.2: Simulated decomposition of winter wheat, spring barley straw and needle litter (Scots Pine). Measured values from mesh bag experiments were adopted from Henriksen and Breland (1999) and Bergmann et al. (1999)

For spring barley straw and winter wheat straw residues, modelled decomposition fits with observed data and the mass loss of C within 800 days is correctly represented. For Scots Pine needle early stage decomposition is not reflected accurately (first 200 days, ref. figure 2.2), but in the long run mass loss of C in Scots Pine needles by decomposition is met by the simulation.

Primary Organic Matter	n	RMSE	Ε	r
Spring barley straw	13	4.9	- 1.5	0.99
Winter Wheat straw	12	4.2	0.6	0.99
Scots Pine needles	7	9.4	- 5.1	0.94

Table 2.3: Representation of statistics describing the model performance of POM decomposition

n = numer of values

In general, simulation of the crop primary organic matter decomposition (winter wheat and spring barley straw) performed better than Scots Pine needle decomposition. This is reflected by the higher r values and lowers RMSE (table 2.3). The values of E are close to zero for the crop types, which indicates low bias in the simulation. Values for r are between 0.94 and 0.99 and hence a high association between simulated and observed values for both forest and crop types is achieved.

Heterotrophic soil respiration

Simulated soil respiration is compared to measurements obtained from the ATB experimental field site (see table 1 for description) and to values cited in literature for measurement sites in Germany (table 2.4).

Simulated soil heterotrophic respiration on cropland (rye – triticale – rye) based on annual sums is met reasonably compared to measurements in the years 1999 – 2001 at the ATB field experimental site (table 2.4).

The year 1999 at the ATB site shows the weakest agreement. This year was a warm and dry year where especially the influence of soil temperature and soil moisture dynamics could not be mirrored correctly by the model. The simulated years 2000 and 2001 delivered an acceptable agreement with the measured annual sums.

The annual soil respiration values cited in literature for deciduous and evergreen forest ecosystems including different soil and climate conditions in temperate zones match well to simulated values. The simulated values for deciduous and evergreen forest are derived from long-term simulations in the Elbe river basin (Central Europe).

Land cover	SR [gC m ⁻² yr ⁻¹] simulated	SR [gC m ⁻² yr ⁻¹] measured	Reference
Crop – Triticale	300 (2000)	250 (2000)	ATB measurements, see table 2.1
Crop – Rye	275 (1999) 250 (2001)	211 (1999) 236 (2001)	ATB measurements, see table 2.1
Forest deciduous	100 – 375	147 292 710	Trüby (2000) Beyer (1991) (Buchmann, 2000))
Forest evergreen	300 - 525	475 - 663	(Beyer, 1991) Granier et al (2000)

Table 2.4: Simulated yearly soil respiration (SR) values for three land cover types compared with literature cited values and measurements

Long-term soil C dynamics

Tests were performed for two plots at the Müncheberg site (figure 2.3 c) and for four plots at Bad Lauchstädt (figure 2.3 a and 2.4 b, plots 1, 6, 13, 18). Fertilisation regimes of the plots are described in table 2.1.

Measured soil carbon contents (0-20 cm) have increased for plots 1 and 6 and have remained practically constant on plots 13 and 18 during the period of 1902 to 2002. The Müncheberg site shows no trend for the fertilised plot with a soil carbon content (0-25 cm) remaining at the same level (figure 2.3 c). The unfertilised plot at Müncheberg shows a decreasing content of soil carbon.



(continues on next page)



Fig. 2.3: Measured and simulated values of total soil organic carbon at Bad Lauchstädt for (a) plot 6 (receiving 30 t ha⁻¹ farmyard manure every two years) and plot 18 (no fertilisation) and (b) plot 1 (receiving 30 t ha⁻¹ farmyard manure every two years and various amounts of inorganic fertilisation) and plot 13 (receiving various amounts of inorganic fertilisation) and for Müncheberg experimental site (c) for a plot receiving no fertilisation and a plot receiving 1.2 [t ha⁻¹ a⁻¹] organic dry matter of farmyard manure to root and tuber crops and various amounts of inorganic fertilisation (162 kg N ha⁻¹ a⁻¹ on average). Lines in (a) and (b) are showing the simulation, dots the measured values with standard deviation bars and dotted lines the long-term linear trend in the measurements

	Field site	Ν	RMSE	Ε	R
a)	fertilised plot	16	8.9	3.9	0.17
a)	unfertilised plot	16	7.1	-2.01	0.81
b)	plot 1	20	9.1	0.02	0.35
b)	plot 6	20	8.6	-0.29	0.36
b)	plot 13	20	11.9	2.04	-0.33
b)	plot 18	20	8.9	-0.07	-0.31

Table 2.5: Representation of statistics describing the model performance in simulating soil carbondynamics for the Müncheberg experimental site (a) and Bad Lauchstädt long-term static fertilisationexperiment (b)

n = numer of values

The simulated soil organic carbon (SOC) contents of the four Bad Lauchstädt plots generally agree with the measured data as do the simulations for the Müncheberg site. The simulations could reproduce well the impacts of organic fertilisation on SOC dynamics. The simulated values lie between the standard error of most of the measured data. The long-term trends in measured SOC contents (dotted lines in figure 2.3 a and b) are met by the simulations, except for plot 13 at Bad Lauchstädt, which show a slightly decreasing trend in the simulation (figure 2.3 b). Statistical analysis shows that *RMSE* values are in the same range as for most of the models used in a soil organic matter model comparison at the Bad Lauchstädt site (Smith et al. 1997b). A low *E* value for all plots indicates that no consistent errors are present in the simulations (table 2.5).

Problems occurred at the Bad Lauchstädt site for plot 13, where the simulation shows a decreasing trend whereas the measurements remain more or less constant. Regular applications of inorganic fertiliser (NPK) seem to stabilise the SOC content at this site. The simulation could not represent this process sufficiently. Inorganic fertilisation effects on crop productivity are not represented correctly, at least for the Bad Lauchstädt site conditions.

2.4.2 Effects of land management practices on long-term SOC trends

A quantification of long-term SOC trends of diverse crop rotations, inclusion of cover crops, fertilisation regimes and crop residual management for the Müncheberg and Bad Lauchstädt sites is given here.

The effect of inorganic and organic fertilisation can be seen in figure 2.4. The extended model properly reflects the influences of organic fertilisation on long-term SOC development. Application of organic fertilisation in form of e.g. farmyard manure generally increases SOM with time. Inorganic fertilisation enhances crop growth and is important for SOM decomposition and mineralization because of nutrient supply for soil organisms.

An increasing SOC content due to organic fertilisation can be stated for the Bad Lauchstädt site in the measurement and in the simulation with an increase from 2.1 % C_{org} in 1951 to 2.3 % C_{org} in 2001 (+ 5.2 t C ha⁻¹ for the simulation period of 51 years, corresponding to a rate of + 0.1 t C ha⁻¹ y⁻¹, figure 2.3 b, plot 1). Plot 6 receiving only organic fertilizer shows an increasing C_{org} content from 2.1 to 2.25 % C_{org} (3.99 t C ha⁻¹ in 51 years and +0.078 t C ha⁻¹ y⁻¹,

figure 2.3 a). At the Müncheberg site organic fertilization resulted in a stabilization of SOC (figure 2.3 c).

Inorganic fertilisation alone does not result in an increase of SOC, but a stabilised SOC content for the Bad Lauchstädt site can be stated for the measurements, not adequately reflected by the simulation. No application of fertilisers results in a decrease of SOC contents at both sites, varying between 0.2 % Corg loss for Bad Lauchstädt and 0.12 % Corg loss for the Müncheberg site.

To simulate the impact of diverse crop rotations and the inclusion of cover crops, a set of typical rotational systems have been established for the two sites (figure 2.4 a and b). Note that for these simulations no fertilisation and standard residual management (as on the original rotations) was assumed to describe the pure effect of diverse cropping systems and cover crops.

For both sites, the behaviour of respective rotations is similar in the long-term trend (figure 2.4 a, b). Following table 2.6 the rotations number 1 to 6, 9, 11 and 12 are losing SOC at an annual rate between -0.013 and -0.0007 t C / ha.

Rotations with root crops (potatoes and sugar beet) and no cover crops in between, and hence a fallow soil period in the rotations, show a decreasing trend in SOC content over the respective years (numbers 1, 2, 3, 5 in table 2.5). Rotations with grain crops and no cover crops (numbers 9, 11 in table 2.5) also show a decrease in SOC over time, but the trend is less pronounced. Inclusion of cover crops in grain – root and grain rotations (numbers 4, 6, 10 in table 2.5) lead to a stable SOC content over time at both sites (figure 2.4 a, b). Rotations including ley-arable use (number 7 and 8 in table 2.5) have an increasing trend in SOC. The 4 years grain and two years ley-arable rotation increased the SOC content over the simulated time period of about 1.6 t C ha⁻¹ (51 years simulation period) at the Bad Lauchstädt site and 1.0 t C ha⁻¹ (37 years simulation period) at the Müncheberg site. The rotation with four years of ley-arable use and two years grain crops resulted in a simulated increase of 2.5 t C ha⁻¹ (51 years simulation period) at the Müncheberg site.



Fig. 2.4: Impacts of crop rotations and cover crops on long-term SOC dynamics [% Corg] for the Bad Lauchstädt (a) and the Müncheberg (b) experimental site. The numbers refer to crop rotations explained in table 2.2

Number	Crop rotation	Cumulative SOC per	[t C ha ⁻¹ simulation iod ⁻¹]	Incremental SC	oC [t C ha ⁻¹ yr ⁻¹]
	4	Müncheberg	Bad Lauchstädt	Müncheberg	Bad Lauchstädt
-	original rotation Müncheberg	- 4.96	1	- 0.13	:
7	original rotation Bad Lauchstädt	;	- 4.6	:	- 0.09
ŝ	grain – maize	- 3.75	- 3.2	- 0.01	- 0.06
4	grain – maize – cover crop	- 1.02	- 0.035	+0.0027	- 0.0007
5	grain – root	- 4.6	- 5.9	- 0.127	- 0.4
9	grain – root – cover crop	- 2.12	- 1.25	- 0.057	- 0.02
5	4 yrs grain -2 yrs grass	+ 1.0	+ 1.6	+0.027	+0.03
8	2 yrs grain - 4 yrs grass	+2.63	+ 2.5	+0.071	+0.05
6	rape – winter wheat	- 4.33	- 4.45	- 0.11	- 0.087
10	rape – winter wheat – cover crop	- 1.96	+0.41	-0.053	+0.008
11	winter wheat – spring barley	-3.38	- 2.72	- 0.091	- 0.053
12	winter wheat - spring barley - cover crop	- 0.93	- 0.28	- 0.025	- 0.0054
13	harvest surplus – 2 t straw ha ⁻¹	- 3.7	- 3.1	- 0.1	- 0.06
14	harvest surplus – 5 t straw ha ⁻¹	- 1.5	+ 1.39	- 0.04	+ 0.027
15	harvest surplus – calculated	- 2.5	+1.38	- 0.07	+ 0.027
16	fertilisation, Bad Lauchstädt, plot 1	:	+5.2	:	+ 0.1
17	fertilisation, Bad Lauchstädt, plot 6	ł	+ 3.99	1	+ 0.078
18	fertilisation, Bad Lauchstädt, plot 13	1	- 3.74	:	- 0.07
19	fertilisation, Bad Lauchstädt, plot 18	ł	- 4.6	ł	- 0.09
20	fertilisation, Müncheberg, unfertilised	- 4.96	ł	- 0.13	ł
21	fertilisation, Müncheberg, fertilised	+ 0.3	1	+0.008	1

Table 2.6: Changes in SOC content for the simulation period (cumulative) and the yearly increment of change for the different crop rotations, grain . The start of the start sites dodonii Maitada Citablication diff. مناطنين



Fig. 2.5: Impacts of grain straw addition on long-term SOC dynamics [% Corg] for the Bad Lauchstädt (a) and the Müncheberg (b) experimental site. The numbers refer to grain straw additions explained in table 2.2

The influence of post harvest residual management is demonstrated with three simulation runs considering input of 2 t ha⁻¹ (minimum value for straw residues, table 2.2), 5 t ha⁻¹ straw (maximum value for straw residues) and the calculated amounts of straw residuals to each grain crop (on average 4.73 t C ha⁻¹ for Bad Lauchstädt and 3.45 t C ha⁻¹ for Müncheberg site). The simulations were done for the original rotations (table 2.2) without fertilisations.

Figure 2.5 a and b shows the effect of straw incorporation on long-term SOC dynamics for Bad Lauchstädt and Müncheberg repectively. At both sites the original rotations show a decreasing trend of SOC contents and the inclusion of 2 t ha⁻¹ straw resulted in a lower decrease. Incorporating 5 t ha⁻¹ straw residuals and the calculated amount of straw residuals resulted in a clear increase in SOC contents at the Bad Lauchstädt site of about 0.027 t C ha⁻¹ y⁻¹ (figure 2.5 a). For the Müncheberg site a slightly decreasing trend of -0.04 t C ha⁻¹ y⁻¹ when incorporating 5 t ha⁻¹ straw residuals and -0.07 t C ha⁻¹ y⁻¹ considering the model calculated amount can be stated. The simulated effects of long-term trend are in general agreement to findings on experimental studies cited in literature (Freibauer et al., 2004; Körschens et al., 2004).

2.5 Discussion

2.5.1 Soil organic matter module

The proposed model integration uses a fairly simple and coupled description of soil C and N turnover processes using a multi-compartment model on the basis of first order reaction kinetics.

Influence of soil temperature, soil moisture and soil pH (where soil pH data are available) on turnover processes are described using established turnover process reduction functions (Van't Hoff, 1884; Stanford and Smith, 1972; Rodrigo et al., 1997). The extension can be assigned to a multi-compartment process-based model (using two SOC pools and three SON pools) and is not explicitly assigning a passive or inert soil organic matter pool with residence times of $10^2 - 10^3$ years. The main reason is that measurement of passive or inert pool sizes are largely unavailable, and simulation runs are usually done for 10 - 50 years only. Using empirical functions as proposed by e.g. Falloon et al. (1998) considering soil textural parameters (mainly clay content) could be integrated, but assessing changes in soil organic matter due to land use / cover changes and climate changes considers time frames of 50 to 100 years (Paustian et al., 2000; Desjardins et al., 2005). Soil C sequestration strategies are referring

to timeframes of around 30 years with an emphasis on maintaining the conducted measures in the long-run as a climate change mitigation tool (e.g. (Smith et al., 2000; Lal, 2004a; Smith, 2004). Therefore an explicit modelling of a stable / inert soil C pool (with turnover times of \geq $10^2 - 10^3$ years) was excluded. The reduction to two soil C pools additionally has the advantage that the pools can directly be referred to observations in field experiments and laboratory experiments.

The decomposition of POM is considered with up to 5 different plant fractions with intrinsic decomposition properties. This allows distinguishing not only different plant species but also different biological and chemical resistance of plant fractions due to their chemical composition (C/N ratio of plant fractions). A different treatment of e.g. stems, twigs and branches, foliage, coarse roots or fine roots in forest ecosystems, or stubble, straw and roots in e.g. croplands is therefore ensured. Further on coarse and fine roots are distributed with soil depth as is the case for above-ground residuals for croplands according to tillage depth (same is true for inorganic and organic fertiliser application). Mineralization properties of SOC are differentiated for the humus layer (grassland and forest ecosystems) or ploughing layer in agro-ecosystems and mineral layers to consider different mineralization properties with soil depth.

The new model extension exhibits a similar level of complexity as other process descriptions in SWIM and is robust in parameterisation for meso- to macro-scale river basins. Through the integration of SOM processes into SWIM an integrated assessment of water quantity, water quality and crop productivity issues alongside with SOM dynamics can be assessed at the river basin scale. The integration of matter fluxes in semi-closed systems (river basins) offers the opportunity to assess ecosystem services and the behaviour of ecosystem function and their interrelations at the regional scale. This allows the reactions of SOM dynamics under different land use strategies and climate change to be assessed in an integrated way.

2.5.2 Testing of soil organic matter processes

The main processes for SOM turnover have been tested for environmental conditions in Central Europe using field experimental sites and literature values. Simulation of decomposition of POM, soil heterotrophic respiration and long-term SOC dynamics show reliable performance in respect to observed data and values cited in literature. Important factors influencing SOM processes like soil temperature, soil moisture dynamics and vegetation growth (crop growth) can be modelled satisfactory (Post et al., 2004; Post et al., 2005a).

Decomposition of POM showed reliable temporal behaviour for the selected plant species (spring barley and winter wheat straw, Scots Pine needle litter). For all main crop types and plant fractions values from incubation and field experiments have been derived, which enable a correct representation of decomposition. Beside the turnover coefficient (rate constant) for POM decomposition (kⁱ_{pom}), the correct representation of the amount of Cⁱ_{POM} entering the C_{AOM} pool (the synthesis coefficient kⁱ_{syn}) is important. Looking at soil heterotrophic respiration values offers a good proof for the representation of kⁱ_{syn}. The annual comparison of soil heterotrophic respiration simulation at the ATB field plot and for values cited in literature reasonably agree with the measurements.

The exact quantification of root/rhizosphere respirations is problematic in comparison of measured total soil respiration with simulated heterotrophic soil respiration. Therefore, the addition of the root/rhizosphere respirations contribution to simulated soil heterotrophic respiration, based on literature values and estimation with soil respiration measurement during bare soil periods introduces a high degree of uncertainty. Additionally the assumption of a constant root/rhizosphere contribution throughout the year is very general, but for comparisons on a yearly basis it seems justified. Due to root growth, priming effects (Kuzyakov et al., 2000), soil water and temperature dynamics the contribution of root/rhizosphere respiration is temporally dynamic. But the aim is not to accurately represent the temporal dynamics of all soil respiration sources (all environmental and biological factors) at this stage. One feasible way to improve the quantification of root/rhizosphere respiration in temperate zones croplands is a recently published method by

Raich and Mora (2005) or by Kutsch and Kappen (1997). Raich and Mora (2005) proposed to use measurements of total soil respiration and soil temperature as input to derive root/rhizosphere contribution to total soil respiration. Incorporating one of these methods would improve the robustness of soil respiration simulations in terms of seasonable dynamics. Additionally recent findings suggest that looking on both pathways of soil respiration (soil heterotrophic respiration and root/rhizosphere respiration) is necessary to quantify impacts of climate change (especially considering higher soil temperatures) on soil CO₂ efflux to the atmosphere (Kätterer et al., 1998; Kuzyakov, 2002; Fang et al., 2005a; Knorr et al., 2005).

To test capabilities of the extended model to simulate soil N and long-term SOC dynamics, two experimental field sites have been evaluated in this respect (chapter 3).

Soil C and N processes have to be considered in a coupled way, because soil C turnover provides energy for N turnover and immobilisation of N can slow down C turnover processes considerably (Liu et al., 2005). Therefore a correct representation of soil N dynamics in respect to temporal dynamics, plant uptake effects, fertilisation effects and lateral/vertical movement is necessary (chapter 3). The extended model showed adequate performance for soil N dynamics at the plot scale for the Müncheberg and Bad Lauchstädt site and is comparable to the original SWIM soil N module performance (chapter 3). The original soil N module was successfully tested and applied for water quality modelling and assessment of diffuse source pollution in river basins (Krysanova and Becker, 1999; Hattermann et al., 2005a; Post et al., 2005a). One advantage of the extended model is the consideration of the ammonification process, which might be neglected in agro-ecosystems, because residence times of ammonia in cropland soils, which are not under anaerobic conditions, is very short. This makes a verification of this process very difficult. But for forest ecosystems and riparian zones/wetlands consideration of this process becomes more important.

The simulated long-term C dynamics, proved on two long-term experimental field experiments under various fertilisation regimes, provided a good agreement to the measured long-term trend. The results obtained with extended SWIM model show similar performance as other soil organic matter models compared on the same sites in a model inter-comparison study (Smith et al., 1997b). Important is the calculation of correct amounts of plant residues (POM) entering the soil, which is seldom measured. The uncertainty in the amount of POM substance to decomposition and the allocation to plant fraction with intrinsic decomposition behaviour is a crucial point. The empirical formulation proposed by (Franko, 1990; Franko et al., 1995) to calculate crop residues using simulated crop yields for major crop types provides reliable calculations of these amounts. The calculated amounts for each crop type are in a general agreement with e.g. analysis of measured crop residual returns to soil conducted by (Klimanek, 1987, 1990a, b) for central Europe.

The described test shows that the SWIM extension to model SOM dynamics can correctly represent decomposition, mineralization, soil heterotrophic respiration, soil N and long-term SOC dynamics under various site conditions.

2.5.3 Effects of land management practices on long-term SOC trends

Land management practices are influencing SOM processes and different sets of recommended land management practices (RMPs) can increase SOM content, which is beneficial in respect to soil fertility and soil C sequestration opportunities e.g. (Smith et al., 2000; Freibauer et al., 2004; Lal, 2004a; Rees et al., 2005; Singh and Lal, 2005). Lal (2004a) stated that the potential soil C sequestration (through land use conversions or RMPs) of managed ecosystems approximately equals the cumulative historic C loss. Therefore it should be possible to enhance SOM contents in managed ecosystems through the implementation of appropriate management strategies. Beside others, Smith et al. (2000) and Freibauer et al. (2004) present a list of measures for increasing soil carbon stocks in agricultural soils with estimates of potentially soil carbon sequestration rates. Next to conservation agriculture, measures like perennial grasses and permanent crops, set-aside, deep rooting crops, application of animal manure and sewage sludge, improved rotations, fertilisation and extensification are proved to offer a potential for soil carbon sequestration, but the underlying estimates incorporate high uncertainties. Inorganic fertilisation does not lead to an increase in SOC in our assessment. Neither the measurements of plots receiving only inorganic fertiliser nor the conducted simulation show an increase. The stabilisation of SOC content due to inorganic fertilisation measured at the Bad Lauchstädt site however shows that enhancement of crop growth due to application of inorganic fertiliser leads to a higher input of harvest residues and may lead to a stabilisation. Effects of organic fertilisation in terms of application of farmyard manure could be successfully reproduced by the model.

Crop rotation impacts on long-term SOC contents might either be beneficial or unfavourable in terms of increasing SOC storage. The simulation of 12 different crop rotations shows that root crops (potatoes, sugar beet) and rotations with long fallow periods show a clear decrease of SOC content at both field sites (- 0.4 to -0.05 t C ha⁻¹ yr⁻¹, table 2.6). This is in accordance with values cited in (Körschens et al., 2004; Körschens et al., 2005), where humus supplies of a crop rotation is calculated on the base of coefficients accounting for the demand of different crops and the compensation of humus by organic fertilizers. Thereby sugar beet and potatoes possess highest humus demands (-760 to -1300 kg humus C ha⁻¹ yr⁻¹), followed by silage maize (-560 to -800 kg humus C ha⁻¹ yr⁻¹) and grain crops (-280 to -400 kg humus C ha⁻¹ yr⁻¹). According to their findings inclusion of ley-arable use, cover crops, straw incorporation account for an increase of around 80 to 600 kg humus C ha⁻¹ yr⁻¹. Simulated inclusion of cover crops resulted in a stable SOC content in the respective time periods. Extensive agricultural production using rotations including two or four years of ley-arable use lead to an increase of 0.02 to 0.07 t C ha⁻¹ y⁻¹. Values from a 37 year experiment in Norway for a three years grain and three years root crop rotation show a decrease of SOC of around 0.078 t C ha⁻¹ y⁻¹ (Singh and Lal, 2005). On the same site a four years grain and two years ley-arable rotation led to an increase of 0.11 t C ha⁻¹ y⁻¹ and two years grain and four years ley-arable to an increase of 0.35 t C ha⁻¹ y⁻¹.

Simulated influences of different sets of crop rotations presented here show the capabilities of adjusted crop use in rotations to increase or stabilise SOC contents in soils. The long-term tendencies of SOC dynamics in the simulations are in general agreement with values

cited in literature and show the model capabilities to quantify crop rotational effects on soil C balance.

Considering incorporation of grain straw residues an increase in simulated SOC content in a magnitude reported in literature (Smith et al., 2000; Freibauer et al., 2004; Körschens et al., 2004) can be stated. As straw residuals can also be used as biofuel or animal food, a total incorporation of straw residues into top soils is seldom. However, in terms of enhanced soil conditions (supply of organic material to increase SOM contents), it is a noticeable measure. Incorporation of all grain straw produced would sequester C at an annual rate of + 0.03 to +0.09 t C ha⁻¹ in comparison to the original rotations in place.

The simulations show the effects of some RMPs for enhancing SOM content in agricultural soils. With the extended model effects of fertilisation, crop rotations and harvest residual returns on SOC development can be quantified. The assessment of side effects (e.g. Nitrate leaching into surface and groundwater) by not properly adapted fertilisation can be considered as well. When applied at the river basin scale different sets of land use and management scenarios and their impacts on water availability, water quality and SOM can be assessed.

In a next step effects of spatially distributed crop rotation schemes and possible changes in crop shares (and hence changes in crop rotation distribution) under future policy assumptions on SOM dynamics will be assessed based on the successful verification and simulation experiments considering some RMPs presented in this study.

2.6 Conclusions

The extension of the eco-hydrological river basin model SWIM for the assessment of SOM dynamics provides reliable simulation results for decomposition of POM, soil heterotrophic respiration and long-term soil C development in comparison to measurements at three experimental field sites and literature studies. The field sites represent different climatic and edaphic conditions and agricultural management practices.

The extension provides a coupled description of soil N and C processes using a processbased multi-compartment approach following first order reaction kinetics. The chosen SOM extension fits into the overall model complexity of SWIM, is robust in model parameterisation using literature cited parameter values and distinguishes SOM pools which relate to measurable quantities.

Mass C loss of POM (decomposition) alongside with heterotrophic soil respiration could be described correctly in terms of temporal dynamics and magnitudes of these processes. Annual soil heterotrophic respiration ranges of literature values for croplands and forest ecosystems could be met by the extended model. A model improvement to better estimate root / rhizosphere contribution to total soil respiration though seems necessary to assess seasonal temporal dynamics and could be implemented using strategies proposed e.g. by (Kutsch and Kappen, 1997; Raich and Mora, 2005).

Simulated long-term soil organic C trends at two field sites under different fertilisation regimes and crop rotations fit good with observed SOC values. In this respect the proposed model extension delivers similar performance as other SOM models used in a model intercomparison study on same datasets (Smith et al., 1997b).

Investigations of different fertilisation, crop rotation and crop residual impacts on longterm SOC dynamics presented in the simulation study show the possibility to adapt management strategies to increase SOC contents, which are beneficial in terms of soil fertility and soil C sequestration potentials. Simulated reactions in long-term SOC trends of these RMPs are in agreement with findings in field experiments described in literature. Judicious use of crop rotation types, fertilisation and additional input of harvest surplus to soils (e.g. grain straw incorporation) lead to SOC increases of around 0.1 t C ha⁻¹ yr⁻¹ at the two field sites. Reducing the period of fallow soils through the use of cover crops, using more crop types in rotational systems, reducing the share of root crops in rotations or extensification by ley-arable use or other set-aside strategies improve soil fertility and SOC contents.

Effects of combination of these sets of management practices on SOM dynamics, vegetation growth, water quality issues (N pollution of water bodies) and water quantity issues

can now be assessed in an integrated way. In a next step a river basin scale assessment regarding impacts management practices on SOM dynamics can be performed.

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Chapter 3

Evaluation of water and nutrient dynamics in soilcrop systems using the eco-hydrological catchment model SWIM (Soil and Water Integrated Model) *

Keywords: *agro-ecosystems, eco-hydrological modelling, plot scale evaluation, crop growth, soil temperature, soil hydrology, soil carbon, soil nitrogen*

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Abstract: An assessment of water and nutrient dynamics in soil - crop systems for different climatic, edaphic, land management practices and time scales requires an integrated modelling framework and a thorough testing of relevant processes and their interactions, which is presented here. The eco-hydrological river basin model SWIM (Soil and Water Integrated Model), recently extended by a process-based, multi-comportment model for soil organic matter turnover (coupled soil nitrogen and carbon turnover), was evaluated against observations on soil temperature, soil hydrology, crop growth, soil nitrogen and long-term soil carbon dynamics for different site conditions in eastern Germany. The successful, integrated representation of water and nutrient dynamics under documented site conditions is a pre-requisite to perform integrated assessments of global change impacts on agro-ecosystems at the regional scale.

3.1 Introduction

Regional scale dynamic environmental modelling investigating the impacts of regional environmental change requires modelling systems that are able to simulate the relevant processes adequately under the constraints of moderate data availability and model parameterisation. A possibility to assess the impact of regional environmental change and management practices on ecosystem dynamics is the use of integrated, process-based ecohydrological catchment models, which are spatially distributed and operate at time steps appropriate for the natural processes described.

Catchments integrate many forces, including land use and climate, fluxes of water, nutrients and pollutants (Krysanova and Becker, 1999). An integrated consideration of hydrological processes, vegetation dynamics, biogeochemical cycles and interactions between these quantities driven by soil, climate, land use and land management information is therefore necessary to assess regional environmental change and the consequences thereof. One prerequisite for the application of regional scale environmental models is a successful evaluation against observed data. Agro-ecosystems are highly altered ecosystems through human interactions and are of high importance in both providing nutrients for humans and being a source of environmental pollution. In this context coupled modelling of soil temperature and water dynamics, crop growth and yield, soil nitrogen and carbon transformations and transport in lateral and vertical dimensions can be useful to assess agro-ecosystem dynamics and their impacts on the environment.

This paper describes the results of the model evaluation exercise during the international workshop "Modelling water and nutrient dynamics in soil-crop systems" at the Leibniz-Centre for Agricultural Landscape Research (ZALF) e. V. Müncheberg, Germany in June 2004. In the frame of this workshop, observed data for soil temperature, soil hydrology, soil nitrogen contents, crop yield and long-term soil organic matter dynamics have been provided for three sites in Germany (Bad Lauchstädt in Saxony-Anhalt, Müncheberg in Brandenburg and Berlin) representing different crop rotations, fertilisation regimes, soil management, soil types and climatic conditions. This comprehensive dataset of documented site conditions offers the opportunity to test the model capability in simulating relevant processes and interactions between them on the field scale and on different time scales for agro-ecosystems. Important in assessing soil organic matter turnover is a coupled representation of soil C and N processes, as C turnover provides the energy for N processes and soil N immobilisation delay C turnover, beside the effect of soil N availability on plant growth (Liu et al., 2005; Russell et al., 2005; Torn et al., 2005).

The Soil and Water Integrated Model SWIM (Krysanova et al., 1998) was used in this model evaluation exercise. It was developed mainly for meso- to macro scale (100 – 100 000 km²) catchment modelling of water quality, water quantity and vegetation growth (e.g. crop yield) assessments under the control of land use, land management and climate (Krysanova et al., 1998, 1999, 2000; Wechsung et al., 2000; Hattermann et al., 2004). In this context a comprehensive field scale evaluation of relevant processes is fundamental. But it has to be mentioned that SWIM was not designed to be used as a field scale agro-ecosystem model for crop yield prediction or a farm scale fertilisation recommendation tool. SWIM was developed for regional environmental change assessment

and therefore the relevant processes and interactions have to be represented in the correct magnitudes and with correct temporal behaviour under the various agricultural management practices relevant at that scale.

Testing ecosystem behaviour under documented site conditions is fundamental to assessing ecosystem behaviour under hypothesized conditions (Grant, 2001). Based on a successful evaluation, useful information on questions related to soil C sequestration and soil quality, soil nutrient and water uptake by plants, soil nutrient loss and water quality issues, soil disturbance and land management impacts on ecosystem can be gained through the application of ecosystem models (Grant, 2001).

3.2 Materials and Methods

3.2.1 Experimental sites

The datasets provided by the workshop organisers are described in full detail for the Müncheberg plots in (Mirschel et al., 2005), for the Bad Lauchstädt plots in (Franko et al., 2005) and for the Berlin datasets in (Diestel et al., 2005). Here we provide an overview of the datasets used for simulation with SWIM (table 3.1) and a general description on the experimental field sites used (table 3.2). For details on measurement techniques, agricultural management practices and experimental setup we have to refer to the citations given in table 3.2. Our aim was to provide an integrated model evaluation by including soil temperature, soil water, soil nitrogen and carbon and crop growth dynamics rather than focusing on a single process. Therefore we present here representative examples for each process for all three measurement sites.

3.2.2 Model description

SWIM (Soil and Water Integrated Model, Krysanova et al. (1998) is a continuous-time, spatially-distributed model. SWIM works on a daily time step and integrates hydrology, vegetation, erosion, nutrients (nitrogen, N and phosphorus, P) and sediment fluxes at the river basin scale (figure 3.1). The spatial aggregation units for river basin modelling are subbasins, which are delineated from digital elevation data. The subbasins are further disaggregated into so called hydrotopes, hydrologically homogenous areas. The hydrotopes are delineated by overlaying of subbasin, land use and soil maps (Krysanova et al., 2000). The model is connected to meteorological, land use, soil and agricultural management data (figure 3.1). For detailed process descriptions, validation studies and data see (Krysanova et al., 1998, 1999, 2000). An extensive hydrological multi-scale and multi-criterial validation of the model in the Elbe basin (Germany) including sensitivity and uncertainty analyses is described in Hattermann et al. (2005b). The relevant processes for the presented work are described briefly.

Field site	Plot	Time frame	Soil temperature	Soil hydrology	Crop yield	N dynamics	C dynamics
	plot 1	6 maara		\checkmark	√	√	—
Muencheberg	plot 2	o years	\checkmark	✓	✓	√	_
	plot 3		•	✓	✓	✓	—
	crop rotation	4 years	✓	\checkmark	\checkmark	\checkmark	\checkmark
Bad	black fallow		_	\checkmark	—	\checkmark	\checkmark
Lauchstaedt	Plot 1	100		_	✓	_	\checkmark
	Plot 6	years,	_	—	✓	_	✓
	Plot 13	51 years	—	—	✓	_	✓
	Plot 18	simulated	_	—	√	_	✓
Donlin	1-4		•	\checkmark	_	_	—
Jeinii -	5-10	3 years	•	\checkmark	_	_	—
Lysineter	11-12	-	•	\checkmark	_	_	_

 Table 3.1: Overview of simulated sites and processes used for model evaluation.

✓ simulated, – no measurement, ● not simulated

The hydrology module is based on the water balance equation, taking into account precipitation, evapotranspiration, percolation, surface runoff and subsurface runoff for the soil column, which is subdivided into several layers according to the soil database (figure 3.1). The water balance for the shallow aquifer includes ground water recharge, capillary rise to the soil profile, lateral flow, and percolation to deep aquifer (Krysanova et al., 1998).

The Priestley–Taylor (Priestley and Taylor, 1972) or Penman – Monteith (Monteith and Unsworth, 1990) methods are used (depending on input data availability) to estimate the potential evapotranspiration. Soil evaporation and plant transpiration are calculated as functions of leaf area index (LAI) using the approach of Ritchie (Ritchie, 1972).

Surface runoff is calculated using a modification of the Soil Conservation Service (SCS) curve number technique. Water, which has infiltrated into the soil, percolates through the soil layers using a storage routing technique (Arnold et al., 1990). The water percolated from the bottom soil layer is defined as groundwater recharge (Hattermann et al., 2004). Lateral subsurface flow or interflow is calculated simultaneously with percolation using a cinematic storage model. Interflow occurs in a given soil layer, if the soil layer below is saturated.

Soil temperature is calculated on a daily basis at the centre of each soil layer. The calculation is based on an empirical relationship between daily average, minimum and maximum air temperature and a damping factor for soil depth. The effect of current weather conditions and land cover (snow, above ground biomass) are considered (Krysanova et al., 2000; Neitsch et al., 2002).

The module representing crops and natural vegetation is an important interface between hydrology and nutrients (figure 3.1). A simplified EPIC approach (Williams et al., 1984) is included in SWIM for simulating arable crops (like wheat, barley, rye, maize, potatoes), using specific parameter values for each crop type. The model uses a concept of phenological crop/plant development based on daily accumulated heat units, according to Monteith's approach (Monteith, 1977) for potential biomass, water, temperature and nutrient stress factors and harvest index for yield partitioning.

Experimental field site	data provider (Reference)	plots presented in paper	site conditions	fertilisation regime	input data for model simulation
Berlin - Dahlem, Berlin, Germany, 52° 28' N and 13° 18' E (1996 – 1999)	Technical University of Berlin (Diestel et al., 2005)	lysimeters 9, 10: shallow groundwater table at 135 cm soil depth; lysimeters 11, 12 deep groundwater table at 210 cm soil depth	Soil: Eutric Cambisol (FAO) Climate: mean annual air temperature: 9.3 °C, mean annual precipitation sum: 545 mm	No fertilization	Climate, soil, management data provided by data holder, land cover. lawn
Müncheberg, State of Brandenburg, Germany, 52° 52′ N and 14° 7 E (1993 – 1998)	ZALF* (Rogasik et al., 2004; Mirschel et al., 2005)	plot 3	Soil: Eutric Cambisol (FAO) Climate: mean annual air temperature: 8.5 °C, mean annual precipitation sum: 531 mm	various amounts of ammonium urea solution, ammonium nitrate lime, farmyard manure (amounts differ in all years)	Climate, soil, management data provided by data holder. Crop rotation: phacelia, sugar beets, winter wheat, winter barley, winter rye
Bad Lauchstädt, State of Saxony- Anhalt, Germany, 51° 24' N and 11052' E. Anort tane 6414	UFZ* UFZ*	crop rotation plot	Soil: Haplic Chemozem (FAO) Climate: mean annual air	Calcium-Ammonium-Mitrate amount differs for all years, organic fertilisation with harvest residuals every 2 years	Climate, soil, management data provided by data holder. Crop rotation: sugar beets, spring barley, potatoes, winter wheat
(1998 – 2002) (1998 – 2002)	Franko et al., 2005)	black fallow plot	temperature: 8.7 °C, mean annual precipitation sum: 483.8 mm	No fertilization	Climate, soil, management data provided by data holder. Field tilled from time to time to remove weeds
		Bad Lauchstädt, Plot 1 (1951 – 2002) Ded Tambér de Proce	Soil: Haplic Chemozem	30 t ha ⁻¹ fresh matter farmyard manure every two years and varying rates of inorganic fertiliser (NPK, amounts between 80 and 170 kg N ha ⁻¹ yr ⁻¹)	
bad Lauchstadt, State of Saxony- Anhalt, Gernany, 51° 24' N and 11° 53' E, long-term static	UFZ* (Körschens and Müller, 1996; Eccels of el 2005)	Dad Laucinstadt, Flot o (1951 - 2002) Dad T conchate A Dict 12	(FAO) Climate: mean annual air temperature: 8.7 °C, mean	30 t ha ¹ fresh matter farmyard manure every two years	Climate, soil, management data provided by data holder. Crop rotation: spring barley / potatoes /
(1902 – 2002)	LIAHKO EL AL., 2000)	(1951 – 2002)	annual precipitation sum: 483.8 mm	received varying rates of inorganic fertiliser (NPK, amounts between 80 and 170 kg M ha ⁻¹ yr ⁻¹)	winter wheat / sugar beet
		Bad Lauchstädt, Plot 18 (1951 – 2002)		no fertilisation	
* ATB - Leibniz-Institute of Agric Research. Leiozig/Halle. Germany:	ultural Engineering Bomim, Germ PIK – Potsdam Institute for Clima	any; ZALF - Leibniz-Centre ate Impact Research Potsdar	: for Agricultural Landscape and m. Germany: FAL – Federal Ag	d Land Use Research, Müncheberg, Germany, UFZ – (d cultural Research Gentre Braunschweig Germany	Centre for Environmental

Table 3.2: Description and site conditions of experimental sites used for model evaluation.



Fig. 3.1: Flow chart of the SWIM model, integrating hydrological processes, crop / vegetation growth, nutrient (nitrogen, N and phosphorus, P) dynamics and soil carbon turnover.

The original nitrogen module includes the following pools: nitrate nitrogen (N-NO₃), active (No-ac) and stable (No-st) organic nitrogen, organic nitrogen in the plant residue (Nres) and the processes: mineralization, denitrification, plant uptake, fertilisation, input by precipitation, wash-off with surface and subsurface flows and leaching to groundwater (figure 3.1). The nitrogen mineralization model is a modification of the PAPRAN mineralization model (Seligman and Keulen van, 1991). Mineralization of fresh organic nitrogen and active organic nitrogen pool depends on the C:N ratio, soil temperature and water content. Denitrification occurs only under the conditions of oxygen deficit and is described as a function of soil water content, soil temperature, organic matter content and mineral nitrogen content. Plant uptake of nitrogen is estimated using a supply and demand approach. The daily plant demand of nutrients is estimated as the product of biomass growth and optimal concentration in the plants. Actual nitrogen uptake is the minimum of supply and demand. The plant is allowed to take nutrients from any soil layer that has roots. The main purpose of the nitrogen module within SWIM is to assess catchment scale water quality

issues like nitrate pollution of groundwater and surface water bodies under regional environmental change.

A process-based, multi-compartment module for the turnover of soil organic matter was recently extended by integrating the soil organic matter module of the forest growth model 4C (Grote et al., 1999; Lasch et al., 2002) into SWIM. This module describes the coupled soil carbon and nitrogen turnover.

The soil carbon (C) and nitrogen (N) turnover is based on the tight relationship between soil and vegetation processes. On the one hand an input exists into the soil by addition of organic material and on the other hand there is a release of CO₂ into the atmosphere. To describe the C and N budget organic matter is differentiated into Active Organic Matter (AOM) as humus pool and Primary Organic Matter (POM) as litter pool. The latter is separated in up to five fractions for each vegetation and crop type as stems, twigs and branches, foliage, fine roots and coarse roots.

The C and N turnover into different pools is represented by first order reaction kinetics (Parton et al., 1987; Franko, 1990; Jenkinson, 1990; Chertov and Komarov, 1997). The C and N change in the primary organic matter pool is controlled by matter (plant type) and plant litter fraction specific reaction coefficients, which control the rate of turnover. The transformation of primary organic matter to active organic matter pools is controlled by a matter (plant type) and plant litter fraction specific synthesis coefficient. The turnover of active organic matter is made up from the synthesised portion and the amount used in the process of mineralization driven by the mineralization coefficient. How much nitrogen is absorbed into the active organic matter and what proportion is mineralised depends on the C/N ratio of both organic fractions and on the carbon used in the synthesis of the active organic matter. Pland N uptake, lateral and vertical transport of N and denitrification is connected to the related process formulations in SWIM (see above). In contrast to the original soil N module, changes of nitrogen in the reserves of ammonia N-NH4 and nitrate N-NO₃ are considered separately. The C and N turnover is influenced by soil water content, soil temperature and pH-value of each soil layer through standard reduction functions (Franko, 1990; Kartschall et al., 1990).
3.2.3 Model parameterization and initialisation

It is beyond the scope of this paper to provide a full description on input data and parameterisation necessary to run the model. Except for the recently extended description for soil organic matter turnover, a detailed description of SWIM including all information on necessary input data and model parameterisation can be found in (Krysanova et al., 2000). Any changes from standard model parameterisations are provided in the respective sections.

Main parameters necessary for soil parameterisation relevant to soil hydrological processes are soil textural information (percentages of clay, silt and sand), bulk density, soil porosity, available water capacity, field capacity and saturated soil conductivity. If saturated soil conductivity is not specified, it is calculated by standard pedotransferfunctions (e.g. Genuchten Van, 1980; Rawls and Brakensiek, 1985). These data should be available for the entire layered soil profile. Related to soil C and N processes, initial organic carbon and nitrogen contents and initial nitrate content have to be provided with agricultural management practices (crop rotation, crop management, fertilisation). General information was provided for the three field sites under study, for which necessary soil parameters have been assigned from standard soil science textbooks or the standard configuration in SWIM for the respective soil type has been used.

The model parameterisation for soil organic matter turnover was done to simulate the relevant processes for agro-ecosystems under eastern German conditions. Therefore related environmental studies in the region and literature were used for parameterisation. Determination of main parameters and coefficients was mainly done either by field experiments (litter bag experiments) or under laboratory conditions (incubation experiments) cited in literature. Main source of these parameters are for agricultural plants investigations by (Franko, 1990; Klimanek, 1990 a, b; McGechan and Wu, 2001).

3.2.4 Statistical evaluation

One way to evaluate model simulation is by visual / graphical comparison of the simulation values produced by the model with actual measured values from the field experiments. Besides this qualitative way of assessing the goodness of the simulation, a statistical assessment of the residuals (the differences between the observed and the simulated values) was performed. Addiscott and Whitmore (1987) stated that using one statistical method alone to quantify the discrepancy between model simulations and measured data can be misleading. It is hence necessary to use a set of statistical methods to determine common strengths and weaknesses in the simulation through distinct statistics to describe different aspects of the accuracy of the simulation (Smith et al., 1996). Therefore we adopted a quantitative method described by Smith et al. (1996, 1997b).

As most observed data are without replicate measurements, we considered altogether eight statistical methods, seven as proposed in the statistical procedure described in (Smith et al., 1996) and the modelling efficiency index (IA) (Willmott, 1982). Table 3.3 provides an overview of the applied statistics and the respective references. Each of these statistics provides a partial insight into model performance. By balancing different aspects of the used statistics allows an appropriate evaluation of model performance.

The RMSE (root mean square error) provides a term for the total difference between the predicted and the observed values. The lower limit is 0, which indicates no difference between measured and simulated values (table 3.3). The modelling efficiency (EF) value compares the variance of predicted from the observed values to the variance of the observed values from the mean of the observations. A value of 1 denotes a perfect match of predicted and measured values. The coefficient of determination (CD) is a measure of the proportion of the total variance in the observed data that is explained by the predicted data (table 3). A value of 1 again indicates a perfect fit. RMSE, EF and CD are measures to prove how closely the simulated values correspond to the measured values and therefore assess the coincidence of two data sets (Smith et al., 1996).

METHOD	NAME	EQUATION	PERFECT FIT [RANGE]	PURPOSE OF METHOD	REFERENCE
RMSE	Root mean square error	$\sqrt{\sum_{i=1}^{n} \left(P_{i} - O_{i}\right)^{2}/n}$	$0 [0:+\infty]$		(Loague and Green, 1991)
EF	Modeling efficiency	$\frac{\left[\sum\limits_{i=1}^{n}\left(O_{i}-\overline{O}\right)^{2}-\sum\limits_{i=1}^{n}\left(P_{i}-O_{i}\right)^{2}\right]}{\sum\limits_{i=1}^{n}\left(O_{i}-\overline{O}\right)^{2}}$	+1 [-∞ : +1]	Total difference and Coincidence between measured and simulated	(Smith et al., 1996)
CD	Coefficient of determination	$rac{\sum\limits_{i=1}^{n}\left(O_{i}-\overline{O} ight)^{2}}{\sum\limits_{i=1}^{n}\left(P_{i}-\overline{O} ight)^{2}}$	+1 [0 : +∞]	values	(Loague and Green, 1991)
E	Relative error	$\frac{100}{n}\sum_{i=1}^n \frac{(O_i - P_i)}{O_i}$	[∞+ : ∞-] 0	Consistency of errors	(Addiscott and
Μ	Mean difference	$\sum_{i=1}^{n} \frac{(O_i - P_i)}{n}$	0 [-∞ : +∞]		Whitmore, 1987)
t(m)	T value of M with critical 2.5% levels (two-tailed)	$\frac{M}{S_d/\sqrt{n}}$		Student's t statistic of M	(Chatfield, 1983)
IA	Modelling efficiency index	$1 - \frac{\sum_{i=1}^{n} (P_i - O_i)^2}{\sum_{i=1}^{n} \left(\left P_i - \overline{O} \right + \left O_i - \overline{O} \right \right)^2}$	+1 [0 : +1]	Measure of agreement between measured and simulated values	(Willmott, 1982)
r	Sample correlation coefficient	$\frac{\sum\limits_{i=1}^{n}\left(O_{i}-\bar{O}\right)\cdot\left(P_{i}-\bar{P}\right)}{\sqrt{\sum\limits_{i=1}^{n}\left(O_{i}-\bar{O}\right)^{2}}\cdot\sqrt{\sum\limits_{i=1}^{n}\left(P_{i}-\bar{P}\right)^{2}}}$	1 [-1 : +1]	Association between simulated and measured values	(Draper and Smith, 1966)
O _i = observed (i measures are th	measured) values, $P_i = predicte$ e respective measurement units	d (simulated) values, \overline{O} = mean of observed v	alues, $\overline{P} = mean$ of predicte	d values, $n=$ number of samples;	Units of the statistical

Table 3.3: Overview of statistics used in the model evaluation procedure.

The sample correlation coefficient (r) and the modelling efficiency index (IA) are measures of the association of two datasets, i.e. the similarity of the shape of plotted simulation values in respect to measured values. A value of 1 for both statistical methods indicates a perfect fit and the same pattern of observed and simulated values.

The relative error (E) and the mean difference (M) are indicators for the bias in the total difference between simulations and measurements. They can be used to assess consistent or inconsistent errors in the simulations in respect to observations. Values of 0 for both indicate a perfect fit between simulation and measurements. The significance of the coherency between simulation and observation can further be tested using Student's t of M. Although it has to be mentioned that using student's t test in this context fails for testing if measured and simulated values are related since they are not completely independent (i.e. calibration of simulations regarding observations, Smith et al., 1997b). Here we test if the simulations and measurements values differ significantly from each other using a two-tailed 2.5 % significance measure.

3.3 Results and discussion

3.3.1 Soil temperature

Soil temperature was simulated at the Bad Lauchstädt site for two soil depths (20 cm and 50 cm) and at the Müncheberg site at 5 and 20 cm soil depths over a period of eight years for the Müncheberg site and six years for the Bad Lauchstädt site. Simulation was performed on a daily basis for the two sites. In general the simulated soil temperature compared satisfactory with the measured data (figure 3.2), especially for the present purpose of soil temperature as an reduction factor for soil carbon and nitrogen turnover.



(continues on next page)



Fig. 3.2: Measured and simulated values of soil temperature for (a) Müncheberg, plot 3, 20 cm, (b) Müncheberg, plot 3, 50 cm, (c) Bad Lauchstädt, crop rotation, 5 cm and (d) Bad Lauchstädt, crop rotation, 20 cm soil depth.

It can be noted that near soil surface simulation of soil temperature performed better than deeper soil depths, which is expressed in lower IA values and higher RMSE values for deeper soil depths (table 3.4). SWIM uses a relatively simple formulation mainly driven by daily average, minimum and maximum air temperature and a damping factor for soil depth, which is dependent upon the bulk density and the soil water content. The influence of plant canopy or snow cover on soil temperature is incorporated with a weighting factor, which is dependent on total aboveground biomass and residues, on the water content and on the snow cover on the current day. This is not a physically based description of soil heat fluxes and results in higher daily fluctuations of the simulations and decreasing goodness of simulation with soil depth compared to the measurements (figure 3.2).

For the Müncheberg plot problems occurred mainly in spring and autumn seasons, where the sandy soil is warming or cooling quicker than soils with higher clay contents. Simulations are not representing this properly, resulting in a significantly biased simulation for the Müncheberg plot at 20 cm soil depth, where t values of M were greater than the critical two tailed 2.5% t value (table 3.4). For the 50 cm soil depth this effect was the strongest, resulting in the lowest association between measured and simulated values (lowest r value of 0.87 of all simulations, table 3.4).

Field site	RMSE	Ε	Μ	t(m) *	t _{crit.}	EF	CD	IA	r
a) 20 cm	3.3	- 14.1	0.81	2.9 **	1.98	0.85	1.75	0.94	0.94
b) 50 cm	3.9	- 57.4	0.61	1.61	1.98	0.69	2.82	0.87	0.87
c) 5 cm	3.1	- 19.6	- 0.02	- 0.09	2.0	0.93	1.39	0.96	0.97
d) 20 cm	3.0	- 41.9	-0.26	-0.96	2.0	0.91	1.46	0.95	0.97

Table 3.4: Representation of statistics describing the model performance in simulating soil temperaturefor a) Müncheberg, plot 3, 20 cm, b) Müncheberg, plot 3, 50 cm, c) Bad Lauchstädt, crop rotation, 5 cm,d) Bad Lauchstädt, crop rotation, 20 cm soil depth.

* t-value, critical at 2.5% (two-tailed)

** significantly biased

The problems described here can partly be solved through calibrating the damping (for soil depth) and weighting (for land cover) factor used in the soil temperature description separately for the black earth and sandy soil. This would lead to a better representation of the measurements and the respective conditions (e.g. current plant cover, soil heat properties) at the two sites but the described discrepancies are seen to be negligible for the purpose of soil temperature as a reduction factor for soil carbon and nitrogen turnover and soil temperature impacts on water movement.

3.3.2 Soil water content

Soil moisture simulations have been performed for all three Müncheberg plots (only plot 3 is shown here), for the two short-term Bad Lauchstädt plots, one representing a crop rotation and one black fallow plot (the latter is not shown) and for the Cambisol soil Lysimeter at the Berlin site (lysimeter 9 - 12).

Different techniques have been applied for measuring soil moisture contents at various depths. The most reliable and accurate measurements are seen to be the gravimetric measured soil moisture contents. Additional techniques used were Tensiometer measurements, Field Domain Reflectometers (FDR) and Time Domain Reflectometers (TDR) measurements. For the Bad Lauchstädt sites three replicate measurements using FDR instruments were conducted. Standard deviations between replicate measurements varied

between 0.7 (Vol. %) and 2.6 (Vol. %) for the crop rotation. At the Müncheberg sites gravimetric measurements were available for comparison with simulations.

Figure 3.3 shows comparisons of soil moisture dynamics for Müncheberg, plot 3 (figure 3.3 a), for Bad Lauchstädt at the crop rotation site (figure 3.3 b) at two soil depths and for the Berlin site the Lysimeters 9 - 12 (0 - 90 cm soil depth) representing a Cambisol soil for different groundwater distances (135 cm and 210 cm) as representative examples over all simulations.

The temporal dynamics and magnitudes of volumetric soil water contents at different soil depths are seen to be reliable represented by the simulations. Important to note is that interactions with soil water uptake by plants and with meteorological variables (precipitation and climatic water balance) are distinguishable and represented by the simulations (and the measurements). The general pattern of these mechanisms is met by the simulations (figure 3.3).

Discrepancies in the above-mentioned patterns (representation of plant water uptake, climatic water balance influences) are most pronounced for the Bad Lauchstädt comparisons. Here the simulations show the influence of plant water uptake and water stress to be too great due to a negative climatic water balance (figure 3.3 b, left and right). In times of plant water uptake during the growing season and of negative climatic water balance an underestimation of soil moisture is seen. The strong underestimation for the 90 cm soil depth plot is likely to be due to an insufficient representation of root water uptake and the assignment of maximal rooting depth as an input parameter. Using a standard maximal root depth parameter for the specific crops as proposed by e.g. Breuer et al. (2003) or Krysanova et al. (2000), might not be the appropriate value for the present soil type and properties. A calibration of this parameter would lead to a better representation but that was not the scope of this exercise. Additionally water uptake by roots is overestimated for deeper soil depths (see figure 3.3 b, right).



Fig. 3.3: Description on next page

black dots gravimetric measurements of soil water content) and (c) Berlin Lysimeter 9 and 10 for 135 cm groundwater distance (affected by	groundwater) and Lysimeter 11 and 12 for 210 cm groundwater distance (not affected by groundwater) on a Cambisol soil. Black lines are Lysimete	measurements and grey lines are the respective simulations for 0 – 90 cm soil depth. At the secondary axis values for precipitation [mm] (left) and	climatic water balance [mm] (right) for the Müncheberg site (a) and Bad Lauchstädt site (b) are shown. For Berlin (c) only climatic water balance	[mm] is given.
Lauchstädt crop rotation plot for 45 cm (left) and 90 cm (right) soil depth (grey lines are simulations, black lines TDR or FDR measurements and	Lauchstädt crop rotation plot for 45 cm (left) and 90 cm (right) soil depth (grey lines are simulations, black lines TDR or FDR measurements and black dots gravimetric measurements of soil water content) and (c) Berlin Lysimeter 9 and 10 for 135 cm groundwater distance (affected by	Lauchstädt crop rotation plot for 45 cm (left) and 90 cm (right) soil depth (grey lines are simulations, black lines TDR or FDR measurements and black dots gravimetric measurements of soil water content) and (c) Berlin Lysimeter 9 and 10 for 135 cm groundwater distance (affected by groundwater) and Lysimeter 11 and 12 for 210 cm groundwater distance (not affected by groundwater) on a <i>Cambisol</i> soil. Black lines are Lysimeter	Lauchstädt crop rotation plot for 45 cm (left) and 90 cm (right) soil depth (grey lines are simulations, black lines TDR or FDR measurements and black dots gravimetric measurements of soil water content) and (c) Berlin Lysimeter 9 and 10 for 135 cm groundwater distance (affected by groundwater) and Lysimeter 11 and 12 for 210 cm groundwater distance (not affected by groundwater) on a <i>Cambisol</i> soil. Black lines are Lysimeter measurements and grey lines are the respective simulations for 0 – 90 cm soil depth. At the secondary axis values for precipitation [mm] (left) and	Lauchstädt crop rotation plot for 45 cm (left) and 90 cm (right) soil depth (grey lines are simulations, black lines TDR or FDR measurements and black dots gravimetric measurements of soil water content) and (c) Berlin Lysimeter 9 and 10 for 135 cm groundwater distance (affected by groundwater) and Lysimeter 11 and 12 for 210 cm groundwater distance (not affected by groundwater) on a <i>Cambisol</i> soil. Black lines are Lysimeter measurements and grey lines are the respective simulations for 0 – 90 cm soil depth. At the secondary axis values for precipitation [mm] (left) and climatic water balance [mm] (right) for the Müncheberg site (a) and Bad Lauchstädt site (b) are shown. For Berlin (c) only climatic water balance
	black dots gravimetric measurements of soil water content) and (c) Berlin Lysimeter 9 and 10 for 135 cm groundwater distance (affected by	black dots gravimetric measurements of soil water content) and (c) Berlin Lysimeter 9 and 10 for 135 cm groundwater distance (affected by groundwater) and Lysimeter 11 and 12 for 210 cm groundwater distance (not affected by groundwater) on a <i>Cambisol</i> soil. Black lines are Lysimeter	black dots gravimetric measurements of soil water content) and (c) Berlin Lysimeter 9 and 10 for 135 cm groundwater distance (affected by groundwater) and Lysimeter 11 and 12 for 210 cm groundwater distance (not affected by groundwater) on a <i>Cambisol</i> soil. Black lines are Lysimeter measurements and grey lines are the respective simulations for $0 - 90$ cm soil depth. At the secondary axis values for precipitation [mm] (left) and	black dots gravimetric measurements of soil water content) and (c) Berlin Lysimeter 9 and 10 for 135 cm groundwater distance (affected by groundwater) and Lysimeter 11 and 12 for 210 cm groundwater distance (not affected by groundwater) on a <i>Cambisol</i> soil. Black lines are Lysimeter measurements and grey lines are the respective simulations for 0 – 90 cm soil depth. At the secondary axis values for precipitation [mm] (left) and climatic water balance [mm] (right) for the Müncheberg site (a) and Bad Lauchstädt site (b) are shown. For Berlin (c) only climatic water balance



For this case the root water uptake description might not be appropriate. The plant water use is estimated using the approach of Williams and Hann (1972), which is driven by the plant water transpiration rate. It is parameterised assuming that about 30% of the total water use comes from the top 10% of the root zone. Simulated soil moisture for the uppermost layer (not shown) is overestimated, indicating that for this case the model has to allow more water to be taken by the plants in these layers. Another factor at the Bad Lauchstädt site is the high loess content of the black earth soil, which causes problems assigning soil physical properties. This is due to the fact, that loess soils have an inherent high variability of soil physical properties like available field capacity or soil porosity. Using general soil parameterisation and pedotransferfunctions (e.g. Genuchten Van, 1980; Rawls and Brakensiek, 1985) are one source of errors in simulating this site. Studies by (Hattermann et al., 2004) using SWIM showed that uncertainties in simulating river discharge in loess regions are highest compared to mountain or lowland regions. This is mainly due to difficult loess soil parameterisation (e.g. soil physical properties), high amounts of macro pores in loess soils and high variability of soil physical properties derived from laboratory measurements.

Consequently simulation performance was weaker at the Bad Lauchstädt plot than the Müncheberg and Berlin plot having higher RMSE values and lower values for IA (except Müncheberg, 90 cm soil depth) and CD (table 3.5). CD values at the Müncheberg plots are close to one or higher, which denote that the deviation of the simulations from the mean of the observed values is less than observed in the measurements, i. e. the model describes the measured data better than the mean of the measurements (Smith et al., 1996). The CD values for the Bad Lauchstädt site lie between 0 and 1, indicating that the deviation of the simulations from the mean observation is greater than observed in the measurements (Smith et al., 1996). This points to problems with model parameterisation presumably related to the above mentioned loess soil properties.

In consideration of the more reliable gravimetric soil moisture measurements at the Müncheberg site, the simulated soil water dynamics performed well. The temporal dynamics are more or less consistent with low bias (M) and good association (r values between 0.6 and

0.75, table 3.5). The effects of plant water uptake and climatic water balance are better represented. The sandy soil leads to higher soil water dynamics than the Bad Lauchstädt soil, which is satisfactory reflected by the simulation.

Table 3.5: Representation of statistics describing the model performance in simulating soil water contents for a) Müncheberg Plot 3 with respective soil depths, b) Bad Lauchstädt crop rotation with respective soil depths, c) Berlin Lysimeter 9,10 (135 cm groundwater depth) and 11,12 (210 cm groundwater depth), *Cambisol* soil.

Field site	RMSE	Ε	М	t(m) *	t _{crit.}	EF	CD	IA	r
a) 30 cm	2.7	0.3	0.53	0.86	2.14	0.54	1.7	0.82	0.75
a) 60 cm	3.6	3.5	0.93	1.55	2.13	0.26	2.2	0.72	0.60
b) 45 cm	5.6	-1.9	-0.47	-0.82	2.01	0.69	0.5	0.54	0.18
b) 90 cm	5.3	1.8	0.28	0.47	2.01	0.58	0.4	0.81	0.27
e) 135 em	3.2	2.2	0.23	0.96	2.03	0.54	0.7	0.58	0.83
c) 210 cm	1.4	3.9	0.42	1.8	2.03	0.42	0.6	0.92	0.81

* t-value, critical at 2.5% (two-tailed)

The Berlin site shows a similar goodness of simulations in respect to measurements like the Müncheberg simulations. For lysimeters 9 and 10 which are affected by groundwater (distance of 135 cm, figure 3.3 c, left) the simulation overestimate the measurements. The simulations further show higher soil water content as for lysimeters 11 and 12 with no groundwater influence (distance of 210 cm, figure 3.3 c, right). Higher soil water content for groundwater influenced sites can be expected beforehand, but is not mirrored by measurements (figure 3.3 c). The overestimation is also expressed in a higher RMSE value for groundwater influenced lysimeters (table 3.5 c). The consistency of this error (the overestimation) is mirrored in low values of E and M, which are close to zero. This indicates a systematic bias, either in the measurements or in the simulation. For the 210 cm groundwater distance lysimeter (11 and 12) the simulations fit well to the measurements (figure 3.3 c, left and right). The general course of simulated soil water dynamics, influenced by climatic water balance and plant water uptake, reflects the dynamics in the measurements. This site shows lowest RMSE values and highest IA of 0.92 and a high r value of 0.81 (table 3.5 c).

3.3.3 Crop yields

The performance of the crop growth model was evaluated using measured crop yields - as an indirect measure for crop growth - for the long-term and short-term field plots at Bad Lauchstädt and the field plots at Müncheberg.

The growth cycle of a plant in SWIM is controlled by plant attributes summarized in the plant growth database (Krysanova et al., 2000; Neitsch et al., 2002) and by the timing of operations listed in the management file. The exact dates of sowing, harvesting and other management practices provided have been implemented into the management routines of SWIM. Related parameters remained unchanged and are set accordingly as for regional impact studies, described e.g. in Krysanova et al., 1998 and 2000. According to Williams et al. (1984) crop growth is mainly driven by solar radiation and adjusted daily considering for plant stress factors (water, temperature, nitrogen and phosphorous) using a simplification of the EPIC crop model. Therefore crop growth and consequently yield simulations are seen to reflect mainly climatic and soil hydrological effects.

For the short-term assessments, the simulations are satisfactory comparing to the measurements. IA and r-values are highest for all comparisons and M values range around 13 (12.6 for the Bad Lauchstädt site and –13.6 for the Müncheberg site, table 3.6 c and a), indicating a mean difference of 13 dt ha⁻¹ for both sites. Although showing considerable differences, the simulation can be evaluated as satisfactory. On one hand the simulations have not been calibrated by adjusting the harvest index or other relevant parameters, on the other SWIM is not designed as a plot scale yield prediction model. Points which need further consideration is a better representation of nutrient influences on crop growth, for long-term studies an introduction of a time dependent harvest index, which reflects technical improvements (improving seed / sort quality) and a higher sensitivity of crop growth on soil properties. As it can be seen in figure 3.4 (a and b) the levels of crop yield in the simulations are less distinctive than in the measurements. The higher soil fertility of the Bad Lauchstädt plot, resulting in general higher crop productivity than the sandy soil at the Müncheberg site is not sufficiently mirrored in the simulations.



Fig. 3.4: Measured and simulated values of crop yield for (a) Müncheberg plot 3, (b) Bad Lauchstädt crop rotation plot and (c) Bad Lauchstädt long-term (plot 1) for winter wheat.

For the long-term picture at the Bad Lauchstädt site, simulations are poor compared to a year-to-year comparison (figure 3.4 c). The average yields however can be met fairly well. In the measurements a clear trend of increasing yields can be seen (figure 3.4 c, dotted black line) which should be probably assigned to technical and management improvements in agriculture during the last 50 years, especially in improving seed quality, higher efficiency of fertilisation and in increasing the harvested plant part in comparison with shoots of a crop. SWIM allocates harvest from total biomass using a harvest index, which is crop specific but doesn't change with time. Thus the technological improvements can currently not be mirrored in the simulations (grey dotted line in figure 3.4 c). Only climatic constraints are influencing crop growth in the simulations. Therefore a direct comparison with measured total biomass and an appropriate representation of technical and management advances in agriculture within the model would be necessary for a long-term assessment at the plot scale. An adjusted harvest index considering technical and management improvements over time would have increased the goodness of the simulations, but correct parameter values are difficult to obtain. Not considering these facts, the long-term comparison shows a low IA value for winter wheat (table 3.6 b).

Table 3.6: Representation of statistics describing the model performance in simulating crop yield for a)Müncheberg plot 3, b) Bad Lauchstädt long-term plot only for winter wheat yields, c) Bad Lauchstädt,
short-term crop rotation plot.

Field site	RMSE	Ε	Μ	t(m) *	t _{crit.}	EF	CD	IA	r
a)	19.1	-28.4	-13.6	-2.25	2.57	0.49	0.93	0.85	0.86
b)	17.3	-8.3	-0.2	-0.04	2.18	0.08	16.9	0.36	0.28
c)	23.4	6.8	12.6	1.42	2.57	0.65	1.63	0.87	0.88

* t-value, critical at 2.5% (two-tailed)

3.3.4 Soil nitrogen dynamics

Temporal dynamics of soil nitrogen contents have been evaluated at two sites. For the Müncheberg plots, results are shown for plot 3 in figure 3.5 (a) and table 3.7. Plots 1 and 2 led to similar results and are not shown here. Plot 3 consists of a sugar beet / winter wheat / winter barley / winter rye rotation starting 1993. Before each rotation phacelia was grown and ploughed under as green manure. Various amounts of inorganic and organic fertilisation have been applied, for a detailed description see (Mirschel et al., 2005). Results are shown for the years 1993, 1994 and 1995 because in this period most measurements were available providing a sufficient basis to perform an appropriate evaluation. Additionally results are shown for 0 - 90 cm soil depth, not considering layers 0-30, 30-60 and 60-90 cm here. Evaluation of soil nitrate concentrations for the Bad Lauchstädt site is shown for the shortterm crop rotation and for the black fallow plot in the compartments 0-20 cm at two sampling dates per year (1998 – 2002, figure 3.5 b and c). The crop rotation consists of winter barley, winter wheat, sugar beet, spring barley, potato, and winter wheat starting 1997. Various amounts of organic manure and mineral N fertiliser have been applied (for details see (Franko et al., 2005). For both sites, the mineral N contents of each soil layer with which the model was initiated were estimated from the measurements. Sowing, harvesting, fertilisation etc. during the model run are on the same dates as those in the field experiments.

Soil N was simulated using the original N module and the newly implemented soil organic matter turnover module (coupled soil N and C processes), whereas both are compared with respective measurements.

For both simulations nitrate contents for plot 3 (Müncheberg) rose following each inorganic fertilisation to comparable levels in the measured data, except for October 1993 where an ammonium urea solution was applied (figure 3.5 a). This did not directly effect nitrate contents, because the solution entered the soil as ammonia and was then transformed to nitrate resulting in increasing nitrate content thereafter, which is more pronounced for the SCN module simulation (figure 3.5 a). The simulated values generally agree with the observation in the correct pattern and magnitudes. The value of CD is greater than 1 (1.8 and 16.1 for the original and the SCN module respectively, table 3.7 a), indicating that the

variation in the observed values is higher than in the simulated values. This means that either the model is not adequately describing extreme values or the experimental measurements are erroneous.

The high value in June 1993 is most likely a measurement error. Under these instances the high RMSE and the high negative E value have to be interpreted. Occurrences of extreme values enlarge E (and RMSE) in a way that does not truly reflect the accuracy of the simulation and should thus be excluded for interpretation. A low M value (0.03 and 1.8, table 3.7 a) and an IA value of 0.48 and 0.38 however indicate a low bias of the simulation.

For the crop rotation field experiment (Bad Lauchstädt) a similar quality of simulation performance can be stated for both simulations as for the Müncheberg plot. Inorganic fertiliser application led to a rapid increase in nitrate concentration in the simulations. But the correct order of magnitude could not be evaluated as measurements at these times are missing. Apart from that, both models correctly represent the general course of nitrate dynamics. The organic fertilisation (November 1999, see figure 3.5 b) is not resulting in a rapid increase of nitrate concentration in the simulation because the main form is ammonium being either transformed to nitrate, washed-out or taken up by the plants or is subject to decomposition. IA of the original module is higher (0.83) than the SCN module (0.5), but both are indicating a good association of simulated and measured values. Notable is the low r value of 0.14 for the SCN module compared to 0.74 for the original module (table 3.7 b). The total difference between the simulated and the measured values is between 2.0 and 4.3 (RMSE, table 3.7 b) and EF value is positive indicating a low coincidence between simulations and measurements for the original module. With M values close to zero (-0.11 and 1.77) it can be stated that no consistent errors are within both model representations.



Fig. 3.5: Measured and simulated values of soil nitrogen (nitrate, NO₃-N) dynamics for (a) Müncheberg plot 3 [kg ha⁻¹], (b) Bad Lauchstädt crop rotation plot [kg mg⁻¹] and (c) Bad Lauchstädt black fallow plot [kg mg⁻¹] using the original soil N module (grey lines) and the coupled soil carbon and nitrogen turnover (SCN) module (black lines). Black rhombi are measurements and black bars are indicating the amount of fertilisation [kg N ha⁻¹].

Statistical values are indicating a better agreement between modelled and measured nitrate contents for the black fallow plot (figure 3.5 c, table 3.7 c). IA and r values are high (between 0.86 and 0.89, table 3.7 c). This plot shows a good temporal representation of the soil nitrate dynamics, but minima and maxima are not fully represented by the original model, whereas the SCN module performed slightly better. This can also be seen in the CD values (2.6 and 2.1, table 3.7 c), which is greater than one, denoting that the deviation of the predictions from the mean observation is less than observed in the measurements and the low RMSE values (3.6 and 3.6, table 3.7 c).

Table 3.7: Representation of statistics describing the model performance in simulating soil nitrogen (nitrate) dynamics using the original soil N module and the coupled soil carbon and nitrogen turnover (SCN) module for a) Müncheberg Plot 3, b) Bad Lauchstädt crop rotation, c) Bad Lauchstädt black fallow plot.

Field site	RMSE	E	Μ	t(m) *	t _{crit.}	EF	CD	IA	r
a) original N module	38	-419	0.03	0.37	2.07	-0.25	1.8	0.48	0.21
a) SCN module	36	-187	1.8	0.2	2.07	0.06	16.1	0.38	0.24
b) original N module	2.0	-27.5	-0.11	-0.16	2.3	0.56	2.29	0.83	0.76
b) SCN module	4.3	-32.8	1.77	1.27	2.3	-1.06	0.73	0.5	0.14
c) original N module	3.3	-21.3	-0.37	-0.3	2.36	0.72	2.6	0.89	0.89
c) SCN module	3.6	-35.5	-1.6	-1.27	2.36	0.66	2.1	0.87	0.86

* t-value, critical at 2.5% (two-tailed)

The simulation results obtained generally agree in the temporal course and levels of measured soil nitrate contents. Although the number of measurements does not allow a more detailed evaluation, as measurements e.g. after fertilizer application are sometimes missing. Nevertheless it can be stated that plant uptake, denitrification and nitrate leaching as calculated in SWIM are performing accordingly as simulations generally meet measurements. The performance of both N descriptions does not differ considerably and SCN module delivers reliable courses of nitrate.

3.3.5 Soil carbon dynamics

Soil organic carbon dynamics have been simulated for the long-term static fertilizer experiment at Bad Lauchstädt (Franko et al., 2005). Data for four plots have been provided. Plot 1 received 30 t ha⁻¹ farmyard manure every two years and varying rates of inorganic fertiliser (NPK), plot 6 received 30 t ha⁻¹ farmyard manure every two years, plot 13 received varying rates of inorganic fertiliser (NPK) and plot 18 received no fertilisation at all. A four year rotation of summer barley / potatoes / winter wheat / sugar beet was in use at all plots. Soil carbon levels (0-20 cm) have increased for plots 1 and 6 and have remained constant on plots 13 and 18 (figure 3.6, a and b).

Simulation of soil organic carbon started 1951, because from 1951 onwards all necessary meteorological input data have been provided. The model was initialised for each plot by simply using the value from 1951 derived from the linear trend of the measured data (1901 – 2002, dotted lines in figure 3.6). We considered only aboveground plant residuals (straw and shoots/stubbles) and belowground plant residuals (roots) as primary organic matter fractions, which have been allocated according to root to shoot ratios as proposed by e.g. Klimanek (1990a and b).

A Monte Carlo based sensitivity assessment of input parameters (chapter 4) indicated, that the amount of dead plant material entering the soil (as evaluated indirectly through crop yield comparisons), the synthesis coefficient of primary organic matter and the turnover coefficient of active organic matter are sensitive parameters of the model. Hence a correct representation of these two parameters and the amount of dead plant material entering the soil column is very important.

Amount of dead plant material entering the soil was derived from simulated crop yields by using an empirical relationship proposed by (Franko, 1990; Franko et al., 1997a) to calculate the carbon inputs. Amount and timing of inorganic and organic fertiliser input, sowing and harvest times and atmospheric N deposition have been provided by the data holders and have been fed into SWIM. The turnover coefficient of active organic matter was calibrated on the long-term experiment in Müncheberg (not part of this evaluation exercise, Post et al., 2004) and remained unchanged for this study. The simulated soil organic carbon (SOC) contents of the four plots generally agree with the measured data. The simulations could reproduce well the impacts of organic fertilisation on SOC dynamics and the pattern of the measurements was matched reasonable by the simulation. The simulated values lie between the standard error of most of the measured data. The long-term trends in measured SOC contents (dotted lines in figure 3.6 a and b) are met by the simulations, except for plot 13, which show a slight decreasing trend in the simulation (figure 3.6 b). Statistical analysis shows that for plot 13 the simulation shows a significant bias (greater student's t-value of M (4.1) than tcrit (2.0), see table 3.8). RMSE values, when using the scaled RMSE values (scaled against the mean of the measurements to give the error in fractional units, as used in (Smith et al., 1997b)), delivering values between 8.6 - 12 % RMSE, are in the same range as most of the models used in a soil organic matter model comparison at the Bad Lauchstädt site (Smith et al., 1997b). EF values are positive for all plots, so the model accurately simulates soil organic carbon dynamics for that site.

Problems occurred at plot 13 where the simulation shows a decreasing trend whereas the measurements remain more or less constant. Regular applications of NPK seem to stabilise the SOC content. The simulation could not represent this process adequately, hence inorganic fertilisation effects on crop productivity are not considered correctly, at least for the Bad Lauchstädt site conditions. Therefore the effects of increasing plant productivity due to inorganic fertilisation on SOC dynamics can currently not be assessed satisfactorily. Although organic fertilisation with farmyard manure and effects of crop rotation on SOC contents have been described correctly.



Fig. 3.6: Measured and simulated values of total soil organic carbon in the top 20 cm of soil at Bad Lauchstädt for (a) plot 6 (receiving 30 t ha⁻¹ fresh matter farmyard manure every two years) and plot 18 (no fertilisation) and (b) plot 1 (receiving 30 t ha⁻¹ fresh matter of farmyard manure every two years and various amounts of inorganic fertilisation) and plot 13 (receiving various amounts of inorganic fertilisation, dots the measured values with standard deviation bars and dotted lines the long-term linear trend in the measurements.

Field site	RMSE	Е	Μ	t(m) *	t _{crit.}	EF	CD	IA	r
a) plot 6	0.11	-0.29	-0.005	-0.53	2.0	0.99	0.36	0.69	0.36
a) plot 18	0.08	-0.07	0.0005	0.08	2.0	0.99	0.34	0.53	-0.31
b) plot 1	0.13	0.02	0.003	0.28	2.0	0.99	0.41	0.46	0.35
b) plot 13	0.13	2.04	0.03	4.1**	2.0	0.98	0.44	0.49	-0.33

Table 3.8: Representation of statistics describing the model performance in simulating soil carbondynamics for the Bad Lauchstädt long-term static fertilisation experiment plots 1, 6, 13, 18.

* t-value, critical at 2.5% (two-tailed)

** significantly biased

3.4 Conclusion

SWIM performed reasonable well in simulating soil temperature, soil water, soil nitrogen, soil carbon dynamics and crop yields at the plot scale using the standard model parameter values. For soil temperature the empirical process formulation shows some disadvantages when evaluated at the plot scale. Probably, more physically based descriptions for soil heat flow (e.g. de Vries, 1963; Suckow, 1984; Grant, 1995) would lead to better representation, especially for deeper soil positions and under various land covers. But soil temperature is mainly used as impact factor on soil carbon and nitrogen turnover processes and impacts on water movement in SWIM and for this purpose the presented agreement is seen to be sufficient.

Comparisons of soil moisture showed that SWIM adequately represents plant uptake and water fluxes in the soil driven by meteorology. Problems occurred for the black earth soil (Bad Lauchstädt) where simulating soil hydrology was weakest mainly due to difficulties in parameterisation of soil physical properties for soils with high loess and organic matter contents. Soil water dynamics play a central role for vegetation growth and soil carbon and nitrogen dynamics. Especially soil nitrogen dynamics highly depend on soil water dynamics and errors in soil water simulations will propagate to soil nitrogen dynamics. Modelling of crop yield for a long period showed the lowest performance in this exercise. The process description is clearly designed to assess crop growth at regional scales and is simplified mainly in the description of phenological processes in order to decrease requirements on input information. Taking this fact into consideration the yield assessments performed satisfactory at the field scale and can be used to calculate plant biomass entering the soil. Especially these quantities are important determinants for soil C and N turnover.

Simulation of soil nitrate contents showed reliable dynamics both in magnitudes and temporal behaviour under the different crop species, fertilisation regimes and soil types. Although a detailed evaluation of soil nitrogen dynamics in soil-crop systems need to consider additional processes in more detail (e.g. ammonification, ammonium and plant uptake of inorganic nitrogen and effects on crop growth and transport with soil water). Since mineral nitrogen content in the soil is the result of multiple simultaneous processes and is highly dependent on crop growth, management practices and soil water dynamics, it is difficult to evaluate these processes (Diekkruger and Arning, 1995). Again, errors in e.g. soil moisture simulations propagate into simulation of soil nitrate dynamics.

The newly added soil carbon and nitrogen turnover module performed accordingly in simulating soil nitrate, and delivered good agreement with plot scale measurements. Considering coupled soil carbon and nitrogen processes in this context is important as carbon turnover is providing energy for soil nitrogen processes and absence of sufficient inorganic nitrogen will inhibit the carbon turnover. Therefore considering explicitly N dynamics together with soil carbon dynamics is important to correctly represent long-term soil C trends. These plot scale results have to be combined with river basin scale validation of nitrate loads and concentrations in streams as shown by (Krysanova and Becker, 1999; Hattermann et al., 2005b) using SWIM. The plot scale findings obtained here for soil N processes together with river basin scale N transport (lateral and vertical with water) and alteration (e.g. retention and wetland processes) delivers a proof of the models capability to assess N dynamics at the catchment scale.

Long-term soil carbon dynamics have been successfully simulated, especially the longterm trend of organic carbon. Impacts of organic fertilisation and plant derived organic matter inputs are well represented, whereas impacts of inorganic fertilisation on crop growth and consequently SOM dynamics needs further consideration.

By evaluating the process dynamics as a whole it can be stated that SWIM is able to reproduce the relevant interaction in soil-crop systems in respect to its purpose as a regional scale eco-hydrological model. A detailed evaluation of processes using field scale measurements is of importance both in checking the models capability and to detect problems and deficits. Without field scale experimental plots and available data out of it, development and improvement of regional ecosystem models is impossible. Combined with evaluations of lateral fluxes of water and nutrients it is possible to perform integrated assessments of global change impacts on agro-ecosystem functions (water quality and quantity, crop growth, soil fertility and soil C sequestration) at the regional scale using the eco-hydrological catchment model SWIM.

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(in review)

Chapter 4

Parameter and input data uncertainty estimation for the assessment of long-term soil organic carbon dynamics

Keywords: *Eco-hydrological modelling, soil carbon, uncertainty analysis, sensitivity analysis, model parameters, input data*

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¹ Potsdam Institute for Climate Impact Research Dep.: Global Change & Natural Systems P.O. Box 60 12 03, 14412 Potsdam, Germany **Abstract:** The use of integrated soil organic matter (SOM) models to assess SOM dynamics under climate change, land use change and different land management practices requires a quantification of uncertainties and key sensitive factors related to the respective modelling framework. Most uncertainty studies hereby focus on model parameter uncertainty, neglecting other sources like input data derived uncertainties, and spatial and temporal properties of uncertainty.

Sources of uncertainties assessed in this study are stemming from uncertainties in model parameterisation and from uncertainties in model input data (climate, soil data, and land management assumptions). Thereby, Monte Carlo based global sensitivity and uncertainty analysis using a latin hypercube stratified sampling technique was applied to derive plot scale (focussing on temporal propagation) and river basin scale propagation of uncertainty for long-term soil organic carbon (SOC) dynamics. The model used is the eco-hydrological river basin model SWIM (Soil and Water Integrated Model), which has been extended by a process-based multi-compartment model for SOM turnover. Results obtained by this study can be transferred and used in other simulation models of this kind.

Uncertainties resulting from all input factors used (model parameters + model input data) show a coefficient of variation between 5.1 and 6.7 % and accounted for +/- 0.065 to +/- 0.3 % soil carbon content (0.06 - 0.15 t C ha⁻¹ yr⁻¹). Parameter derived uncertainty contributed most to overall uncertainty. Concerning input data contributions, uncertainties in soil and climate input data show off. On the river basin scale, cropland and forest ecosystems, loess and gleyic soils possess the highest degree of uncertainty. Quantified magnitudes of uncertainty stemming from the examined sources vary temporally and spatially due to specific natural settings and deliver useful information for interpreting simulation results on long-term soil organic carbon dynamics under environmental change.

Derived from this analysis, key sensitive model parameters and interactions between them could be identified, where the mineralization rate coefficient, the carbon use efficiency parameter (synthesis coefficient), parameters determining the soil temperature influence on SOM turnover (mainly Q10 value) and soil input related data (soil bulk density and initial soil C content) introduced the highest degree of model uncertainty.

4.1 Introduction

Assessing changes of soil organic matter (SOM) due to land management practices, land use and climate change plays a vital role in the fields of climate change mitigation (soil carbon sequestration), land – atmosphere interactions and soil fertility. SOM is an important soil component as it influences soil structure and aggregation, soil moisture conditions, soil nutrient status and soil biota, and hence influences ecosystem functioning.

Due to the complex interactions of processes affecting SOM dynamics, the use of integrated dynamic ecosystem models are seen as a useful tool to assess SOM dynamics. Dynamic modelling is an effective approach to characterise the system by integrating various processes, and as a tool for mechanism understanding, estimating, predicting, and policy making (Zhang et al., 2002).

In the context of model simulations, the quantification of attached modelling uncertainties on model outputs and information on how the uncertainty in the model output can be apportioned to different sources of uncertainty in the model input (sensitivity analysis) are meanwhile necessary information (Hattermann et al., 2005b; Janssen et al., 1994; Saltelli et al., 2000; Zähle et al., 2005). Recently, a number of studies have been carried out to quantify the uncertainties in simulation models and their propagation in the model. Thereby most studies focus on model parameter uncertainties and on the calculation of which parameters are attributing most to this uncertainty (Janssen et al., 1994; Saltelli et al., 2004). Parameter uncertainty is mainly stemming from errors in the measurements used for parameterisation, the method used to scale point measurements to the scale the model operates or from parameter and input data estimation of semi-empirical process descriptions (e.g. not readily measurable parameters, soil parameters derived from standard soil measurements, Zähle et al., 2005). But beside parameter uncertainties, uncertainties related to input data (e.g. soil, land use, climate input data, land management practices) and scaling issues have to be considered as well.

Aim of the paper is to give a quantification of model uncertainties stemming from different sources as well as model parameter and input variables sensitivities using the integrated process-based eco-hydrological river basin model SWIM (Soil and Water Integrated Model, Krysanova et al., 1998), which was recently extended to assess SOM dynamics (Post et al., 2004; Post et al., 2005c). Thereby the maximal contribution of these sources to model uncertainty is disclosed. This information is necessary to better interpret SOM model results related to investigation of climate change and land use change (change in land cover and land management practices) impacts in the context of soil carbon sequestration and soil fertility issues.

4.2 Materials and methods

4.2.1 The Soil and Water Integrated Model SWIM

SWIM (Soil and Water Integrated Model, Krysanova et al., 1998) is a continuous-time, spatially distributed model. SWIM works on a daily time step and integrates hydrology, vegetation, erosion and nutrients at the river basin scale. The spatial aggregation units are subbasins, which are delineated from digital elevation data. The subbasins are further disaggregated into so called hydrotopes, hydrologically homogenous areas. The hydrotopes are defined by uniform combinations of subbasin, land use and soil type (Krysanova et al., 2000). The model is connected to meteorological, land use, soil and agricultural management data. For detailed process descriptions, validation studies and data requirements it is referred to publications by (Hattermann et al., 2004, 2005b; Krysanova et al., 1998, 2000), and for the SWIM extension on SOM turnover processes (see next section) a detailed description can be found in (Post et al., 2005 a and c).

4.2.2 Model extension for SOM turnover

The coupled carbon and nitrogen turnover module is based on the tight relationship between soil and vegetation processes. On the one hand an input exists into the soil by addition of organic material through accumulating litter, dead fine roots and organic fertilizer, and on the other hand there is a withdrawal from the soil of water and nitrogen by the vegetation, release of CO₂ into the atmosphere and export of inorganic nitrogen by soil water flows (e.g. leaching into the groundwater and lateral flow processes).

To describe the carbon (C) and nitrogen (N) budget organic matter is differentiated into Active Organic Matter (AOM) as soil organic matter pool and Primary Organic Matter (POM) as litter pool. The latter is separated into five fractions for each vegetation and crop type (stems, twigs and branches, foliage, coarse roots and fine roots). For all pools of active and primary organic matter the carbon and nitrogen content is considered.

The carbon and nitrogen turnover into different stages (pools) is implemented as a first order reaction (Chertov et al., 1997; Franko, 1990; Parton et al., 1987) and can be described as multi-compartment process-based concept of soil organic matter turnover. The processes are controlled by matter specific reaction coefficients. Heterotrophic (substrate induced) soil respiration is calculated through the decay of C_{POM} and C_{AOM} pools per day. Effects of soil temperature, soil water content and soil pH status on mineralisation and nitrification is considered through reduction functions (Franko, 1990; Kartschall et al., 1990).

4.2.3 Quantification of uncertainty and sensitivity

Quantifying the variability and magnitude of model output due to incomplete knowledge of real world processes described in model simulations (Uncertainty Analysis, UA, Janssen et al., 1994) and the apportion of this uncertainty to different sources in the models (Sensitivity Analysis, SA, Saltelli et al., 2004) is more and more becoming an integral component for integrated environmental assessment studies.

The method employed here uses Monte Carlo analysis (Rubinstein, 1981), whereas other methods like analytical (e.g. variance propagation, Morgan and Henrion, 1990) or numerical methods can be used as well (e.g. differential uncertainty analysis, Worley, 1987; non probabilistic methods like fuzzy sets; possibility theory, Ferson and Kuhn, 1992; firstorder analysis employing Taylor expansion, Scavia et al., 1981; or screening designs Scott et al., 2000). These methods are mostly referred to local SA, and are used for studying the error propagation of models with simple equations or linear models (Scott et al., 2000). Screening designs might be appropriate to isolate the most important factors from a large number that may affect a particular model response. Typical screening designs are "one-at-a-time" experiments. Here the impact of changing the value of each factor is evaluated in turn (e.g. Scott et al., 2000). But local approaches do not account for any interactions between inputs, if they exist (Muleta and Nicklow, 2005). Therefore a Monte Carlo based approach was chosen.

Monte Carlo analysis uses multiple evaluations with randomly selected model input and considers the entire range of input factors and possible interactions of them in respect to model output. A Monte Carlo analysis typically consists of the following steps (Saltelli et al., 2000): (1) definition of model variables (input factors) X_i used for the analysis, (2) selection of ranges and the Probability Distribution Functions (PDF) for each X_i, (3) generation of samples within the PDF's (sampling), (4) evaluation of the model output for each element of the input factor sample, (5) uncertainty analysis and (6) sensitivity analysis. For the assessment of sensitivity and uncertainty the software tool Simlab (Version 2.2, Saltelli et al., 2004; Tarantola, 2001) developed by the Joint Research Center (JRC) in Ispra (Italy) has been used.

4.2.4 Definition of model variables and selection of the Probability Distribution Functions

In this study we focus on model parameters and input factors related to the soil organic matter turnover module. SA and UA of hydrological processes using SWIM have been conducted in a recent study (Hattermann et al., 2005b).

Alongside all model parameters driving the model extension for SOM turnover, sensitivity for input data such as climate data (temperature, precipitation and global radiation), soil data (initial soil organic carbon content, bulk density and clay content), and agricultural management practices (fertilisation and crop harvest surplus management) is assessed.

A crucial and fuzzy aspect in SA is the assignment of Probability Density Functions (PDF's) for each input factor (Muleta and Nicklow, 2005; Xu et al., 2005). In most cases there is an absence of information about ranges and distributions for the input factors.

Input factor PDF's were derived through literature review and based on an expert inquiry carried out during two workshops at Aberdeen University, UK (COST 627 meetings, results of expert inquiry can be found at http://www.abdn.ac.uk/modelling/cost627/Question naire.htm, as of 01/03/2005). There, modellers and experimental scientists provided their estimates on input factor ranges and probability distributions. Factors ranges have been narrowed for plot scale assessments, as input factors can be better constrained at the plot scale through the incorporation of more detailed site information (table 4.1). For example field soil respiration measurements in the study area suggest a Q10 value in a range 1.8 to 2.2. Furthermore, we relied on simple distributions like Gaussian Normal, Triangular or Uniform distributions as they seem to be sufficient for explorative SA studies (Haan et al., 1998; Helton, 1993). This kind of best guess of PDF's may introduce additional uncertainty, but since the estimation of parameters in ecological studies is mainly done in laboratories or at the field scale and then scaled up to landscape or global level, an exact estimation of PDF's (through e.g. formal statistical procedures) is not feasible. Table 4.1 gives an overview of the input factors PDF's.

Sampling

In MC analysis different sampling techniques exists (random sampling, stratified sampling, quasi-random sampling). Details on the first two can be found in (McKay et al., 1979) and on the third in (Sobol, 1990). Since Monte Carlo analysis is computationally expensive, an appropriate sampling method may reduce computational time.

ut factor	description	type	distribution of PDF	range (reference value)	reference
k_{aom}	turnover coefficient of active organic matter $[d^{1}]$ first soil lotter (humor lotter) $k = 1$ others 2 = 5	parameter	triangular	[0.0001 : 0.0003] / [0.00015 : 0.00025]* (0.0002)	
k aom_r	Instruction layer (multus layer), k_{hum} , layers $z_{,,hl}$ - (mineral layers); $k_{hum_{1}}$	parameter	triangular	[0.00005:0.0002] / [0.00005:0.00015]* (0.0001)	Franko, 1990; Klimanek and Franko, 1990; Klimanek and
k _{nit}	nitrification coefficient $[\dot{a}^1]$	parameter	triangular	[0.001:0.004] (0.0025)	Senuz, 1997)
Kan ag		parameter	uniform	[0.55:0.80]	(Franko, 1990; Klimanek
^{ری} ایت_ bg	synthesis coefficient of primary organic matter [d ⁻¹], " "carbon use efficiency parameter"	parameter	uniform	[0.55 : 0.80]	and Schulz, 1997; Lettau and Kuzyakov, 1999; Nicolardot, 2001)
oom ag	- [¹ 4]	parameter	uniform	[0.1:0.45]	(Franko, 1990; Klimanek
pom bg	unnover coefficient of printary organic matter [u]	parameter	uniform	[0.1:0.45]	and Schulz, 1997)
fre ag		parameter	triangular	+/- 20 %	(Franko, 1990; Klimanek,
frc_bg	allocation of below and above-ground residuals	parameter	relation	-1.0 * frc_ag	1987; Klimanek and Schulz, 1997)
enr ag		parameter	uniform	+/- 20 %	(Franko, 1990; Klimanek
cm bg	Carbon / Nitrogen ratio	parameter	uniform	+/- 20 %	and Schulz, 1997; Schulz, 1997)
010	Q10 value of soil temp. reduction function	parameter	triangular	$[1.5:2.5]/[1.8:2.2]^*$ (2.)	(Fang and Moncrieff, 2001; Kätterer et al., 1998)
topt	optimal temp. for mineralization, part of soil temp. reduction function [°C]	parameter	triangular	[30:40]/[33:37]* (35)	(Franko, 1990; Kartschall et
<i>wsat</i>	limit of saturated water content, part of soil water reduction function [Vol. %]	parameter	triangular	[0.4:0.6]	au., 1990, Koungo et au., 1997)
temp.	temperature [°C]	climate	normal	$+/-2 \circ C$ $\mu = 0, \sigma = 1.0$	Workshop Aberdeen
precip.	precipitation [mm]	climate	normal	+/-10% $\mu = 0.05$	Workshop Aberdeen
glob	global radiation $[\mathrm{MJ}/\mathrm{m}^2]$	elimate	normal	+/-30% $\mu = 0, \sigma = 0.15$	Workshop Aberdeen
stinorg	inorganic fertilisation [kg/ha]	agric. management	normal	$+/-15$ % $\mu = 0, \sigma = 0.075$	Workshop Aberdeen
fertorg	organic fertilisation [kg/ha]	agric. management	normal	$+/-15$ % $\mu = 0, \sigma = 0.075$	Workshop Aberdeen
dins_vi	crop harvest surplus [kg/ha]	agric. management	uniform	+/- 20 %	own estimate; (Smith et al., 1997)
dens	bulk density [%]	soil	triangular	+/- 10 %	Workshop Aberdeen
clay	clay content [%]	soil	triangular	+/- 10 %	Workshop Aberdeen
nit soc	initial soil carbon content [%]	soil	triangular	+/-10%	Workshon Aherdeen

In our case we adopted Latin Hypercube Sampling (LHS, McKay et al., 1979). Hereby the range of each input factor is divided into N intervals of equal marginal probability (1/N), and one observation of each input factor is made in each interval (Saltelli et al., 2000). This method yields to a reduced amount of samples to be drawn out of the PDF (in comparison to random sampling) and guarantees randomness in sampling the full range of the PDF (fully stratified).

This method allows the consideration of correlation dependencies in input factors / input distributions. In our case the plant residual allocation parameters (frc_ag and frc_bg, table 4.1) PDF's are negatively correlated (frc_ag = - frc_bg) to ensure that the amount subtracted due to e.g. the above-ground fractionation is added with the same amount from the below-ground fraction.

The fourth step in MC analysis is to evaluate each input factor creating a sequence of results. This can be done simply through scatter plots or cow webs to get a first impression on single input sensitivity to model results.

Uncertainty analysis

Uncertainty is assessed by the quantification of model outputs and the use of basic statistics like minima, maxima values, percentiles, expected value (mean), median and variance. Additionally the quantification of model outputs can be compared to measurements as reference data.

In our case we considered the long-term development of total soil C. Further on we assessed the uncertainty at the plot scale at a certain time and the temporal course and on the spatial scale (river basin). Beside the overall uncertainty including all model parameters and input data (later referred to as "all factors"), an assessment for uncertainty of model parameters ("parameters"), soil input data ("soil", including initial soil carbon content, bulk density and clay content), climate input data ("climate", including temperature, precipitation and global radiation) and agricultural management practices (fertilisation, crop harvest

surplus) has been carried out to apportion the overall uncertainty to the different sources (table 4.1).

For the uncertainty assessment the coefficient of variation (deviation of a variable from its mean, "standard error", COV in %) was calculated according to equation 4.1 to quantify the uncertainty to the mean value and to make a comparison between the different sources of uncertainty possible, with n = number of simulation runs, \bar{x} = mean value of output, x_i = output value, sd = standard deviation:

$$COV[\%] = \frac{1}{n-1} \sum_{i=1}^{n} \left\| \left(\overline{x} - x_i \right) \right\| * \frac{100}{\overline{x}} = sd * \frac{100}{\overline{x}}$$
(eq. 4.1)

Sensitivity analysis

To identify the relative importance of a particular input factor to the total model output uncertainty, different indices are proposed in literature. They can be grouped in correlation based (Partial Correlation Coefficients (PCC), Pearson product moment correlation coefficient (PEAR), Spearman coefficient (SPEA)) indices, regression based (Standardised Regression Coefficients (SRC)) index, variance based indices (Fourier Amplitude Sensitivity Test (FAST), Sobol' sensitivity indices) or their rank transformations (Helton, 1993; Saltelli, 1999; Saltelli and Sobol, 1995). These indices are used to screen model input factors based on the absolute value of the regression, variance or correlation coefficients. For a discussion on sensitivity indices it is referred to (Helton, 1993; Saltelli et al., 2000; Saltelli and Sobol, 1995). In our case, we adopted the PCC, because it provides a measure of variable importance that tends to exclude the effects of other variables. Additional correlation based methods offer the possibility to include input factors interdependencies.

In the calculation of PCC first the correlation r_{xjy} is calculated between the input variable X_j (input factor) and the output Y. The output variable Y and the input variable X_j are then assessed from the use of a sequence of linear regression models (Saltelli et al., 2000)

to calculate the PCC (with: \hat{Y} = estimated value of the output value Y and \hat{X}_j = estimated value of the particular parameter (j) obtained from the regression model; b₀, c₀, b_h, c_h are regression coefficients; j and h are respective input factors).

$$\hat{Y} = b_0 + \sum_{h \neq j} b_h x_h$$
 and $\hat{X}_j = c_0 + \sum_{h \neq j} c_h x_h$ (eq. 4.2)

As linear regression and correlation based sensitivity indices are impractical for nonlinear models (poor linear fit to non-linear model output), the use of rank transformations can overcome this problem (Saltelli and Sobol, 1995). Thereby the original input and output variables are replaced by their respective ranks. Although it has to be proved that the model behavior is monotonic (e.g. higher X_j leading to higher Y). If the coefficient of determination R_{y^2} (determines the fraction of variance of the model output explained by the linear regression method used) of the ranked transformed data is higher than of the R_{y^2} of PCC, the Partial Rank Correlation Coefficients (PRCC) can be used. If the PCC values are much smaller / different than PRCC (the absolute values) a non-linear sensitivity of the model to that specific parameter is present (Saltelli and Sobol, 1995). In our cases R_{y^2} on the raw values were higher than on the rank transformed PCC values, indicating that the model behaviour in not non-linear. Therefore the PCC sensitivity index is used and factors are ranked according to their absolute values of PCC (|PCC|).

Model outputs considered were the total soil carbon content (Ctot) and heterotrophic soil respiration (Cresp) for the respective areas under study (table 4.2). For plot scale assessment the Ctot and Cresp values for the last simulation year were used. The same applied to the spatial scale assessment, but here the averaged values for the Nuthe river basin were taken.
ation	rovided by er barley / ư beet	rovided by iter rye, et, spring	rovided by agricultural / winter		
input data for model simul	Climate, soil, management data p data holder. Crop rotation: summ potatoes / winter wheat / sugs	Climate, soil, management data pi data holder. Crop rotation: win potatoes, winter wheat, sugar be barley	Climate, soil, management data pi data holders. Crop rotati on for all i sites: summer barley / potatoes wheat / sugar beet		
fertilisation regime	1.2 [t ha ⁻¹ yr ⁻¹] organic duy matter of farmyard manure to root and tuber crops and various amounts of inorganic fertilisation (162 kg N ha ⁻¹ yr ⁻¹ on average)	1.2 [t ha ¹ yr ¹] organic dry matter of farmyard manure to root and tuber crops and various amounts of inorganic fertilisation (162 kg N ha ¹ yr ¹ on average)	1.2 [t ha ⁻¹ yr ⁻¹] organic dry matter of farmyard manure to root and tuber crops and various amounts of inorganic fertilisation (162 kg N ha ⁻¹ yr ⁻¹ on average)		
description	long-term static fertilizer experiment, soil organic carbon measurements in 0- 20 cm soil depth, loess soil	long-term field experiment V140, soil organic carbon measurements in 0-20 cm soil depth, sandy soil	Pleistocene lowland river Basin area: ~ 1900 km2, 560 mm average Precipitation, 9 °C average Temp. Land Use: 47% cropland, 42% forest Soils: mainly sand to (loamy) soils, Cambic Arenosols and Gléyic podzols (FAO)		
data provider (Reference)	UF2* (Franko et al., 2005, Körschens and Müller, 1996)	ZALF* (Rogasik and Schroetter, 1999; Rogasik et al., 2004)	Land use: Conine data Oollinger and Strobl, 1996) oils: Buek 1000 (Hartwich et al., 1995) Climate: PIK database		
location (simulation period)	 åad Lauchstädt, Plot 18 (1951 – 2002) Müncheberg, fertilised plot (1963 – 2000) Nuthe river basin (1981 – 1997) 				
Process Output	Long - term soil C dynamics				

Table 4.2: Description of experimental sites and study area used in this assessment.

* ZALF - Leibniz-Centre for Agricultural Landscape and Land Use Research, Müncheberg, Germany, UFZ – Centre for Environmental Research, Leipzig/Halle, Germany,

4.2.5 Data sets and study area for uncertainty analysis

For the point scale assessment of uncertainty and sensitivity the field experimental sites Müncheberg (long-term field experiment V140) and Bad Lauchstädt (static fertiliser experiment) have been used. Main characteristics and detailed descriptions of these sites can be found in (Franko et al., 2005; Körschens and Müller, 1996 and chapters 2, 3) for the Bad Lauchstädt site and (Mirschel et al., 2005; Rogasik and Schroetter, 1999; Rogasik et al., 2004 and chapters 2, 3) for the Müncheberg site.

For the spatial assessment of uncertainty the Nuthe river basin was chosen as a test case. The Nuthe river basin is located in Brandenburg, Germany, south of Berlin (figure 4.1). It covers an area of approximately 1900 km². Mean annual precipitation is 590 mm and mean annual air temperature is 9°C. Land use is dominated by cropland (43 % of total area), grassland (13 %) and forest (36 %). Main agricultural area is in the southern region of the basin with mainly Luvic Arenosols on loess sediments (figure 4.1). Soils are mainly characterized by sandy to loamy soil texture (Cambic Arenosols, Podzols and Gleyic podzols) developed on glacial sediments.



Fig. 4.1: Location of the Nuthe river basin and distribution of major soil types and land use classes based on BUEK1000 (soils, Hartwich et al., 1995) and CORINE data (land use, Dollinger and Strobel, 1996).

4.3 Results and discussion

4.3.1 Factors sensitivity and importance

The coefficient of determination of the sensitivity index (PCC), determining the fraction of variance of the output explained by the linear regression method (see section 2.3.4), is showing high values between 0.99 and 0.82, except for the Cresp assessment at the Müncheberg site (0.62, table 4.3). Hence, the determination of the linear regression method is weaker for the Müncheberg site, presumably because of non linear effects of input factors on model output and accordingly a less distinctive picture of input factors sensitivity for that site.

Through interpretation of correlation plots between each of the input factors and the respective model output (Ctot and Cresp) a threshold of |PCC| = 0.20 could be identified. Input factors below this threshold do not show any notable dependency to model output. This led to a reduction of the number of input factors showing substantial importance to long-term SOC dynamics (slashes in table 4.3).

In general it can be stated that the model parameters describing the mineralisation dynamics of SOM (kaom, kaom_r) and the carbon use efficiency (synthesis parameter, ksyn), can be identified as most important factors (high |PCC| values, table 4.3). The synthesis coefficient of primary organic matter (ksyn_ag, ksyn_bg) determines the amount of primary organic matter carbon which is stored in the active organic matter pool and the reciprocal value determines the amount of C which is respired during decomposition of primary organic matter ("carbon use efficiency" parameter). A higher value of ksyn consequently increases storage in the active organic matter pool and reduces heterotrophic soil respiration. The high sensitivity index shows the importance in determining this parameter. kaom and kaom_r in turn determine the mineralization rate and hence the turnover speed of active organic matter. The mineralization rate for humus layers (kaom) and for the mineral layers (kaom_r) is of similar high importance. Higher mineralization rates (and hence higher kaom and kaom_r values) quicker decrease active organic carbon in soils and increase soil respiration rates.

	C _{tot} Bad 1	Lauchstädt	C _{tot} Mün	tcheberg	C _{tot} Nut	he river	Cresp Bad	Lauchstädt	Cresp Müı	ncheberg	Cresp Nu	the river
rank	factor	PCC ($\mathbb{R}^2 = 0.99$)	factor	$\mathbf{PCC} \\ (\mathbf{R}^2 = 0.82)$	factor	$\mathbf{PCC} \\ (\mathbf{R}^2 = 0.96)$	factor	\mathbf{PCC} ($\mathbf{R}^2 = 0.98$)	factor	$\mathbf{PCC} \\ (\mathbf{R}^2 = 0.62)$	factor	PCC ($\mathbb{R}^2 = 0.96$)
1	kaom	-0.989	init_soc	0.762	$\mathcal{O}I\mathcal{O}$	0.938	kaom_r	0.982	ksyn_ag	-0.592	010	-0.953
7	οīδ	0.986	010	0.653	init_soc	0.926	$\mathcal{O}1\mathcal{O}$	-0.960	$\mathcal{O}I\mathcal{O}$	-0.462	kaom_r	0.929
3	ksyn_bg	0.971	kaom	-0.620	kaom	-0.914	dens	0.945	kaom	0.394	topt	-0.812
4	temp	-0.963	ksyn_bg	0.585	topt	0.776	topt	-0.884	topt	-0.337	kaom	0.453
ŝ	topt	0.962	dens	-0.538	temp	-0.340	init_soc	0.869	harv_surp	0.291	init_soc	0.306
9	init_soc	0.935	topt	0.406	ksyn_ag	0.299	kaom	0.742	dens	0.283	dens	0.284
٢	dens	-0.912	ksyn_ag	0.400	ksyn_bg	0.298	temp	0.697	kaom_r	0.250	ksyn_bg	-0.236
æ	ksyn_ag	0.885	glob	0.334	frc_bg	-0.253	harv_sup	0.640	temp	0.222	fertinorg	0.167
6	fertorg	0.880	temp	-0.282	cnr_ag	-0.186	precip	0.604	glob	0.204	temp	0.153
10	harv_surp	0.866	harv_surp	0.221	fertorg	-0.184	kpom_bg	-0.601	ksyn_bg	-0.162	ksyn_ag	-0.140
11	glob	0.835	fertorg	0.200	glob	0.169	glob	-0.502	precip	0.161	kpom_bg	-0.138
12	precip	0.505	frc_{bg}	0.138	dens	-0.157	clay	0.447	fertorg	0.094	glob	-0.133
13	frc_bg	-0.353	fertinorg	0.079	kpom_bg	0.136	fertorg	0.383	init_soc	0.083	harv_surp	0.127
14	kaom_r	-0.078	disaid	0.060	kpom_ag	0.117	ksyn_bg	-0.293	frc_bg	-0.082	frc_{bg}	0.112
15	cnr_ag	-0.057	knit	0.058	knit	-0.111	frc_bg	0.269	cnr_bg	0.055	knit	0.107
16	cnr_bg	0.040	cnr_ag	-0.043	harv_surp	-0.080	ksyn_ag	-0.112	kpom_bg	0.053	fertorg	0.088
17	wsat	0.037	wsat	0.042	wsat	0.069	cnr_ag	0.076	kpom_ag	0.044	wsat	0.068
18	knit	0.026	clay	-0.036	$kaom_r$	0.051	kpom_ag	0.052	fertinorg	0.040	kpom_ag	0.036
19	kpom_bg	0.023	kpom_bg	0.0265	fertinorg	-0.046	cnr_bg	-0.037	clay	0.039	precip	-0.033
20	kpom_ag	-0.014	cnr_bg	-0.0261	clay	0.045	fertinorg	-0.012	cnr_ag	0.024	cnr_{bg}	0.023
21	clay	0.009	kpom_ag	0.018	cnr_{bg}	0.029	knit	0.006	wsat	0.007	clay	-0.010
22	fertinorg	0.003	kaom_r	-0.003	precip	0.004	wsat	-0.002	knit	0.001	cnr_ag	0.006
						fm_a	$g = frc_b g$					

Table 4.3: Description on next page

 R^2 – coefficient of determination ag = above-ground, bg = below-ground Table 4.3: Sensitivity of input factors based on Partitial Correlation Coefficient (PCC) calculated for soil carbon content (Ctot, 0 – 20 cm soil depth) at the end of the respective simulation period (Bad Lauchstädt and Müncheberg experimental site, see table 2), spatial averaged at the end of the simulation period (Nuther river basin, see table 2) and for heterotrophic soil respiration (Cresp) for the whole soil profiles used as yearly sum for Bad Lauchstädt and Müncheberg and as spatially averaged yearly sum for the Nuthe river basin. Abbreviations of input factors are explained in table 1. Ranking was performed based on the absolute PCC values. Slashes are indicating the |PCC| value threshold of 0.2.

Alongside with these, the parameters regulating the influence of soil temperature on SOM turnover (Q10, topt) are of high importance. The Q10 value shows high sensitivity at all sites with |PCC| values ranging between 0.99 and 0.46 (table 4.3). Soil temperature effect on SOM turnover is described according to the Stanford approach (Stanford et al., 1973; Stanford and Smith, 1972). Higher Q10 and topt values decrease the value of the reduction function, which in turn reduce the reaction coefficients (kaom, kaom_r and kpom) governing the SOM turnover. Consequently, for this case, the turnover of SOM is reduced. The positive sign of the PCC values (table 4.3) for Q10 and topt for Ctot shows, that an increase of these two parameters leads to a relative increase of soil carbon and a decrease of soil respiration (Cresp, negative PCC values, table 4.3). This highlights the strong influence of soil temperature on soil decomposition and mineralization and of its driving variables Q10 and topt.

Also noteworthy are the high importance of the soil factors initial soil carbon content (init_soc) and bulk density (dens). Obviously init_soc determines the level of soil organic carbon trends and a correct assessment is central in this approach. Bulk density (dens) is a key factor in determining the soil wilting point and field capacity, which in turn are the important drivers of soil water dynamics. Higher bulk densities in soils increase soils wilting point and reduce soils field capacity, which in turn leads to stronger influence of soil moisture on SOM turnover through higher soil water contents. Higher bulk densities hence reduce turnover of SOM. Further on bulk density is also used in the calculation of soil temperature, where higher bulk densities increase the damping factor of soil temperature. Soils with high bulk density show a smoothed annual soil temperature dynamic and are warming and cooling slower than soils with low bulk densities. This effect tends to smooth and reduce soil temperature dynamics and may reduce turnover of SOM.

Effects of variations in air temperature and global radiation (as climate drivers) also show a considerable impact on soil carbon and soil heterotrophic respiration dynamics. At the Bad Lauchstädt site, with a loamy black soil (Tchernozem), changes in air temperature cause stronger impacts on soil carbon and respiration than at the Müncheberg site (higher absolute PCC values, table 4.3). This can to a large extent be explained by the different thermal properties of these contrasting soil types. The sandy Müncheberg soil is warming and cooling faster as the dark loamy soil (Tchernozem) at Bad Lauchstädt. Additionally the dark soil possesses a higher heat capacity and hence higher temperatures increase soil temperatures stronger and enhances SOM turnover (negative PCC value for this factor at the Bad Lauchstädt site for Ctot and positive for Cresp, table 4.3). All other model parameters show weaker sensitivity and are hence of minor importance, expressed with low absolute PCC values (table 4.3).



⁽continues on next page)



Fig. 4.2: Input factors with |PCC| values above the threshold of 0.2 for Ctot (a) and Cresp (b) and all cases (Bad Lauchstädt, Müncheberg and Nuthe river basin).

Considering input factors with |PCC| values above 0.2 threshold (figure 4.2 a and b), similar tendencies and factors importance can be stated regarding the PCC values for the model outputs Ctot and Cresp for the respective sites. For the Bad Lauchstädt case more input factors are of importance than for the other cases (e.g. fertorg, harv_surp, glob, precip, figure 4.2). This shows that variations in agricultural management and climate related factors impact stronger on Ctot and Cresp for the fertile Tchernozem soil (Bad Lauchstädt) than for the sandy soil (Müncheberg).

Out of the 23 factors included in the sensitivity assessment about ten (Q10, kaom / kaom_r, topt, ksyn_ag / ksyn_bg, temp, glob, init_soc, dens, table 4.3) are showing overriding influence on the simulation of soil carbon and soil respiration dynamics. This is to some extent due to the transient model simulation, because of changing environmental conditions and a system which is not in equilibrium (e.g. croplands are at present not in equilibrium because of crop harvest exportation). Especially for SOM degraded agricultural soils (due to land management practices, e.g. intensive cropping), parameters determining the carbon use efficiency and the mineralization of SOM show higher influence as this

would be the case for equilibrium conditions. For eqilibrium conditions parameters driving biomass growth would dominate more (Zähle et al., 2005). The same holds for parameters determining soil temperature effect on SOM turnover constants (Q10 and topt).

The importance of the parameters of soil temperature reduction function on SOM turnover is especially relevant when investigating climate change effects on SOM dynamics. Here a correct representation of the Q10 value and the temperature reduction function used under changing climatic conditions is crucial. Recent findings suggest that labile and resistant soil C pools are sensitive towards changing soil temperatures (Fang et al., 2005a; Knorr et al., 2005) and that soil temperature effects on soil carbon turnover is a key processes of the impact of climate change on soil-stored carbon (Fang et al., 2005a). The temperature sensitivity in our investigation is clearly dominating the factors importance expressed mainly by the Q10 value, which is apparently a critical parameter. Our approach uses a bulk Q10 value, not distinguishing a temporally or spatially variable Q10 or variability with soil depth and for different soil pools. Present-day understanding of temperature sensitivity on SOM decomposition (Q10 relationship) is not yet sufficient and different approaches of Q10 relationships introduce a high degree of uncertainty (Fang et al., 2005a; Joos et al., 2001). Additionally a scientific consensus about different temperature sensitivities (in terms of temperature sensitivity on SOM turnover rate constants in a process model) of e.g. labile and slow soil C pools or organic and mineral soil C pool is not yet achieved (Fang et al., 2005a; Giardina and Ryan, 2000; Hyvonen et al., 2005; Reichstein et al., 2005a). Soil temperature sensitivity (Q10 dependency) is pivotal in assessing SOM dynamics in our assessment, which is also supported by other ecosystem studies (Joos et al., 2001), laboratory and field experiments (Fang et al., 2005a; Knorr et al., 2005; Reichstein et al., 2005b).

Kaom and kaom_r have to be determined using long-term field experimental sites under different land use and soil conditions or using laboratory incubation experiment. Incubation experiments are also used to derive ksyn relationships of primary organic matter fractions turnover. Especially the changing properties of these parameters under changing environmental conditions (climate change, land use change) are not sufficiently resolved yet. Considering the results presented, constraining these parameters, through e.g. benchmarking sites, is important.



Fig. 4.3: Description on next page

Fig. 4.3: Temporal development of uncertainty for experimental sites Bad Lauchstädt (right) and Müncheberg (left) for 51 and 37 years simulation period respectively considering a) all factors, b) parameters, c) soil, d) climate, e) crop harvest management (harv_surp) and f) fertilisation. Results shown are 5, 25, 50, 75, 95 percentile values based on 500 model runs expressed in percent of soil organic carbon content (Corg, 0-20 cm soil depth). In a) simulation using standard parameterisation (grey line) and measurements at the respective sites are shown. Please note that for Bad Lauchstädt no measurement were conducted for the fertilisation scheme used in this study (1.2 t C ha⁻¹ yr⁻¹, various amount of NPK, see table 4.2) and measurements representing 2 t C ha⁻¹ yr⁻¹ (black circles) and no organic fertilisation (black rhombic sign) are shown.

Beside the model parameters for SOM turnover, soil input data impacts, mainly initial soil carbon content and bulk density, and soil temperature impacts on soil carbon processes show off in this study. This underlines the relevance of soil mapping and long-term soil surveys of soil physical properties for regional impact studies and the importance of dynamic assessment of soil temperature, soil water and soil nutrient processes to simulate SOM turnover. The identification of these most important input factors might also be transferable to other model of this kind, as these parameters are central also for other process models (Bergmann et al., 1999; Franko, 1997a; Lettau and Kuzyakov, 1999).

4.3.2 Assessment of uncertainty

Following the concept described for the sensitivity and uncertainty assessment, we assess the uncertainty in model results due to model parameters, agricultural management practices, soil input data and climate input data and a combination of all mentioned input factors.

Hereby it was distinguished between the inherent uncertainty at the plot scale for the long-term field experimental sites at Bad Lauchstädt and Müncheberg and the inherent uncertainty distribution and magnitudes at the spatial scale (the Nuthe river basin). Further on a quantification of land use and soil related uncertainty distribution is assessed.

Plot scale assessment

The evolving of uncertainty with time at the plot scale is demonstrated for a 51 years time series at Bad Lauchstädt and for a 37 years time series at Müncheberg field experimental site for long-term trends of soil organic carbon content.

Uncertainty stemming from variations of model parameters shows the highest effect on soil organic carbon trends at both sites (figure 4.3 b) with a range of 0.55 % C_{org} (+/- 0.275 % C_{org} , +/- 0.13 t C ha⁻² yr⁻¹ Bad Lauchstädt) and 0.11 % C_{org} (+/- 0.055 % C_{org} , 0.05 t C ha⁻² yr⁻¹ Müncheberg, table 4.4) at the end of the simulation period. Overall uncertainty introduced when considering variations of all input factors is for the Bad Lauchstädt site 0.63 % C_{org} (+/- 0.315 % Corg, +/- 0.15 t C ha⁻² yr⁻¹) and 0.13 % C_{org} (+/- 0.065 % Corg, +/- 0.06 t C ha⁻² yr⁻¹) for the Müncheberg site (table 4.4).

The sources soil and climate are contributing less to the overall uncertainty in model output, whereas variations in crop harvest surplus and fertilisation show the least effects (figure 4.3 c – f). Soil and climate input variations lead to 0.17 to 0.2 % C_{org} for Bad Lauchstädt and 0.07 to 0.03 % C_{org} for Müncheberg site (table 4.4). The agricultural management (variations in fertilisation and harvest surplus) contributions to uncertainty are quantified between 0.09 % C_{org} and 0.01 % C_{org} for Bad Lauchstädt and Müncheberg respectively (table 4.4).

Beside the dominating contribution of parameter uncertainty, variations in soil and climate inputs are also of considerable importance. The effect of variations in climate on soil carbon contents is increasing with time showing the long-term and delayed influence of climatic variations for SOC dynamics. In contrast, soil input data variations (initial SOC content, bulk density and clay content) contribution to uncertainty with time remains the same (Müncheberg) or decreases (Bad Lauchstädt).

The relative contribution to overall uncertainty of the respective sources is for both sites of the same order, but the absolute values are lower for the Müncheberg conditions. Additionally same agricultural management practices (same amount of fertilisation for both sites for this study) is resulting in a slightly decreasing soil organic carbon trend for Bad Lauchstädt and an increasing soil organic carbon trend for the Müncheberg site. The tendency of the long-term trend based on all simulation runs of the uncertainty study is in agreement with the long-term trend in measurements for the Bad Lauchstädt site, whereas the Müncheberg site shows a slight increasing trend of all simulation runs when compared to the measurements. For the Bad Lauchstädt case it has to be noted, that the measurements represent 2 t ha⁻¹ yr⁻¹ organic dry matter farmyard manure and no organic fertilisation (figure 4.3 a), whereas the simulation was conducted with 1.2 t ha⁻¹ yr⁻¹ organic fertilisation to ensure same fertilisation schemes for both sites. Nevertheless it can be stated that variations in measurement are of similar magnitude than variations in overall model uncertainty.

For both cases the uncertainty in model simulations increases with time, except for soil related uncertainty at the Bad Lauchstädt site. For the Bad Lauchstädt site, uncertainty of all factors and of model parameters delivers an increasing and decreasing SOC content. This shows that for particular site conditions variations in model parameter values might introduce either an increase in soil carbon (and hence a sequestration of C in soil) or a decrease of SOC content. For the Müncheberg case although, parameter introduced uncertainty shows the same long-term trend of SOC development as the measurements. Further on the absolute range of uncertainty is lower for the Müncheberg case possessing a low soil organic carbon content. This suggests that poor soils (with low soil organic matter contents) are less sensitive to variations in model parameter than soils with high fertility (high soil organic matter contents). In turn changing environmental conditions (e.g. changing climate) introduces higher absolute changes for soil with higher soil organic carbon contents. This is in line with recent findings of Bellamy et al. (2005), where it was found for topsoils in England and Wales that losses in SOC due to changing environmental conditions are proportional to soil organic carbon contents (e.g. losses are higher for soils with higher organic carbon).

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_	Bad Lau([% C	chstädt ^{∝g}]	Münch [% C	eberg «ể]	Bad Lauchstädt	Müncheberg	Difference E	(95 – 5 percentile value) 3ad Lauchstädt	Difference	(95 – 5 percentile value) Müncheberg
	mean start	m ean end	mean start	mean end	90 % confidence [9	 range of uncertainty 6 C_{αz} 	[% C _{org}]	tC ha ⁻² / tC ha ⁻² yr ⁻¹	[% C _{org}]	$tC ha^2 / tC ha^2 yr^1$
	2.1	1.98	0.56	0.62	1.66 - 2.29	0.55 - 0.68	0.63	+/- 7.57 / 0.15	0.13	+/- 2.3 / 0.06
	2.1	1.98	0.56	0.62	1.72 - 2.27	0.55 - 0.65	0.55	+/- 6.62 / 0.13	0.11	+/- 1.9 / 0.05
	2.1	1.86	0.56	0.67	1.77 - 1.94	0.63 - 0.70	0.17	+/- 2.0 / 0.04	0.07	+/- 1.2 / 0.03
	2.1	1.85	0.56	0.67	1.74 - 1.94	0.65 - 0.68	0.2	+/- 2.4 / 0.047	0.03	+/- 0.5 / 0.013
	2.1	1.86	0.56	0.67	1.81 - 1.90	0.66 - 0.68	0.09	+/- 1.1 / 0.02	0.02	+/- 0.36 / 0.0097
	2.1	1.86	0.56	0.67	1.81 - 1.90	0.66 - 0.67	0.09	+/- 1.1 / 0.02	0.01	+/-0.17/0.0046

River basin scale assessment

For the Nuthe basin the spatial scale propagation of uncertainty was assessed for the same sources as for the plot scale (parameters, climate, soil, fertilisation, harvest surplus and all factors). For comparison of variability between the different sources of uncertainty the coefficient of variation (COV %, see equation 4.1) was used, which describes the variation around the mean value of the model realisations. It has to be mentioned that land cover classes like urban areas, industry, water bodies and peat soils (soil organic carbon contents greater than 20 %) have been excluded here, which explains the value 0 % COV. Broad land cover classes croplands, grasslands and forest, and major soil types have been assessed here.

COV [%] ranges for the uncertainty assessment of all input factors is between 4.26 % and 6.74 % COV, for parameters between 2.06 % and 6.37 % COV, followed by soil (2.5 % - 4.76%), climate (0.33 % - 2.5 %), harvest surplus (0.14 % – 0.45 %) and fertilisation (0.14 % – 0.39 %, table 4.5). This introduces a maximal uncertainty of +/- 2.9 t C ha⁻¹, 0.18 t C ha⁻¹ yr⁻¹ for the basin and all factors (mean organic C content in the basin is 43 t C ha⁻¹, first 30 cm in soil). As for the point scale assessment of uncertainty, parameter variations introduce the largest degree of uncertainty. The contribution of input related uncertainty shows the same ranking as for the plot scale assessment, although the magnitude of soil input variations is stronger at the spatial scale with higher COV values (table 4.5). The same can also be stated for climate input variations, but there it is less pronounced. In terms of mean COV values (figure 4.5), soil input derived uncertainty (mainly through init_soc, see section 4.3.1) is even higher than the parameter contribution.

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Fig. 4.4: Spatial distribution of uncertainty for the Nuthe river basin expressed as coefficients of variation values (COV in %, see equation 4.1) for a) all factors, b) parameters, c) soil, d) climate, e) crop harvest management (harv_surp) and f) fertilisation.

The pattern of the spatial uncertainty distribution regarding variations of all factors and parameter variations is similar with clearly distinguishable areas of high and lower uncertainty (figure 4.4 a and b). Especially the southern region of the Nuthe river basin shows high values of COV. There are also some spots with high COV values located in the northern and central part of the basin. In these areas, Luvic Arenosols with high loess contents and croplands with Cambisols are dominating (see figure 4.1). Regarding the sources soil and climate, the pattern is different than for the parameter contribution (figure 4.4 c and d). Parameter induced spatial uncertainty distribution therefore is different than soil or climate induced uncertainty. The agricultural management factors "fertilisation" and crop harvest surplus ("harv_surp", no values for non cropland ecosystems, figure 4.4 e and f) show highest COV values in the north-eastern part and in the southern area of the basin.

When comparing mean COV values with respective standard variations as zonal statistics for the broad land use types cropland, forest and grassland it can be stated that croplands possess the highest COV values and standard variation considering all factors and soils (figure 4.5 a). Slightly different is the ranking for parameter variations with forest and croplands showing similar COV values. Variations in climate, however, are leading to higher COV values in forest ecosystems.

Looking at soil type contribution to uncertainty in terms of COV values, it can be recognised that Gleyic soils (Gleyic Luvisol and Gleysol) and Luvic Arenosol (loess sediments) possess highest COV values both considering all factors and the different sources (parameters, soil, climate, crop harvest surplus and fertilisation, figure 4.5 b). Uncertainty in simulating river discharge and river basin water balance using SWIM was found to be highest in loess regions when compared to other landscapes in the German part of the Elbe river basin (Nuthe river basin is a subcatchment of the Elbe river basin, Hattermann et al., 2005b). Soil physical properties of loess soils (driving the soil water dynamics) are difficult to characterize as loess soils possess an inherent high variablity of soil physial properties like available field capacity or soil porosity (Post et al., 2005a).



Fig. 4.5: Contributions of broad land use types (a) and major soil types (b) in the Nuthe river basin expressed by zonal mean values and standard variations (black lines) of coefficient of variation (COV in %, see equation 1) considering 1) all factors, 2) parameters, 3) soil, 4) climate, 5) crop harvest management (harv_surp) and 6) fertilisation.

These uncertainties stemming from soil properties (and consequently soil temperature and soil water dynamics) are considerably impacting long-term SOC dynamics. Also notable is the highest mean COV value for Gelysol soils in terms of climatic variations. Soils influenced by high water contents and typically higher soil organic carbon contents deliver the highest degree of uncertainty. Here variations of input factors show the highest impacts on soil carbon contents. Parameter variations (especially Q10 and topt, see section 4.3.1) and climate variations change the temperature sensitivity of SOM turnover and delivers higher variability in long-term SOC dynamics.

Parameter variations and variations in soil input data are the clearly dominating sources of uncertainty related to soil types and broad land cover contributions (figure 4.5 a and b). Soils with high soil carbon content (Gleyic soils and Luvic Arenosol on loess sediments) show higher rates of increase or decrease in SOC when soil data (mainly initial SOC content and bulk density, see section 4.3.1) and parameters (mainly kaom and ksyn, see section 4.3.1) are increased or decreased. As noted for the plot scale assessment, soils with higher clay contents are more sensitive to variations in model parameter and input data (soil and climate). The results based on soil types and broad land cover classes are however interrelated with each other, because fertile soils are associated with croplands and less productive soils are associated with forest or grassland. Nevertheless the assessment results in a detection of sensitive sources both in the model system and in spatial pattern of soils and land cover types for the study area.

4.3.3 Implications for long-term soil organic carbon dynamics

The quantified uncertainty provides useful information to interpret simulation experiments to assess e.g. land management impacts on long-term SOC dynamics. For example, crop types and rotational systems impact long-term SOC dynamics (Freibauer et al., 2004; Smith et al., 2000). Beside other studies, crop rotation impacts on long-term SOC contents are estimated around -0.078 to +0.36 t C ha⁻¹ yr⁻¹ (Singh and Lal, 2005) in Norway and -0.13 to +0.1 t C ha⁻¹

yr¹ for the study area (Post et al., 2005c). As noted by Freibauer et al. (2004) and Smith (2004), the related uncertainty of crop rotation impact is very high but was not quantified. According to Post et al. (2005c, chapter 2), the influences of typical crop rotations on long-term SOC trends were estimated for the experimental field sites Bad Lauchstädt and Müncheberg. Relating the here quantified uncertainty contribution stemming from model parameters to crop rotation impacts on long-term SOC dynamics shows that uncertainties are considerable but do not interfere with simulated long-term trends of crop rotation impacts on SOC dynamics (figure 4.6). It has to be mentioned that parameter derived uncertainty, as estimated here, still is rather an overestimation, as for example the synthesis coefficient (ksyn, see table 4.1) is used with a bulk range for all plant types present in the model's data base and not concerning the ranges for the plant types present in the crop rotation only. This implies that the model structure is capable of representing crop rotation impacts under the quantified uncertainty ranges in which (in this case) crop rotational impacts alter long-term SOC dynamics.

Combining plot and spatial scale results for uncertainty stemming from all factors and the examined sources alone shows that the magnitudes are temporally and spatially different. This implies that different natural settings lead to different characteristics of uncertainty magnitudes and that a temporally and spatially quantification of model parameter and input data derived uncertainty is necessary.

Soils with high fertility (as the Bad Lauchstädt soil with high SOM content and loess substrate) and croplands are more sensitive towards variations in model parameters and model input data and feature highest changes in soil carbon dynamics. For croplands, management practices additionally alter the SOC dynamics and variations in these contribute to the higher uncertainty. Soil and climate induced uncertainty is considerable and is more pronounced at the river basin scale. Here the effects of climate and soil condition variations are more effective than at the plot scale, with maximal COV values of 4.76 and 2.5 at the river basin scale compared to 3.4 and 1.7 at the plot scale respectively (table 4.5). For croplands impacts of management practices show stronger effects at the plot scale with

higher maximal COV values (0.3 % for the river basin and 0.7 to 0.26 at the plot scale, table 4.5, figure 4.4 a).



Fig. 4.6: Parameter based uncertainty related to crop rotational impacts on long-term soil organic carbon dynamics (Post et al., 2005c) for the Müncheberg site considering the original rotation (see table 4.2) and a lay arable use (2 years grain crops and 4 years grass) under unfertilised conditions.

The absolute contributions of the uncertainty ranges (expressed here with COV values) however are dependent on the correct assignment of the parameter distribution function definition (PDF, see section 4.3.1). Especially for agricultural management practices the distribution or variation in e.g. application of fertiliser or harvest surplus management might be higher, probably leading to higher COV values. Therefore absolute COV values have to be interpreted regarding the chosen PDF. But relative contributions of the sources assessed here provide relevant information.

Table 4.5: Comparison of uncertainty for the plot scale assessment (Bad Lauchstädt and Müncheberg sites) and river basin scale assessment (Nuthe river basin) expressed as coefficient of variation values (COV in %, see equation 4.1) for all considered sources a) all factors, b) parameters, c) soil, d) climate, e) crop harvest management and f) fertilisation.

Input factors	Nuthe river basin [COV %]	Bad Lauchstädt [COV %]	Müncheberg [COV %]
a) all factors	4.26 - 6.74	6.1	5.1
b) parameters	2.06 - 6.37	4.6	3.4
c) soil	2.5 - 4.76	3.3	3.4
d) climate	0.33 - 2.5	1.7	0.99
e) harv_surp	0.14 - 0.45	0.71	0.53
f) fertilisation	0.14 - 0.39	0.74	0.26

4.4 Conclusion

The assessment reveals that model parameters describing the rate of mineralisation of soil organic matter, the carbon use efficiency parameter (synthesis parameter) and the Q10 value describing the influence of soil temperature on SOM dynamics introduce the highest degree of uncertainty and are the most important factors. Beside the parameter contribution to uncertainty, which dominate both at plot and river basin scale, in particular soil input data and less pronounced climate input data are important, especially at the river basin scale. Here mainly initial SOC content, bulk density and air temperature are important factors. The high importance of the Q10 value is especially relevant for climate change impact studies. But changes in Q10 under changing climatic conditions in spatial and temporal domains is currently not properly resolved (Fang et al., 2005a; Hyvonen et al., 2005; Reichstein et al., 2005b) and needs further research efforts.

For the river basin scale assessment, Gleysol and Luvic Arenosols on loess sediments alongside with croplands could be identified as areas with highest uncertainty in modelling long-term soil carbon dynamics. This is mainly due to difficulties in parameterising soil physical properties of loess soils and due to the fact that variations in SOC contents are higher for soils with higher level of C content (Bellamy et al., 2005). Variations in agricultural management practices (variations in the fertilisation scheme and in crop harvest surplus management) are contributing least to overall uncertainty. But especially here, incomplete knowledge of factors probability distribution functions (PDF), which ranges might be estimated too narrow, might lead to an underestimation of uncertainty. The assignment of factors PDF is central in this approach for the assessment of uncertainty, but was performed using maximal ranges and typical distributions found in literature, based on expert enquiries and own estimates. The fact that PDF's were set to a large range, to assess uncertainty when transferring the model to another regional setting, and not properly reflecting the knowledge of parameter values and their ranging for the study area, rather leads to an overestimation of uncertainty. Model constraining using benchmarking sites and field measurements in the study area would considerably narrow the presented model uncertainty, but was not the scope of this study as we wanted to disclose sources of uncertainty and their possible magnitudes.

The uncertainty assessment for the plot and river basin scale discloses the input data and model parameter related sources of uncertainty. The results obtained are transferable to other temperate regions and can be seen as surrogate for other process-based SOM turnover models based on the present model conceptualisation. Magnitudes of uncertainty are dependent on land cover and soil properties where variations of model factors lead to different impacts on SOC dynamics both spatially and temporally.

This study delivers a spatially and temporally distributed assessment of model parameter and input data uncertainty and importance ranking of the relating factors and provides necessary information to better interpret integrated simulations of long-term soil organic carbon dynamics under changing environmental conditions.

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Chapter 5

Integrated modelling of soil carbon storage in croplands under climate and agro-economic change in a central European river basin

Keywords: *croplands, soil C balance, C flux, climate change, land use change, agro-economy, bioenergy*

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¹Potsdam Institute for Climate Impact Research Dep.: Global Change & Natural Systems P.O. Box 60 12 03, 14412 Potsdam, Germany **Abstract:** Changes in climate and land use caused by socio-economic changes, greenhouse gas emissions, agricultural policies and other factors, are known to affect soil Carbon (C) storage. This study provides an assessment of present day (1951 – 2000) soil C dynamics and of effects of plausible regionalized climate and agro-economic change impacts on soil C storage and net C fluxes to the atmosphere for croplands in the German part of the Elbe river basin for the period 2001 to 2055. Beside possible future climate change impacts, regionalized agro-economic change impacts on soil C storage have been assessed. An increase of surplus-arable land (land which falls out of agro-economic use and becomes abandoned) of approx. 30 % cropland area is anticipated. Based on four scenario runs (surplus land converts to (1) set-aside with black fallow use, (2) ley-arable use, (3) bioenergy crops, and (4) use of harvest by-products for energy generation) trajectories of agro-economic change effects on soil C storage and land-atmosphere fluxes of C have been investigated.

Results indicate that currently (average of 1991 to 2000 period) croplands are a net source of carbon (net annual flux of 11 g C m⁻² yr⁻¹ to the atmosphere). Climatic trend present for the years 1951 to 2000 (+ 0.8 ° C in summer and + 1.4 °C in winter mean temperature) already causes a net flux of 7 g C m⁻² yr⁻¹ to the atmosphere. Future climate change only effects results in an increased net flux of additional 3 g C m⁻² yr⁻¹, but this effect is less than agro-economic changes, assuming set-aside (black fallow use) on surplus arable land, yielding an extra flux of 12 g C m⁻² yr⁻¹ on a basin scale average. Uncertainty stemming from climate change scenario ranges was low with only small alterations in simulated soil C components.

Other uses of surplus arable land (bioenergy crops or ley-arable) lead to a considerable reduction of net flux to the atmosphere with ley-arable use converting the basin from a source to an overall C sink. Additionally substitution effect of fossil fuel resources by bioenergy crops and harvest by-products is substantial (~ 162 800 TJ yr⁻¹, 10¹²Joule). The use of harvest by-products as bioenergy resource although has to be seen critically, as harvest by-products are important for soil C reproduction and for maintaining soil fertility.

Based on this study a present day assessment of soil C balance was obtained together with future soil C development under possible environmental changes. Furthermore, regions suffering largest changes and regions offering potential for soil C sequestration in the Elbe basin could be identified. Hence, this assessment may deliver useful information for decision making in environmental change mitigation.

5.1 Introduction

Changes in the soil carbon (C) pool influence the atmospheric C pool and the soil fertility status as soil C is important for soil aggregation, nutrient availability, water holding capacity and soils buffering ability (Carter and Stewart, 1996). Thus protecting and enhancing soil C is important in terms of climate change mitigation and in terms of sustaining soil fertility as soils are important resources for society. Furthermore, soils contain large amounts of C, approximately twice that of the atmospheric pool (\sim 770 Pg C, 1 petagram = 10¹⁵ g) and 2.5 times that of the biotic pool (\sim 610 Pg) at the global scale (Batjes, 1998; King et al., 2004) and this storage of C in soils is influenced mainly by land use (land cover and land management) and climatic driving forces.

High amounts of soil C (approx. 1-2 Pg C yr⁻¹ during the 1980ies, Houghton, 1996, 1999) have been lost to the atmosphere due to human alterations (e.g. cultivation of soils, changes in land use and cover) beside the atmospheric increase of CO₂ and other Greenhouse gases (GHG) mainly caused by fossil fuel combustion and cement manufacturing. Additionally climate change possibly enhances decomposition and mineralisation and consequently increases the C flux from soils to the atmosphere (Kirschbaum, 1995; Bellamy et al., 2005). The losses of soil C not only increase atmospheric C content but also degrade soils fertility status. This leads to complex series of interactions between the biosphere, hydrosphere, and the atmosphere, which makes integrated assessment of the relevant hydrological, vegetation and biogeochemical processes driven by land use, land management and climate necessary.

It is now widely recognized that it is desirable to protect and enhance soil C contents as this offers a possibility for climate change mitigation (soil C sequestration) and for the improvement of soil quality. Sustainable or recommended land management practices and land uses play a central role in this context (Lal, 2004a). Many studies show that by adopting recommended soil and land management practices considerable amounts of C can be sequestered in soils (e.g. Paustian et al., 1997; Lal and Bruce, 1999; Smith, 2004). Furthermore, protecting and enhancing soil carbon contents are meanwhile central themes in national (e.g. Bundesbodenschutzgesetz BBodSchG, UmwR, 2005) and international regulations (e.g. UNFCCC (UNFCCC, 2005), Kyoto protocol). Quantifying of changes in soil carbon storage in the recent past and under possible future scenarios of climate and land use properties is therefore of pivotal interest.

Hereby croplands play an important role as human intervention was and is high and heterogeneous and therefore croplands soil C status has been affected more intensively than other ecosystems. According to a European scale assessment, croplands are currently estimated to act as a source of carbon, denoting a net carbon flux from land to atmosphere of 300 Tg C yr⁻¹ (1 Tg = 10^{12} g), whereas other ecosystems are estimated to be C neutral or a sink of C (Janssens et al., 2003).

Quantifying the recent past and current state of soil C dynamics in croplands and providing information on how soil C dynamics might unfold under anticipated regionalised climatic and agro-economic changes are presented in this paper for a central European region, the German part of the Elbe River. The basin is dominated by agricultural land use and expects considerable future land use and climate changes. Consequently, following objectives are addressed in this paper:

- Quantifying present-day soil C dynamics in croplands considering a representation of county level crop share distributions, management schemes and climate properties,
- determining future possible trajectories of soil C storage under regionalised agro-economic and climate change scenarios and quantifying climate and land use contribution to soil C storage changes,

• assessing impacts of bioenergy crops, removal of harvest by-products for energy generation beside extensification of agriculture (e.g. ley-arable rotations) and effects of set-aside (black fallow) on future soil C storage.

Furthermore following questions are posed:

- How much carbon input to the soil is necessary to protect or enhance (sequester) soil C stocks in the study area?
- Do anticipated changes in climate deplete soil C stocks, is it due to changes in temperature and/or precipitation?
- What are the impacts of land management and use (crop rotations, harvest byproducts, extensification) on soil C stocks?
- How are the relative contributions of agro-economic and climate change on soil C changes?
- What are the consequences of bioenergy crops for energy generation (bioenergy crops, harvest by-products) on soil C storage and how much fossil energy resources could be substituted?

The study focuses on a spatially and temporally explicit and dynamic assessment of soil C dynamics and tries to derive patterns and magnitudes of soil C changes. The applied model is the eco-hydrological river basin model SWIM (Krysanova et al., 1998). SWIM was recently extended by a process-based, multi-compartment soil organic matter turnover module (Post et al., 2004; Post et al., 2005c). The extended part is a submodel of the forest growth model 4C ("FORESEE" - FORESt Ecosystems in a changing Environment, Grote et al., 1999; Lasch et al., 2002).

The established modelling tool allows an integrated, process-based simulation of hydrological, vegetation and biogeochemical processes in meso- to macro-scale river basins and is used for the transient simulation of soil C dynamics for recent past climate and agro-economic properties and regionalised global scenarios of climate and agro-economic change.

Thereby a newly developed algorithm to generate spatially distributed crop cover patterns on arable land was implemented for a better description of regional properties and differences for croplands in the Elbe river basin. The adopted modelling tool and simulation setup allows assessing different ecosystem services (changes in water quantity and availability, crop growth and yields, soil C and N development). Changes in water availability and crop yields under recent past conditions and future anticipated global changes in the Elbe basin using the same simulation setup is given in a recent study (Hattermann et al., 2005a).

5.2 Methods

5.2.1 SWIM-SCN

The Soil and Water Integrated Model (SWIM, Krysanova et al., 1998) is based on two older model developments, the basin scale eco-hydrological model SWAT (Soil and Water Assessment Tool, Arnold et al., 1994), and the regional model MATSALU (Krysanova and Luik, 1989).

A three-level spatial disaggregation scheme from river basin to subbasins and to hydrotopes is used. Hydrotopes are sets of elementary units in the subbasin, which have the same geographical features like land use, soil type, and average water table depth.

SWIM is a continuous-time, semi-distributed river basin model, which integrates hydrological processes (water percolation, surface runoff, interflow, groundwater recharge, plant water uptake, evapotranspiration, soil evaporation, and river routing), soil temperature, vegetation growth (using a simplified EPIC approach, Williams et al., 1984), water erosion, sediment fluxes and nutrient dynamics (using the PAPRAN model for mineralization, Seligman and Keulen van, 1991) at the river basin scale (Krysanova et al., 1998, 2000). Adjustment of net photosynthesis to altered CO₂ to reflect the CO₂ fertilisation effect on crops is considered through a semi-empirical approach (Krysanova et al., 1999) based on a modification of a mechanistic model for leaf net assimilation (Harley et al., 1992), which takes into account the interaction between CO₂ and temperature. In our assessment, a

possible reduction of potential leaf transpiration due to higher CO₂, was neglected as this effect has only inferior impacts at the scale considered.

SWIM is driven by climate, soil properties (up to ten soil layers are distinguished), land use, and land management and is designed to investigate effects of climate and land use change on hydrologic processes, vegetation growth, and water quantity and quality issues. SWIM has been validated for hydrology, vegetation growth, erosion and nitrogen dynamics for river basins (mainly for the Elbe basin and 12 basins therein) according to a multi-scale, multi-site and multi-criteria approach (Krysanova et al., 1998; Krysanova and Becker, 1999; Hattermann et al., 2005a).

Recently SWIM was extended by a process based, multi-compartment model of soil organic matter dynamics (coupled soil Nitrogen and Carbon turnover, SWIM-SCN). The adopted description is a sub module of the forest growth model 4C describing soil organic matter dynamics for forest ecosystems (Grote et al., 1999; Lasch et al., 2002). The model extension implemented fits to the level of process complexity of other process descriptions in SWIM, and was developed taking into account constrains of data availability and model parameterisation (Post et al., 2005c).

In order to describe the carbon (C) and nitrogen (N) budget, organic matter is differentiated into Active Organic Matter (AOM) as soil organic matter pool and Primary Organic Matter (POM) as litter pool. The latter is separated into up to five fractions for each vegetation and crop type (stems, twigs and branches, foliage, coarse roots, and fine roots). For all pools of active and primary organic matter and each soil layer the carbon and nitrogen content are considered. The carbon and nitrogen turnover into different stages (pools) is implemented as a first order reaction (Parton et al., 1987; Franko, 1990). The processes are controlled by matter specific reaction coefficients. Heterotrophic (substrate induced) soil respiration is calculated through the decay of POM and AOM pools per day. Effects of soil temperature, soil water content and soil pH status on decomposition, mineralisation, ammonification and nitrification are considered through reduction functions (Franko, 1990).

The soil C and N quantity (POM) entering the soil is calculated for crops using the simulated crop yield according to an empirical relation for main crops (Franko, 1990; Franko et al., 1997a), and is then allocated based on literature surveys on crop harvest residues (above and below ground, Klimanek, 1987, 1997). The empirical relationship is based on a meta-analysis of measured crop residue amounts in the study area (Klimanek, 1987, 1997) and provides reliable estimates of C and N entering the soil (Franko et al., 1997b; Post et al., 2005a, chapter 2).

Further on, standard literature values for C content and C/N ratios in POM fractions, vegetation types and organic fertiliser determine the C and N quantities in the POM fractions (Franko et al., 1997a; Klimanek and Schulz, 1997; Nicolardot, 2001). The fine and coarse roots are further distributed into the soil layers according to rooting depth and a root mass allocation scheme (Jackson et al., 1996).

A detailed description and an assessment of land management impacts on soil C dynamics using the extended Model SWIM-SCN can be found in (Post et al., 2005c, chapter 2), testing of related processes (soil water and temperature dynamics, crop growth and yield assessment, soil Nitrate dynamics and long-term soil C trends) is documented in (Post et al., in print and chapter 3) and a quantification of input data and parameter uncertainties at the plot and river basin scale is described in (Post et al., 2005b and chapter 4).

The combination of empirical and physically based descriptions allows applying the model on a daily time step at the regional scale, considering the spatial heterogeneity of the landscape and possible feedbacks between vegetation, hydrological processes, nutrient transport and retention and soil C and N dynamics. SWIM can be assigned to hydrological models of intermediate complexity (HYMIC, Bronstert, 2003).

5.2.2 The Elbe river basin

The Elbe is one of the largest rivers in Central Europe and drains into the North Sea. The assessment was undertaken for the German part of the Elbe river basin. It covers an area of 80 256 km² (total basin area is approx. 148 000 km²) from the Czech border to the North Sea. About 52 % of the basin area is covered by croplands, 29 % by forest, 6 % by settlements and industry and 5 % by lakes, mining pits and other land use forms.



Fig. 5.1: Overview of broad landscape units (lowland alluvial formed, lowland periglacial formed, loess area and mountains) present in the German part of the Elbe river basin.

Climatically, the Elbe basin marks a transition from atlantic to continental climate. The basin is one of the driest regions in Germany, with mean annual precipitation below 500 mm in the lee of the Harz mountains (western part of the basin), where the loess plains with high agricultural productivity are located. The long-term mean annual precipitation over the whole basin is 659 mm in the period 1951-2000 (ATV-DVWK, 2000).

Hydrologically, the area can be subdivided into three main subregions (see Figure 5.1): (1) the mountainous area in the south, approximately 20 % of the total area, (2) the hilly mountain foreland, predominantly covered by loess soils (approximately 28 %), and (3) the undulating northern lowlands, approximately 52 % of the total area (see Figure 5.1). The northern lowlands are formed by mostly sandy glacial sediments (periglacial landscape) and drained by slowly flowing streams with broad river valleys and alluvial soils. They have a low agricultural productivity and water holding capacity. The soils in the loess region, chernozems and luvisols, are mostly loamy and tend to have layers with low water permeability. The sediments normally have high field capacities and nutrient supply, and therefore the loess subregion is an area with very intensive agricultural land use. The soils in the mountains, mainly thin cambisols, are formed by weathering products and redeposited rocky materials. The mountainous areas are often covered by forests and grassland.

5.2.3 Characterisation of climate

Reference situation

Necessary climatic data on a daily time step were obtained from 84 meterological stations (minimum, maximum and average daily air temperature) and from 369 precipitation stations (precipitation, global radiation and relative humidity) located in and around the Elbe basin. Continuous time series are available from 1951 to 2000 and were used for climate interpolation using an inverse distance technique, taking the digital elevation model as additional information for the spatial interpolation (Hattermann et al., 2005a).

Analysis of reference climate data (1951 – 2000) showed that the average yearly precipitation of 659 mm in the study area is significantly lower than the German average (789 mm). Due to the transition from atlantic / maritime to continental climate from northwest to southeast in the Elbe basin, the north western regions feature higher precipitation and lower average yearly temperatures than the south eastern regions. Important for regional climate are the mid mountain ridges in the southern and southwestern part of the basin. In the lee regions of the mid mountain ridges, precipitation amount are lowest, ranging below 500 mm. The amount of precipitation in the Elbe basin is higher during the summer period than during the winter. The loess region (see figure 5.1), with intensive agricultural use, features the lowest annual precipitation. Average temperature from 1951 to 2000 in the basin is 8.6 °C, lowest in the mountain regions (7.7 °C), 8.8 °C in the loess region and 8.7 °C in the lowlands.

The observed significant climatic trend in the Elbe basin (1950 – 2000, Wechsung et al., 2005) for precipitation indicates a decrease in summer precipitation of about 46 mm and an increase in winter precipitation of about 50 mm. The increase in temperature of 0.8 °C for the summer season is lower than the increase of 1.4 °C for the winter season. The significant increase of temperature, especially in the winter season, together with long-term trends in precipitation are important for plant growth, hydrological properties and soil C and N processes.

Regionalized climate change scenario

The climate change scenario is based on results of the Hamburg ECHAM4-OPYC3-T42 Global Circulation Model (GCM) (Röckner et al., 1999) driven by the IPCC SRES (Intergovernmental Panel on Climate Change – Special Report on Emission Scenarios) emission scenario A1 (Nakicenovic and Swart, 2000). The IPCC SRES A1 temperature scenario selected gives a rather moderate temperature increase of approximately 1.4 °C up to 2055. The resulting climate patterns were regionalised by Gerstengarbe and Werner (2005) using the statistical downscaling model STAR (STAtistisches Regionalmodell, Gerstengarbe et al., 1999, figure 5.2). Long-term transient time-series of the possible future climate (2000 - 2055) were calculated in such a way, that they reflect the temperature changes calculated by the GCM in the given scenario. Furthermore they reflect the observed climate properties (frequency distribution, annual and inter-annual variability and persistence of the main climate characteristics) of meteorological stations (1951 – 2000).

All other meteorological variables are adjusted consistently applying a non-hierarchical cluster analysis (Gerstengarbe et al., 1999) in relation to the temperature changes (using the anticipated air temperature trend) ensuring the persistence of their statistical properties. This leads to regionalized climate change scenario for each meteorological station.

STAR produced 100 long-term transient time series of the possible future climate (2000 – 2055) under the consideration of observed long-term climate patterns of the meteorological stations in the Elbe river basin by incorporating a conditioned Monte Carlo approach in the downscaling process (Gerstengarbe and Werner, 2005). The 100 realizations cover the possible range of climate change under various scenario conditions in the German Elbe basin.

Six realisations have been selected based on simulated precipitation (mean of the 2046 to 2055 period) properties (temperature trend is the same for all realisations in the scenario period) as climate change scenarios. One realisation representing the most probable scenario for the study area (realisation 32), two representing most wet and most dry conditions in the period 2046 – 2055 (realisations 56 and 68 respectively), one representing the statistical median of 100 realisations (realisation 50) and two representing the 5 and 95 percentiles (realisation 77 and 5 respectively). Realisation 32 (Gerstengarbe and Werner, 2005) as most probable was used for regionalised climate change assessments, the others to derive scenario uncertainty (figure 5.2, step 1).

5.2.4 Characterisation of land use and crop share properties

Explicit knowledge of crop rotations and crop sequences at models lowest disaggregating levels (e.g. hydrotopes in our case or raster cells in other models) generally are not considered in regional scale modelling, and broad simplifications are used instead. Most often one typical crop rotation (or even one major crop) for the study area is used (lumped approach) or several runs are performed one after the other changing the crop rotation (or crop). For some research questions this assumption might be appropriate. But explicit, spatially disaggregated information on crop rotations and crop shares is important because different crops and associated management practices influence regional soil C dynamics. Therefore in our case, a so called "crop generation" algorithm has been developed (for a detailed description see Wechsung et al., 2006) and implemented into SWIM to derive reference and scenario crop cover patterns meeting the respective regional crop spectrum and crop shares.

Reference situation

To translate county level agricultural land use statistics (crop shares at county or district level) onto the lowest level of the spatial disaggregation scheme (the hydrotopes) in SWIM, 23 typical crop rotation types for the study area were assigned (table 5.1). Further on, each hydrotope was assigned to one of seven soil fertility classes. The seven soil fertility classes were derived based on climate and soil properties as expressed in potential winter wheat simulations. Based on simulated potential winter wheat yields in the study area, 7 percentile yield classes were derived and assigned as soil fertility class to each hydrotope in a pre-processing step. The commercially more valuable crop shares with generally higher nutrient and water demand were allocated to areas with fertile soils and vice versa, as recorded in the local crop statistics. In a pre-processing step (for details see Wechsung et al., 2006) probabilities of occurrence of each crop rotations are calculated (table 5.1). Thereby the constraint that the simulated crop distributions agree with the county statistics (based on average statistics of 1996 to 1999) is ensured (Wechsung et al., 2006).
able 5.1 : Overvi

Rotation	crop \$	ied nem	ies and	c rop n	umb er	2		cumulative	o rob ab ilities p	ter fertility cl	lass - referenc	e (scenario)		crop type acronyms st
Number	I	I		I			class 1	class 2	class 3	class 4	class 5	class 6	class 7	
1	36	25	36	52	38	53	(0) O	(0) O	0) 60:0	0) 60:0	0.14(0)	0.13(0)	000	WB CC SM WB CC SB WB CC SB
11	4	4	4	, 22	4	25	0.16 (0.16)	0.09 (0.09)	0.16(0)	(0) 60 0	0.14(0)	0.13(0)	000	PG FG WR CC SE WR CC SM
en	4	4	22	4	, 8	5	0.16 (0.16)	0.09 (0.09)	0.16 (0.06)	0.12 (0.01)	0.14(0)	0.13 (0)	0	KL KL CC SB WW WB WW
4	4	25	4	4	4	25	0.28(0.19)	0.09 (0.09)	0.16 (0.06)	0.12 (0.01)	0.14(0)	0.13 (0)	00	wr öc sm wr wr oc sm
÷	4	30	4	4	우	43	0.36 (0.19)	0.22(0.1)	0.24(0.06)	0.23 (0.01)	0.24(0)	0.33(0)	0.1 (0)	wr cc pot wr wr ra wr
Q	4	육	4	4 2	4 9	42	0.36 (0.19)	0.22 (0.1)	0.36 (0.06)	0.23 (0.01)	0.24(0)	0.33 (0)	0.1 (0)	ŴŴ_ŔA_ŴŘ_ŴŴ_ŔÂ_ŴŔ
۲	4	육	4	4	े वि	4	0.52 (0.19)	0.31 (0.1)	0.36 (0.09)	0.27 (0.03)	0.28 (0)	0.33(0)	0.1 (0)	WR_RA_WR_WR_RA_WR
œ	71	11	71	, 23	4	22	0.54 (0.21)	0.32 (0.11)	0.37(0.1)	0.27 (0.04)	0.29 (0.02)	0.34(0.01)	0.1 (0)	FG_FG_FG_CC_SU_WW_CC_SB
6	4	4	23	4	8	25	0.54(0.21)	0.32(0.11)	0.37(0.1)	0.32 (0.12)	0.33 (0.02)	0.37 (0.07)	0.22 (0.16)	KL KL CC SU WW WB CC SM
10	71	11	71	, 23	4	22	0.57 (0.23)	0.34(0.12)	0.42 (0.15)	0.34(0.14)	0.34 (0.04)	0.38 (0.08)	0.22(0.17)	FGFGFGCCSUWWCCSB
II	53	52	4	52	5	5	0.57 (0.23)	0.45 (0.2)	0.44 (0.17)	0.43(0.17)	0.57 (0.24)	0.63 (0.25)	0.43 (0.26)	cc su cc sb ww cc sb ww ww
11	4	4	20	8	4	25	0.57 (0.27)	0.45 (0.23)	0.45 (0.17)	0.43(0.17)	0.57 (0.28)	0.63 (0.25)	0.43 (0.27)	KL KL CC FOT WB WR CC SM
13	8	4	36	4	25	52	0.57 (0.3)	0.45 (0.31)	0.45 (0.17)	0.43 (0.17)	0.57 (0.3)	0.64(0.4)	0.51 (0.3)	cc_pot_wr_wb_wr_cc_sm_cc_sb
14	52	4	4	52	4	22	0.57 (0.3)	0.49 (0.31)	0.45 (0.2)	0.43 (0.22)	0.57 (0.3)	0.64 (0.4)	0.51 (03)	SM_WR_WR_CC_SM_WR_CC_SB
15	52	8	4	4	4	25	0.57 (0.31)	0.49 (0.32)	0.45 (0.28)	0.43 (0.33)	0.57 (0.34)	0.64(0.47)	0.51 (0.45)	CC SB CC POT WW WR WW CC SM
16 1	25	4	25	بر	न	32	0.59 (0.31)	0.7 (0.32)	0.61 (0.28)	0.69 (0.33)	0.58 (0.34)	0.65 (0.47)	0.52 (0.45)	SM WR CC SM WB RA CC SB
71	52	4	8	4	 8	25	0.59 (0.31)	0.7 (0.32)	0.61 (0.28)	0.69 (0.33)	0.71 (0.39)	0.75 (0.47)	0.73(0.47)	CC_SM_WW_WB_RA_WB_CC_SM
18	25	99	4	8	98	25	0.59 (0.31)	0.7 (0.32)	0.61 (0.28)	0.69 (0.33)	0.71 (0.39)	0.75 (0.47)	0.73 (0.47)	cc_sm_wb_wr_wb_wb_cc_sm
19	4	4	-	52		52	0.59 (0.31)	0.7 (0.39)	0.61 (0.28)	0.69 (0.33)	0.71 (0.44)	0.75 (0.47)	0.73(0.47)	WR_WR_CC_ST_CC_SM_CC_ST_CC_SM
20	Я	52	1	52	-	52	0.91 (0.37)	0.79 (0.39)	0.85 (0.4)	0.69 (0.39)	0.71 (0.44)	0.75 (0.47)	0.73(0.47)	WB_CC_SM_ST_CC_SB_CC_ST_CC_SB
21	4	4	육	5	5	육	0.94(0.4)	0.82 (0.44)	1 (0.44)	0.88 (0.46)	0.95 (0.52)	0.94(0.58)	0.95 (0.62)	WW_WW_RA_WW_WW_RA
ដ	4	4	39	ر	5	39	0.98 (0.41)	0.93 (0.48)	1(0.48)	0.93 (0.54)	0.95 (0.63)	0.94 (0.66)	0.95 (0.7)	ww_ww_wb_ww_wb
33	1	1	1	1	1	1	1(1)	1(1)	1(1)	1(1)	1(1)	1(1)	1(1)	ST_ST_ST_ST_ST_ST
23 set-aside	п	-	-		-	1	1(1)	1(1)	10	10	1(1)	13	1(1)	ST_ST_ST_ST_ST ST_ST_ST_ST_ST
23 ley arab le	52	23	12	ខ	२ १	ន	<u>:</u>	() () ()	<u>:</u>	<u>:</u>	3	<u>:</u>	() () ()	FG FG SU WW SB
25 bioenrgy	₹	4	3	3	a a	3	1(1)	1(1)	1(1)	1(1)	1(1)	1(1)	1(1)	KA WK SM SM SM CC SB
* crop rotat	ions:	first	year	alway	ys sp.	ning	barley (S	B), please	note that	some rot	ation inclu	ude cover	crops (CC)	between main crops.
abbreviat	ions: (20-	Cov	er Cr	op, 1	WB-	- Winter]	Barley, SN	M - Silage	: Maize, S	3B – Sprir	ng barley,	FG – Field	Grass (ley-arable use),
WR - WI	nter R	ye, 1	- MW	- Wii	nter	Whe:	at, POT –	Potato, R	A - Wint	er Rape,	SU – Šug	ar Beet, K	L - Clover,	ST – set-aside.

Regionalized agro-economic change scenario

The land use scenario is based on anticipated global crop market developments for the IPCC-SRES A1 storyline (liberalisation of markets), which were produced by the global agroeconomic model WATSIM (World Agricultural Trade Simulation Model, von Lampe, 1999, figure 5.2).



Fig. 5.2: Flow chart of modelling procedure and used modelling tools (adopted from Hattermann et al., 2005a).

Under the SRES A1 an increase in set-aside area (land which falls out of agro-economic use becoming surplus to the requirement of food and fibre production) is anticipated for Europe (Rounsevell et al., 2005). Results obtained by WATSIM were then used by RAUMIS (Regionales Agrar- und Umweltinformationssystem für Deutschland, Henrichsmeyer et al., 1996) to optimize the potential operational income of farmers under socio-economic change at the county level (figure 5.2). The optimization was performed for the timeframe 2016 to 2025. It has to be noted that land use change scenarios are static (no land use change with time), assuming that future change occurs immediately for the first year in the simulation period 2001 to 2055.

Under these assumptions an increase of set-aside arable land (arable land falling out of use due to economical constraints) of approx. 30% cropland area is anticipated (Gömann et al., 2005). Locally, on poor soil, the set-aside land area is up to 60 % under this scenario assumption. The cereal production in the Elbe basin, as example, will decrease by about one third. Especially rye production will decrease considerably on poor soils.

RAUMIS calculates corresponding county specific crop distributions, which are then translated in a pre-processing step onto the hydrotope level in SWIM based on the "crop generator" algorithm (step 2 in figure 5.2, Wechsung et al., 2006). The agro-economic changes at the county level are consequently translated onto the hydrotope level in SWIM (steps 2 and 3 in figure 5.2 and table 5.1).

5.2.5 Characterisation of agricultural management

Beside the characterisation of crop shares at the hydrotope level of SWIM, meeting the constraints of reference and scenario county level crop share statistics and soil fertility, further agricultural management practices have to be assumed for the study area. Here mainly fertilisation practices and harvest management have to be described.

Fertilisation amount and timing has been parameterized based on good management practices and general fertilisation recommendation provided by national authorities (MLUR, 2000). Each crop type receives typical amounts of inorganic (NPK fertiliser) and organic (farmyard manure) fertilisation.

The amount of farmyard manure is applied to root and tuber crops. As farmyard manure contains amounts of straw and other harvested by-products, this amount was considered in the parameterisation of harvest by-products (grain straw, potato haulm sugar beet leaves and so on) removal from the fields. The amount and timing of organic and Table 5.2: Parameterisation of fertilisation properties (organic and inorganic) for the timing (DOY, day of year) and the amount of fertilisation for each crop type.

crop name	acronym	crop	time of fertilisation	amount of	type and unit
potato	POT	number 20	110	IETUIISAUUTI 60	inorganic: ka N ha ⁻¹
			295	20000 *	organic farmyard manure, kg fm ha ⁻¹
summer barley	SB	22	79	50	inorganic; kg N ha
sugar beet	SU	23	100	80	inorganic; kg N ha-1
I			270	2000	organic farmyard manure, kg fm ha
silage maize	SM	25	110	20	inorganic; kg N ha- ¹
			295	2000	organic farmyard manure, kg fm ha-'
winter barley	82	36	60 - 110	60 - 60	inorganic; kg N ha- ¹
rape	RA	40	90 - 120	100 - 80	inorganic; kg N ha- ¹
winter nye	R	42	60 - 110	60 - 50	inorganic; kg N ha- ¹
winter wheat		45	60 - 110 - 140	60 - 50 - 50	inorganic; kg N ha- ¹
field grass	Ð	47	90 - 155 - 185	100 - 50 - 50	inorganic; kg N ha- ¹
cover crop	00	51	ı		no fertilisation
clover	Ϋ́	71	ı		no fertilisation
Set-aside	ST	, -			no fertilisation

inorganic fertilisation remains the same throughout the simulation period from 1951 to 2055 as only effects of land cover and climate change are investigated here.

Further on it is assumed in this study that there is a closed budget of harvest byproducts in the system. That means that over a certain time period all produced harvest byproducts are entering the soil either as crop residuals directly or in form of organic fertilisation. Thereby a loss of 10% is supposed due to e.g. harvest management and straw decomposition in livestock farming.

Regional scale information on the fraction of harvest by-products (e.g. grain straw) remaining on the fields is sparse, especially for the 1950 to 1980 period (Smith et al., 1997a). Descriptions on straw management in the UK and extrapolated to the European Union are provided by Smith et al. (1997a) assuming that until starting 1980 only 2 % of straw was incorporated in the soils, increasing to about 18 % in the late 1980ies (Stainforth, 1982; Smith et al., 2000). Main reason for the low fraction of straw incorporated is given due to straw burning at the fields, whereby as a result of straw burning regulations in the middle 1980ies the straw fraction increased. But straw burning played (if at all) only a minor role in the study area (M. Roschke, MLUR Brandenburg, personal communication 21.12.2005). Prior to German reunification agriculture was organised in so called "Landwirtschaftlichen Produktionsgenossenschaften, LPG". Here, straw predominantly remained at the fields or was used in livestock farming and returned as organic fertiliser to the fields. Investigations by Schmidt and Osterburg (2004) for Germany estimate the amount of harvest by-products remaining on the fields with \sim 80 % of harvest by-products produced, whereby 17 – 28 % of harvest by-products produced serve as fodder and farmyard straw incorporation. Changes of harvest by-products vary with crop yields and did not change significantly throughout the recent past (Schmidt and Osterburg, 2004). The amount of harvest by-products is calculated based on the simulated crop yields and standard main product to by-product ratios per crop species are used (MLUR, 2000; Lal, 2005). Carbon content of by-products is crop specific based on literature values (Franko, 1990; Klimanek, 1997; Klimanek and Schulz, 1997).

acronym	crop number	ratio	source
POT	20	1:0.2	Lal (2005), MLUR (2000)
SB	22	1:0.9	MLUR (2000)
SU	23	1:0.7	MLUR (2000)
SM	25	-	
WB	36	1:0.9	MLUR (2000)
RA	40	1:1.5	Lal (2005)
WR	42	1:0.9	MLUR (2000)
WW	45	1:0.9	MLUR (2000)

Table 5.3: Dry weight ratio of harvest by-product to crop yield for different crops.

Harvest by-product management remains the same throughout the simulation period (1951 - 2055). Although harvest by-products have the potential being used as energy source (biomass burning, biogas production), beside the incorporation into the soil for soil C reproduction and the use in livestock farming.

For the reference situation (1951 to 2000) four simulation runs have been performed to mirror the impacts of harvest by-product incorporation into the soils on soil C dynamics (table 5.4).

Table 5.4: Description of simulation assumptions during the reference period (1951 to 2000) for theparameterisation of harvest by-product percentage remaining on the fields. Please note that Ref07assumptions are used also for future scenario cases (2001 to 2055).

	Acronym	Description	Model drivers	Annotation
	Ref00	Reference period, Harvest by-products remaining on fields: 0 %	nate	unts est ctices
e peri	Ref05	Ref erence period, Harvest by-products remaining on fields: 50 %	nd clin	to be 2000_2
erenci 1951 -	Ref07	Ref erence period, Harvest by-products remaining on fields: 70 %	use al refere	isatior cording gemer MLUR
()	Ref08	Ref erence period, Harvest by-products remaining on fields: 80 %	land	Fertil acc manag

Thereby fractions of 0.0 ("ref00"), 0.5 ("ref05"), 0.7 ("ref07") and 0.8 ("ref08") of total harvest by-products have been assigned to each simulation run to derive both the

uncertainty in field straw incorporation and the consequences of harvest by-products on soil C storage (table 5.4).

5.2.6 Simulation set up, scenario assumptions and target results

Necessary pre-processing steps, calibration and validation of hydrological and crop growth processes for the study area is described in detail in Hattermann et al. (2005a), where the same simulation set up was used to investigate changes of water availability and crop yields under global change impacts in the Elbe basin. Spatial input data used are the European land cover data set CORINE (Dollinger and Strobl, 1996) to describe land use, and the soil map of the Federal Republic of Germany (scale 1:1,000,000, (Hartwich et al., 1995)).

Concerning the reference simulation, climate and agricultural land use is assumed as described above. A fraction of 0.7 (70 % of harvest by-product remaining on fields) is assumed for the scenario period. As reference climate (1951 to 2000) already shows a trend in temperature (increase of 0.8 K for summer and 1.4 for winter period), one run was created using meteorology of 1965 (typical meteorological year in the reference period as derived from data analysis, Krysanova et al., 2005), to assess the impacts of the climate trend present from 1951 to 2000 on soil C dynamics ("ref07_1965" case). The year 1965 can be characterized as average in terms of seasonal dynamics of evapotranspiration, runoff and precipitation amounts for the reference period (Krysanova et al., 2005). Average temperature for that year is 7.6 °C and one degree lower than the mean of the period 1951 to 2000.

To assess climate and land use change and combined effects in the scenario period, three simulation runs were performed (CCo, LCo, CLC1, table 5.5). Uncertainty of climate change on soil C dynamics was derived based on six runs, which are described in table 5.5 (CLC2 to CLC6).

The land use scenario (see above) anticipates an increase of set-aside agricultural land of approx. 30 % cropland area ("surplus" arable land). Different land use properties can be assigned to this area (table 1), to evaluate their impact on soil C storage. Four cases of surplus

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		Acronym	Description (simulation period)	Model drivers	Annotation
reference conditions		Ref07	Ref erence period (1951 - 2000)	land use and climate reference	Fertilisation amounts according to best management practices (MLUR 2000), harvest by-products remain to 70 % on the fields (Schmidt and Osterburg, 2004)
	and w) on th set- tuse	ပိပ	Climate Change effects only (2001 - 2055)	land use reference and climate scenario	Fertilisation amounts and harvest by-products as Ref condition, climate change scenario realisation 32 (most probable)
	and lanc ffects wi lack fallo lack fallo lack fallo	LCo	Land Use Change effects only (2001 - 2050)	land use scenario with surplus arable land as set-aside (blak fallow) and climate reference	Fertilisation amounts and harvest by-products as Ref condition, surplus arable area: set-aside use (black fallow, see table 1), observed reference climate
รเ	climate change e aside (b surplu:	CLC1	Climate and Land use Change effects (2001 - 2055)	land use scenario with surplus arable land as set-aside (blak fallow) and climate scenario	Fertilisation amounts and harvest by-products as Ref condition, surplus arable area: set-aside use (black fallow, see table 1), climate change scenario realisation 32 (most probable)
no condition	Climate change scenario uncertainty	CLC2 CLC6	Climate change scenario uncertainty (2001 - 2055)	land use scenario and climate scenarios	Fertilisation amounts and harvest by-products as Ref condition, surplus arable area: set-aside (black fallow, see table 1), climate scenarios: most wet and most dry scenarios, 5 and 95 percentiles, median realisation
euaos	and se uses of s change	CLC1-Ley	as CLC1 but Ley. arable rotation on surplus arable land (2001 - 2055)	land use scenario with surplus arable land as ley-arable rotation and climate scenario	Fertilisation amounts and harvest by-products as Ref condition, surplus arable area: ley arable use (3 yrs grass, 3 years cash crops, see table 1), climate scenario 32 (most probable)
	nd land use h alternativ lus arable l	CLC1-Bio	as CLC1 but bio energy rotation on surplus arable land (2001 - 2055)	land use scenario with surplus arable land as bioenergy rotation and climate scenario	Fertilisation amounts and harvest by-products as Ref condition, surplus arable area under scenario conditions: bioenergy rotation (see table 1), climate scenario 32 (most probable)
	climate a effects wit surp	CLC1-Harv	as CLC-Bio and exporting 80 % of Harv est by- products from fields (2001 - 2055)	land use scenario with surplus arable land as bioenergy rotation and climate scenario	Fertilisation amounts as Ref condition, surplus arable area: bioenergy rotation and 80% of croplands harvest by-products exported from fields for energy generation, climate scenario 32 (most probable)

arable land use are distinguished. First, surplus arable land is used as set-aside area, which is kept open by the farmer and used as black fallow (e.g. weed-killing) ("set-aside", table 5.1 and CLC1 in table 5.5). This case states an extreme future use as ley-arable or other extensified agricultural uses are more probable. Second surplus arable land is used extensively through a ley-arable rotation ("ley-arable", table 5.1 and CLC1-Ley in table 5.5), third a typical bioenergy rotation as expected for the study area and based on the fact that surplus arable land is located on less productive soils ("bioenergy", table 5.1 and CLC1-Bio in table 5.5) and fourth the same bioenergy rotation as described but in addition a usage of harvest by-products (80 % of harvest by-products exported from the fields) as bioenergy source on total cropland area (CLC1-Harv, table 5.5).

The assessment focuses on soil carbon dynamics, whereby the development of the carbon content in the topsoil (up to the ploughing depth of 30 cm) and the entire soil is considered. The entire soil is defined as the soil depth where water still is available for plants (rooting depth).

Further on the exchange of carbon between the biosphere and the atmosphere (Net Biome Exchange, NBE), the Net Primary Production (NPP) and the Net Ecosystem Exchange (NEE) of C is considered alongside with heterotrophic soil respiration. To characterise the amount of C entering the soil, information on plant derived C input, harvest by-products and C input from organic fertilisation are given. NEE and NBE is calculated as follow:

$NEE = R_h - NPP$	(eq. 5.1)
$NBE = NEE + L_d;$	(eq. 5.2)
$L_d = H - F$	(eq. 5.3)

Where L_d is the loss by major episodic disturbances determined here as input of C with organic fertilisation (F) and C removed by harvested crop yields (H). Other ecosystem disturbances as e.g. fire are not considered. Negative values of NBE denote a net flux of C from the atmosphere to the land, e.g. an increase of soil C.

fertility class	2	9	9	4	3
rotation number scenario	21	23	23	23	20
rotation number reference	11	21	21	16	10
soil	12 - Gelysol	26 - Podzoluvisol	46 – Luvic Arenosol (loess. Sedim.)	59 – Cambic Arenosol	59– Cambic Arenosol
landscape unit	lowlands (alluvial)	lowlands (periglacial)	loess region	core officiations	
acronym	lowland-1	low/and-2	loess-1	mount-1	mount-2

Table 5.6: Selected hydrotopes to exemplary describe local effects of climate and land use change on soil C storage and fluxes.

The temporal dynamics are given for the entire basin and croplands only, excluding organic soils with C contents above 15 %. In addition results for selected sub-regions (table 6) based on the landscape units, characteristic soil types, typical rotations and their changes under scenario conditions are provided.

Furthermore maps are provided for the periods 1991 – 2000 (reference baseline) and 2046 – 2055 (scenario baseline) highlighting the spatial changes in soil C storage.

5.3 Results

5.3.1 Regionalisation of agricultural land use

The study area consist of 125 counties for which agricultural statistics on the crops shares were translated by the "crop generation" algorithm to the hydrotope level in SWIM. Comparisons for generated crop shares with agricultural statistics for the period 1996 to 1999 are presented for results aggregated on the state level (German Bundesländer).

Shares for arable crops in the State of Brandenburg as derived through agricultural statistics (years 1996 -1999) are in good agreement with the generated representation in SWIM. Main crop types with highest shares (as winter wheat, winter rye, winter barley, summer barley, rape, silage maize) comprise about 77 % of total crop area derived through statistics and 76 % after re-allocation using the crop generation algorithm. The correlation between state level statistics and generated crop shares for the Elbe basin per states and crops (table 7) are between 0.99 (State of Brandenburg and Mecklenburg-Western Pomerania) and 0.91 (State of Saxony).

a) statistics



b) after re-allocation



Fig. 5.3: Use of arable crop land in Brandenburg: a) taken from statistics b) after reallocation applying the crop allocation algorithm (adopted from Wechsung et al., 2006).

_	Western States		Eastern	n States		
-	Schleswig-Holstein (SH)	Brandenburg	Mecklenburg- Western Pomerania	Saxony	Saxony- Anhalt	Thuringia
_	0.95	0.99	0.99	0.91	0.99	0.94

Table 5.7: Correlation between original and re-allocated crop shares for the Elbe basin per state and
across crops (1996 – 1999).

The regional agro-economic model RAUMIS provided county level changes of crop shares for the period 2016 – 2025. The changes under assumed liberalization of global crop markets are considered in the land use scenario based on the IPCC SRES A1 storyline. The area of set-aside arable land increases from about 7.0 % to 29.8 % on average for the Elbe basin, with a strong regional variation (poor soils fall out of use). The share of winter wheat drops from 26.4 % to 21.7 % and that of silage maize from 7.0 % to 2.0 % (Hattermann et al., 2005a). A spatial figure of arable land cover patterns for one year in the reference situation and for one year under future land use change is given in figure 5.4, high lightening the areas becoming set-aside.

5.3.2 Reference period (1951 – 2000)

C input derived from organic fertilisation (farmyard manure) is the same for all cases (ref00, ref05, ref07, ref07 and ref07_1965) and accounts for 20 g C m⁻² yr⁻¹ on average. Average soil C input from crop residuals is 88, 147, 171, 183 and 185 g C m⁻² yr⁻¹ for ref00, ref05, ref07, ref08 and ref07_1965 respectively (table 5.8). Simulation under climate conditions for the year 1965 (ref07_1965) yields highest soil C input from crop residuals (table 5.8) and also average yields where higher as ref07.

Simulation of soil water content delivered no significant trend throughout the reference period with mean soil water content of 140 mm and a standard deviation of 5.6 mm as a basin average. Soil water content features same temporal patterns as yearly amounts of precipitation.



Fig. 5.4: The change in crop distributions for one year in the reference period (top) and in the scenario period (down).

The observed temperature trend in the reference period translates into simulated soil temperature in the topsoil. Average soil temperature is 8.3 °C with a standard deviation of 0.57 based on yearly basin scale averages and increases by 0.67 °C in the reference period.

Soil carbon storage in the first 30 cm (topsoil) increased for the ref07_1965 case by 4.5 g C m⁻² yr⁻¹ on average from 1.53 % Corg (6631 g C m⁻²) in the year 1951 to 1.6 % Corg (6892 g C m⁻²) in the year 2000. Ref_07 and ref_08 show a slight increase of soil C content, whereas soils C content for ref_05 and ref_00 decreased for the reference period (figure 5.5 a). A loss of 0.2 % Corg (818 g C m⁻²) can be stated for the ref_00 run, the case that all harvest by-products are exported from the fields. Considering the changes in soil C storage for the whole soil (figure 5.5 b), a decrease for all runs was obtained as a basin scale average. Clearest decrease of about 1320 g C m⁻² in the reference period can be stated for ref_00, and losses of 182, 395, 509 and 725 g C m⁻² for ref07_1965, ref_08, ref_07 and ref_05 respectively (table 5.8). The simulated decrease of soil C storage consequently results in a net C flux from land to atmosphere, mirrored in positive NBE values (figure 5.5 c) as respective soil C inputs remain the same. All runs, except ref08 and ref07_1965 show for all years positive NBE values.

Annual net C flux from land to atmosphere decreases with increasing amount of harvest by-products remaining on the fields. NBE of ref_00 delivers an average annual net flux to the atmosphere of 28 g C m⁻² yr⁻¹ and shows a decreasing trend for the reference period. Reason for this is the increase in NEE for ref_00 due to increasing NPP in the reference period. Heterotrophic soil respiration for ref_00 remains stable over time (136 g C m⁻² yr⁻¹ on average, table 5.8). The climatic trend in the reference period stimulates more plant growth and biomass production than soil heterotrophic respiration, leading to increasing NEE and decreasing NBE towards the end of the reference period for that case. With increasing litter input (harvest by-products remaining on the fields) for ref_05, ref_07 and ref_08, NBE values are lower (15.5, 10.8, 8.4 g C m⁻² yr⁻¹ respectively on average, table 5.8) and feature no significant temporal trend. Lowest NBE values are found for the ref07_1965 simulation run (figure 5.5 c) with an average yearly NBE of 4 g C m⁻² yr⁻¹.



Fig. 5.5: Simulated changes in topsoil C storage (g C m⁻², a), total soil C storage (g C m⁻², b) and Net Biome Exchange (g C m⁻², c) for different assumption of harvest by-product amounts remaining on the fields (ref 00, 0 % remaining; ref 05, 50 % remaining; ref07, 70 % remaining and ref08, 80 % remaining on fields) and reference climate of 1965 (ref07_1965).

Looking at spatially distributed properties of average values for topsoil C storage and NBE in the period 1991 to 2000 for the Elbe river basin deliver the baseline situation of C storage and land – atmosphere fluxes and are shown in figure 5.6.



Fig. 5.6: Map of average topsoil C storage (g C m⁻², a) and Net Biome Exchange (g C m⁻², b) for croplands only in the Elbe basin and for the time period 1991 to 2000 based on reference conditions.

Highest topsoil C storage (12000 – 30000 g C m⁻²) are located in the loess landscape with fertile soils and for alluvial soils in the lowlands (dark black, figure 5.6 a). Lowest values (< 8000 g C m⁻²) are found for the mountain areas and the periglacial formed part of the lowlands, dominated by sandy soils dominating. Average annual C flux to the atmosphere (NBE) is highest (85 - 195 g C m⁻² yr⁻¹) in the loess landscapes and alluvial formed parts of the lowlands (blue areas in figure 5.6 b). Riparian zones of the Elbe river feature positive NBE values. In general it is visible that most areas are net sources of C with positive NBE values. Only parts of the lowlands (periglacial landscape with sandy soils) and eastern loess areas (see figure 5.1) are detected as sinks of C (negative NBE values, figure 5.6 b).

	Acronyms	Average input of C	Change in topsoil	Change in totalsoil C	Average yearly soil	Net annual flux to atmosphere.	NBE standard	Change in topsoil C storage per	Change in totalsoil C storage per
	- -	to soils م 7 m ⁻² رس ⁻¹	c content م ر _{m-2}	content م 7 m ⁻²	respiration م 7 m ⁻² س ⁻¹	NBE	deviation م 7 m ⁻² س ⁻¹	year	year مرسم م
	CIII	y ال	<u>م</u> ر =	u د =	y ال	g l l j	y الا	של ווי או	של יוי ש
19 {	Ref00	88	-819	-1320	136	28.0	4.9	-16.4	-26.4
0) 46 950	· Ref05	147	-224	-725	183	15.5	4.9	-4.5	-14.5
00)) p Iali	Ref07	171	ο	-509	201	10.8	5.4	-0.2	-10.2
efe oin 2 -	Ref08	183	104	-395	211	8.4	5.7	2.1	-7.9
b6 L	Ref07_1965	185	260	-182	209	4.0	3.9	5.2	-3.6
) po	ပိပ	162	-278	-720	158	14.0	5.8	-5.1	-13.1
ina 155	LCo*	125	-592	-1082	196	23.0	5.0	-11.8	-21.6
· 50	CLC1	120	-824	-1400	158	27.0	5.6	-15.0	-25.5
bine - M	CLC1-Ley	203	480	206	211	ကု	10.7	8.7	3.7
500 Sua	CLC1-Bio	167	114	-181	196	4	4.7	2.1	
;) ios	CLC1-Harv	107	-462	-757	146	10.3	5.4	-8.4	-13.8

5.3.3 Scenario period (2001-2055)

Climate change only (CCo)

Keeping the land use as it is in the reference period (as Ref07 case, table 5.5) and considering climate change only (most probable realisation) leads to a decreasing soil C content both in the topsoil and for the entire soil. Average loss in the scenario period is 278 g C m⁻² for topsoil and 720 g C m⁻² for the entire soil. In comparison to the reference condition (ref07), climate change leads to a decrease in topsoil C storage (figure 5.7 a). Average net flux of C to atmosphere increased from 10 g C m⁻² yr⁻¹ in the reference period to 14 g C m⁻² yr⁻¹ under climate change (table 5.8). Due to climate impacts only, a significant positive trend (p < 0.001) in NBE can be stated from 1951 to 2055 (figure 5.7 c). NEE remains on the same level under climate change as under reference conditions. NPP decreases slightly under climate change only, so do the crop yields with heterotrophic soil respiration also decreasing slightly without a significant tendency. Hence, litter input derived soil C input under climate change is less than for the reference case (ref07).

Comparison of changes in topsoil C storage and NBE for the reference conditions (ref07, 1991 to 2000) and climate change only (CCo, 2046 - 2055) is given in figure 5.8 (a and b). Highest loss of topsoil C with 9577 g C m⁻² is located in the loess area (south-western part of the Elbe, see figure 5.1) and in the alluvial areas of the lowlands with some gains (maximum value of 3650 g C m⁻²). Only minor changes are obtained for the eastern loess regions, the periglacial formed lowlands and parts of the mountain landscape (figure 5.8 a).



Fig. 5.7: Basin scale average for croplands only for four scenario assumptions (land use reference and climate reference Ref07 as black line, land use scenario and climate scenario CLC1 as black line and rectangles, land use reference and climate scenario CCo as bright grey with triangles, land use scenario and climate reference LCo as dark grey with circles) for topsoil C storage (g C m⁻², a), total soil C storage (g C m⁻², b) and Net Biome Exchange (g C m⁻², c).



Fig. 5.8: Difference map for mean topsoil C storage (g C m⁻²) for a) Climate Change only (CCo) minus reference condition (ref07), c) Land use change only (LCo) minus reference condition and qualitative illustration in changes of Net Biome Exchange (NBE) for b) Climate Change only (CCo) minus reference condition and d) Land Use change only (LCo) minus reference condition. Please note that averaged values of the periods 1991 to 2000 for the reference conditions and 2046 to 2055 for the scenario conditions are used. Topsoil C storage values below zero denote a loss of C under scenario conditions compared to reference conditions. Abbreviations are explained in table 5.5.

Areas with losses in topsoil C storage can also be identified as areas of net annual flux to the atmosphere (sources of C, red areas in figure 5.8 b). Largest areas in the Elbe basin could be identified as sources of C with some hotspots in the southern part with a conversion of sinks to sources of carbon due to climate change only (CCo). Identified sinks in the basin in general are getting smaller, staying as sinks of C under climate change only but nevertheless are loosing C in comparison to the reference situation (bright blue areas in figure 5.8 b).

Climate change scenario uncertainty

Climate change scenario induced uncertainty related to the target results is relatively low based on six simulation runs covering the range of 100 climate change realisations (wet and dry realisation, 5 and 95 percentile realisation, most probable and median realisations, table 5.5). As the temperature change of all realisations possesses the same increase of 1.4 K from 2001 to 2055 based on the IPCC SRES A1 scenario, only precipitation properties differ for the selected realisations (precipitation range of 607 mm to 758 mm per year on average from 2046 to 2055). The scenario uncertainty for altered precipitation patterns translates to small ranges of change in soil C dynamics. Differences in state variables (maximal value – minimum value of the respective mean value for the selected realisations in the period 2046-2055) are low: for topsoil C (38 g C m⁻²), for total soil C (29 g C m⁻²), NBE (1.6 g C m⁻²), NEE (11 g C m⁻²), Cresp (4 g C m⁻²) and litter input (4 g C m⁻²). A soil C decrease for all cases can be stated, both for topsoil and total soil storage, with 850 and 1400 g C m⁻² respectively. The tendency of soil C changes under climate change only remains the same as in the climate scenario uncertainty assessment.

Agricultural land use change only (LCo)

The anticipated change for croplands under land use scenario conditions (liberalization scenario) deliver a decrease in cropland area which is economically profitable. Approximately 30 % of agricultural land (see figure 5.4) is falling out of economical profitable use ("surplus arable land"). Using the spatially disaggregated change in crop shares and land cover at county level, we assigned set-aside (black fallow) use to these areas (see table 5.1). Other potential uses are described in the following section. To derive the agro-economic change only effects on soil C balance, one run was performed using the reference climate (LCo see table 5.5).

Both topsoil and total soil C storage show a clear decrease over time of about 590 and 1082 g C m⁻² on average respectively. In comparison to the reference simulation (ref07) a decrease of ~600 g C m⁻² of totalsoil storage can be stated attributable to the agro-economic change. Average NBE is positive and 23 g C m⁻² yr⁻¹ as a basin scale average over the simulation period and shows a slight decreasing trend over time. Hence there is a higher net C flux to the atmosphere due to anticipated agro-economic change than for the reference situation. Decreasing average yearly values are also found for heterotrophic soil respiration and dry matter production, whereas NEE increases over time as a basin wide figure. In comparison to the reference situation (ref07, 171 g C m⁻² yr⁻¹), the C input to the soil (through crop residuals and harvest by-products) decreases to 125 g C m⁻² yr⁻¹ (table 5.8). Input of soil C for set-aside areas is considerably lower than under agricultural use resulting in lower soil C inputs, increased C flux to atmosphere and losses of soil C.

Concerning the spatially distributed changes in topsoil C storage, one can recognize that areas loosing soil C in comparison to the reference condition are increasing. Areas loosing topsoil C are practically the same as described for the climate change only case (CCo), but additional areas in the eastern loess areas and lowlands are obtained. The absolute magnitude of topsoil C loss is slightly less for agro-economic change than for the climate change only simulation run (-9346 and -9577 g C m⁻², brownish areas in figure 5.8 a and c). But less productive areas falling out of agricultural use and assigned to set-aside, are located mainly in areas with slight changes or gains of soil C concerning climate change and agroeconomic reference conditions. Consequently these areas convert to regions loosing soil C.

This effect is clearly visible looking at changes in NBE (figure 5.8 d). There is an increase in areas assigned as "sinks getting sources" of C (dark brown areas, figure 5.7 d). Additionally it can be stated that areas loosing soil C (sources with reddish colours in figure 5.7 d) are dominating the picture and only some regions acting as sinks of soil C, mainly in the mountain landscape and some parts of the periglacial formed lowlands.

Combined land use and climate change effects

Under scenario conditions, for both anticipated agro-economic and climate change, four cases have been considered. Based on the land use scenario, the cropland area falling out of use has been utilized to investigate different usage of these areas under expected climate change with four simulation runs (see table 5.5).

For set-aside use (CLC1, table 5.5), extensified arable use (ley-arable rotation CLC1-Ley, table 5) and bioenergy rotation (CLC1-Bio table 5.5) on surplus arable land, results are shown for soil C storage and NBE. Additionally one case with a bioenergy rotation and the use of crop harvest by-products on all croplands as potential energy resource was considered (CLC1-Harv, table 5.5).

Strongest decreases in topsoil and total soil C content were obtained for the set-aside use with a total loss of soil C of 1400 g C m⁻² (figure 5.9 a and b). Also a loss of soil C can be stated for the "CLC1-Harv" case, but is less pronounced than the set-aside case (CLC1). Here total soil C decreased by 757 g C m⁻². Placing a bioenergy rotation on surplus arable land (CLC1-Bio) stabilizes soil C over time for the entire soil with a slight increase for the topsoils C storage (figure 5.9 a and b). A clear increase in soil C storage for total and topsoil is obtained for the extensified agricultural use (ley-arable rotation CLC1-Ley, figure 5.9 a and b)). The gain of C in soil for this case is calculated as about 206 g C m⁻². Accordingly, net annual C flux to atmosphere (NBE) is highest (27 g C m⁻² yr⁻¹ on average) for the set-aside case (CLC1), followed by CLC1-Harv case (10.3 g C m⁻² yr⁻¹), CLC1-Bio (4 g C m⁻² yr⁻¹) and CLC1-Ley (-3 g C m⁻² yr⁻¹) cases (figure 5.9 c). Litter input and soil respiration is highest for CLC1-Ley case, with 203 and 211 g C m⁻² yr⁻¹ respectively. Litter input and soil respiration decreases from CLC1-Bio (166 and 196 g C m⁻² yr⁻¹ respectively) to CLC1 (120 and 158 g C m⁻² yr⁻¹ respectively) and then to CLC1-Harv (107 and 146 g C m⁻² yr⁻¹ respectively) with organic fertilizer input being 24 g C m⁻² yr⁻¹ for CLC1-Bio and CLC1-Harv and 11 g C m⁻² yr⁻¹ for CLC1-Ley and CLC1.

Regionalized climate and agro-economic change (CLC1, table 5.5) translates to a spatial figure for the Elbe river basin with a major part loosing topsoil C (up to 10750 g C m⁻², figure 5.10 a, left) and acting as a source of C with a net flux to the atmosphere (reddish areas in figure 5.10 a, right). A considerable area in the Elbe basin converts to a source from a sink (dark red areas in figure 5.10 a right). Only some regions can be assigned as sinks of C in soils, with most of them getting smaller, and consequently are also loosing C in respect to the reference condition. Areas acting as a source are most dominant in loess areas (figure 5.10 a right). A reas acting as source in the scenario period have considerably increased under climate and agro-economic change in comparison to reference conditions.

Placing an extensified arable use (CLC-Ley) on surplus arable land leads to storage of topsoil C and a sink of C in the soils (figure 5.10 b left and right) for the affected areas in comparison to the "CLC1" case. Magnitudes of gains (4660 for CLC1-Ley to 3990 g C m⁻² for the CLC1 simulation run) and losses (- 9580 to -10750 g C m⁻² respectively) are weaker. The south eastern part of the basin (loess areas) remains a source of C with some spots converting from sinks to sources. But for this case, areas acting as C sinks (bluish areas in figure 5.10 b) are clearly dominating and areas converting from sources to sinks (violet areas in figure 5.10 b right) are visible. Hence, for this land use assumption most areas, except the intensive agricultural areas in the loess landscapes (south western part of the region), are acting as C sinks.



Fig. 5.9: Basin scale average for croplands only for five scenario assumptions (Ref07 as black line, CLC1 as black line and rectangles, CLC1_Ley as black line and crosses, CLC1-Bio as bright grey line and circles and CLC1-Harv as dark grey and rhombi) for a) topsoil C storage (g C m⁻²), b) total soil C storage (g C m⁻²) and c) Net Biome Exchange (g C m⁻²). Abbreviations used are explained in table 5.5



(Fig. 5.10 continues next page)



Fig. 5.10: Maps of topsoil C storage difference (g C m⁻², left) and qualitative expressions for Net Biome Exchange (NBE, right) for a) CLC1 minus Ref07, b) CLC1-Bio minus Ref07, c) CLC1-Ley minus Ref07 and d) CLC1-Harv minus Ref07. Please note that averaged values of the periods 1991 to 2000 for the reference conditions and 2046 to 2055 for the scenario conditions are used. Topsoil C storage values below zero denote a loss of C under scenario conditions compared to reference conditions. Scenario acronyms are explained in table 5.5).

In general the same pattern can be recognized for the case of a bioenergy rotation on surplus arable land (CLC1-Bio, table 5.5). Concerning soil C storage, most regions are gaining C under that land use assumption in a similar manner as under the ley-arable conditions (CLC1-Ley, almost same magnitudes). Clearest gains can be seen for the lowland and mountain landscapes. Same tendencies and patterns in net flux to the atmosphere (NBE, figure 5.10 c right) for CLC1-Bio are visible as for the CLC1-Ley case, again with dominating losses of C for loess and lowland (alluvial) landscapes. Soils in most regions are storing C under this land use assumption and climate change. Hence, beside the possible use of bioenergy crops as energy resource, soil C storage increases with a decrease of net C flux to the atmosphere in the affected areas.

Harvest by-products offer the potential being used as energy resource (CLC1-Harv case, table 5.5). The effects on soil C storage and NBE for the case that 80 % of harvest by-products are removed from the soils is demonstrated in figure 5.10 (d). Consequently the absolute magnitude of topsoil C loss is highest than for the previous cases (- 10 820 g C m⁻²). The spatial pattern of increase and decrease of topsoil C in respect to the reference condition is similar to the "CLC1" case. Also the pattern of sources and sinks is similar, with increased areas as C source in comparison to the bioenergy (CLC1-Bio) and ley-arable (CLC1-Ley) cases, but slightly less as the "CLC1" case. Here the set-aside assigned areas are stronger sources of C than for CLC1-Harv (please note that for the "CLC1-Harv" case the bioenergy rotation is in place on surplus arable land). As a consequence, assigning bioenergy crops on surplus arable land and exporting harvest by-products leads to higher topsoil C storage compared to set-aside (CLC1) conditions.

Selected regional effects

To represent local effects of climate and agro-economic changes for each landscape unit some hydrotopes have been selected (see table 5.6) based on main soil types. For five hydrotopes development of topsoil C content from 1951 to 2055 is illustrated in figure 5.11.

For lowland-1 the soil C content increases for the reference period (ref07) with rotation number 11 in place (see table 5.1). For the period 2000 to 2055, climate change only (CCo, table 5.5) causes a clear decrease in topsoil C storage. Due to agro-economic change, the crop sequence changes from rotation 11 to 21 in the scenario period. Keeping the reference climate and land use change only (LCo) leads to a decrease in soil C which gets

stronger under climate change conditions (CLC1, figure 5.11 a). Changing crop sequences (here summer barley – winter wheat rotation 11 to winter wheat – rape rotation 21) results in a decrease in soil C storage.

For the lowland (periglacial) landscape one hydrotope (lowland-2, table 5.6) was chosen representing a Podzoluvisol (soil 26, table 5.6) and a crop rotation change from number 21 to 23 (see table 5.1). Rotation 23 is assigned to surplus arable land, with different possible future uses (set-aside, ley-arable, bioenergy rotation). Soil C storage increased during reference period which continues also under climate change keeping the reference land use (CCo). For climate and agro-economic change conditions ("CLC1", figure 5.11 b) with set-aside on rotation 23, soil C storage clearly decreases. Same effect was obtained with agro-economic change only (LCo, figure 5.11 b). Consequently, climate change has no significant impact for these site conditions. For CLC1-Bio or CLC1-Ley cases a clear increase in topsoil C of about 0.6 % Corg (~ 2500 g C m⁻²) can be stated.



(Fig. 5.11 continues next page)



Fig. 5.11: Topsoil C storage changes for selected hydrotopes for a) loess region, b) lowland (alluvial), c) lowland periglacial), d) moun_1 and e) mount_2 representing main landscapes, soil types and changes in crop rotations for five scenario assumptions (Ref07 as black line, CLC1 as black line and rectangles, CLC1-Ley as black line and crosses, CLC1-Bio as bright grey line and circles and CLC1-Harv as dark grey and rhombi) for a) topsoil C storage (g C m⁻²). Acronyms for selected hydrotopes are explained in table 5.5.

The selected hydrotope for loess landscape (loess-1) represents soil 46 (Luvic Arenosol on loess sediments) and a change in crop rotation from number 21 to 23. In the reference period (ref07) under rotation 21 a decreasing trend in soil C is obtained, which continues under climate change and land use reference conditions with similar rates (CCo, figure 5.11 c). Again for the "CLC1" case (rotation 23 as set-aside) and for LCo a clear decrease in soil C

of about 0.6 % Corg (-2500 g C m⁻²) is visible. Assigning a bioenergy and ley-arable rotation on surplus arable land (CLC1-Bio and CLC1-Ley) leads to an increase of soil C of about 0.2 % Corg (950 g C m⁻²).

Two hydrotopes were selected for the mountain landscape both on a Cambic Arenosol (figure 5.11, d and e). Mount1 feature a crop rotation change from number 16 (see table 5.1) to 23. Under reference conditions (ref07) an increase in soil C storage is obtained which is only slightly reduced because of climate change (CCo), but increasing trend is preserved. For "CLC1" conditions soil C is clearly decreasing, although bioenergy or ley-arable rotations (CLC1-Bio and CLC1-Ley) result in an increase in soil C. Same tendencies are obtained for the mount-2 case, with increases of soil C for the reference period (ref07) and a small impact of climate change (CCo) on that increase. Changing from rotation 10 (a rotation with a three years field grass sequence, see table 5.1) to rotation 20 (summer barley, winter barley, silage maize and two years set-aside) results in decreasing soil C. Climate change only (CCo) delivers no significant effects on soil C storage for this case.

Bioenergy production

Crop biomass can be used for energy generation, which is a renewable energy source. Here we assessed the biological energy potential of biomass neglecting factors like economic feasibility, biomass quality, transportation and storage. A full energy balance accounting (considering also energy consumption by machinery, labour, transportation, fertilisation and so on) is not considered here.

Instead we give a rough estimate on energy potential of biomass and energy crops for two scenario cases: First, a bioenergy rotation on surplus arable land (CLC1-Bio) and second the use of 80% of grain straw residues for energy generation (CLC1-Harv, table 5.5). The potential energy gains are then compared to resulting changes in soil C storage for these cases. Table 5.9 gives average values on energy potential of harvest by-products and bioenergy crops (grains, oilseed).

		I			I 1	I							
Oil equivalent	10 ³ barrel yr ¹	2738	1053	3316	7107	2193	1016	3159	1477	2564	11877	22286	29393
Other studies **	TJ yr ⁻¹		6313 ^c	20880 ^d					4859 ^c			86900-177393 ^e	132098-269657 ^e
Energy equivalent	TJ yr ¹	12478	5984	18842	37304	12464	4623	17954	8395	14570	67486	125492	162796
net calorific value	10 ⁻⁶ TJ kg ¹	q	26.5	17.4		17.5	q	17.5	26.5	17.4	17.2		
biomass production	10 ⁶ kg	10557	226	1083	11866	712	3920	1026	317	837	3923	10735	22601
Area	km^2	4856	2428	2428	9712	1759	1799	2176	1869	2100	8970	18673	28385
biomass	kg km ⁻²	2174000	93000	446000		405000	2179000	471600	169500	398700	437400		
bioenergy type		biogas ^a	biofuel	biofuel		biofuel	biogas ^a	biofuel	biofuel	biofuel	biofuel		
usage		complete	oilseeds	grains		harvest by - products	complete	harvest by - products	oilseeds	harvest by - products	harvest by - products		
crop		silage maize	rape seed	winter rye		summer barley	silage maize	winter barley	rape seed	winter rye	winter wheat		
		CLC1- Bio						-LC1-	Harv			TOTAL	TOTAL BOTH

a calculation of biogas generation from silage maize: 1 t of maize equals 171 m³ biogas; 1 m³ biogas equals 1.92 kWh; 1 kWh equals 3.6 10⁻⁶ TJ (FNR, 2005) and www.fnr-server.de

b net calorific value derived from (FNR, 2005)

c according to (IER et al., 2005) d according to (Scholz and Ellerbrock, 2002) e according to (Scholz and Ellerbrock, 2002) e according to (Scholz and Ellerbrock, 2002) e accroding to (Lal, 2005), lower value is energy value of harvest by-products estimated for world, higher values estimated for US croplands. Scaled to respective area in this study, please note that values by (Lal, 2005) are for harvest by-products only, whereas in this study for CLC1-Bio also grains or complete biomass and for CLC-Harv complete biomass for silage maize are considered

The bioenergy rotation (CLC1-Bio, with an area of 9712 km² energy crops maize, rape seed and winter rye) yields an energy equivalent 37304 TJ (10^{12} J) per year (table 5.9). The potential energy equivalent here would substitute approximately 7107 10³ barrel oil per year. Scholz and Ellerbrock (2002) assessed the energy potential of winter rye to ~ 11 TJ km⁻² yr⁻¹ on an energy plantation in the study area, corresponding to 20880 TJ yr⁻¹ scaled to the respective area of winter rye. Our estimate of 18842 TJ yr⁻¹ is comparable in magnitude to that study (table 5.9). According to IER et al. (2005) rape seeds deliver an average net energy equivalent (accounting also for attached energy consumption in the process chain) of 2.6 TJ km⁻² yr⁻¹. Our estimates deliver for the CLC1-Bio case ~ 2.46 TJ km⁻² yr⁻¹ and for CLC1-Harv ~ 4.5 TJ km⁻² yr⁻¹ but are rather biologically (gross) potential estimates.

Using crop residuals of the entire area of croplands would have an estimated annual potential of 125 492 TJ and would substitute 22286 10³ barrel oil (table 5.9). Looking at the combined energy gains (bioenergy rotation and harvest by-products of the remaining cropland area) would results in an annual energy equivalent of ~ 162796 TJ. The total gross energy equivalent of 162 000 TJ per year is roughly 1% of total annual German primary energy consumption (~ 14 500 000 TJ BMU, 2005) and equals a substituted amount of 14.6 Mt CO₂ (1 Mt = 10^{12} g). The latter is roughly 1.6 % of annual CO₂ emissions in Germany (year 2002: 878 Mt CO₂, BMWI, 2006).

5.4 Discussion

Changes in climate (mainly temperature and precipitation) and in land use (land cover and land management) alter soil C storage. This alteration is mainly caused either by changes in turnover properties of soil organic matter in soils (mineralisation and decomposition) but also by changes in the amount and quality of C inputs. Both, climate and land use, directly or indirectly influence these properties.

Changing climate, as already observed and expected to continue for the study area, will lead to increase in temperature and decrease in precipitation, except winter precipitation in the western mountain areas (Harz and Thüringer Wald) which will most probably increase (Gerstengarbe and Werner, 2005). Increase in temperature will speed turnover processes of soil organic matter, but changing precipitation patterns (future decrease in precipitation amount for most of the basin) counteract the temperature effect. Soil moisture properties anticipated for the Elbe basin (decrease in soil water content) will reduce the temperature effect on soil C storage. Additionally increase of temperature and atmospheric CO2 concentration will enhance NPP. Although expected changes in crop yields (considering the same regionalized climate change scenario and fertilisation effect caused by an increase of CO₂ concentration) reduces C3 crops yields (e.g. winter wheat, summer barley) by 11 to 17 %, whereas C4 crop yields (e.g. silage maize) will not be significantly affected on average (Hattermann et al., 2005a; Wechsung et al., 2005). Hence amount of soil C added will consequently decrease. The land use factor alters mainly the amount and quality of added C to soil beside the impacts of land management practices on soil properties (e.g. tillage). Quality of added C directly affects decomposability by soil organisms. Consequently properties of crop rotations and crop sequences together with fertilisation impact soil organic matter dynamics.

Positive and negative effects of crop rotations, harvest surplus management and fertilisation regimes (organic and inorganic fertilisation) on soil C storage are documented in many studies (Smith et al., 2000; West and Marland, 2002; Freibauer et al., 2004; Desjardins et al., 2005; Post et al., 2005c; Singh and Lal, 2005).

To address the consequences of changes in climate and land use properties for croplands at the regional scale a simulation set up was established to create characterisation of regionalized climate and agro-economic properties for the time frame 1951 to 2055. Special emphasis lied on the regionalization of these external driving forces for the study area to ensure a spatially distributed representation of local climate and agro-economic properties both for reference conditions (1951 to 2000, based on measurements and statistics) and for future conditions (2001- 2055, based on regionalisation of global climate and agro-economic change scenarios). The regionalized climate change scenario (produced by the model STAR, Gerstengarbe et al., 1999), maintains the statistical properties (frequency
distribution, annual and interannual variability and persistence) of observed climate properties at the local scale. Hence local meteorological properties are maintained in the climate change scenarios.

The crop generation algorithm (Wechsung et al., 2006) ensures a spatially distributed representation of crop shares at the county level. The algorithm furthermore considers soil fertility aspects (combination of climate and soil properties) and assigns typical rotational systems at the sub-regional level. The explicit consideration of local crop share properties and their changes under anticipated future agro-economic properties ensures an adequate representation for croplands heterogeneity. This development forms a necessary requirement to mirror local crop share properties which considerably affect soil carbon dynamics. Hence an enhanced present-day and future soil C assessment considering county level of crop shares properties and changes was achieved.

The regionalization of the major external driving forces climate and land use not only delivers an adequate representation of croplands heterogeneity but also allows consideration of feedbacks between trend in climate and its impact on land use.

5.4.1 Reference period

The fractions of harvest by-product remaining on the fields considerably impact soil C storage both for topsoil and totalsoil C contents. The soil C loss due to exportation of harvest by-products from the fields is roughly 1 t C m⁻² in relation to the reference case. The quantity remaining on the fields through typical harvest practices is difficult to estimate. Additionally harvest practices and hence the amounts of harvest by-products remaining on the fields are heterogeneous and vary locally. Also the common practice of harvest management changes with time. In Great Britain for example, where straw burning was common until the straw burning regulation in the early 1980ies, the fraction of harvest by-products remaining on the fields changed. Based on these developments, fraction of harvest by-products could be estimated for Great Britain (18 % of cereal straw was ploughed-in,

Christian and Ball, 1994) and were extrapolated for a European scale assessment (Smith et al., 2000). Figures derived for the study area although suggest a fraction between 70 and 80 % remaining on the fields (Schmidt and Osterburg, 2004). Additionally straw burning did not play a significant role in eastern Germany and the assumption that the fraction of incorporation is not changing considerably for the reference period (1951 – 2000) seems appropriate. Hence, for the Elbe basin a fraction of 70 % of harvest by-products remaining on the fields was adopted, which results in stable soil C development for the topsoil and a slight decrease for the total soil as basin scale average.

For a basin scale assessment the assumption that harvest by-products are incorporated sooner or later into the soil (via direct incorporation or in form of e.g. farmyard manure) with a loss of 10 % is adequate. Considering the different simulation runs with different fractions of by-products remaining on the fields illustrate the importance of e.g. straw incorporation to stabilize or enhance soil C contents. For topsoil C reproduction a fraction between 50 and 70 % of by-products incorporated to the soil seems necessary for soil C reproduction and soil C stabilization for the basin scale situation based on our simulations. Investigations by Röschke (MLUR Brandenburg, personal communication 21.12.2005) for the State of Brandenburg yield a fraction of 50% incorporation for soil C reproduction based on long-term measurements (Zimmer and Roschke, 2001).

Concerning the net annual C flux to the atmosphere (NBE, figure 5.5) as a basin average show that for all cases croplands are a net source of C with average NBE of + 10.8 g C m^{-2} yr⁻¹ for the reference case (ref07, figure 5.5). With no incorporation (only application of organic fertilization remains the same for all cases) net C flux to atmosphere is approx. three times higher (28.0 g C m^{-2} yr⁻¹, ref00). To stabilize soil C contents an additional input of approx. 11 g C m^2 is necessary. Another option to increase soil C contents is the adoption of recommended management practices (e.g. no tillage, Lal, 2004b).

Average net annual NBE is calculated here between 8.4 and 28.0 g C m⁻² yr⁻¹ depending on percentage of harvest by-product incorporated to soils. In comparison, mean annual soil C losses based on measurements and the up scaled to the national scale are e.g. 24 g C m⁻² yr⁻¹ for Austria and 76 g C m⁻² yr⁻¹ for Belgium (Janssens et al., 2003). Rinklebe and Makeschin (2003) report mean annual soil C losses between 0.59 g C m⁻² yr⁻¹ and 25.9 g C m⁻² yr⁻¹ for a loess landscape in lower Franconia (Germany) based on measured soil C changes for a period of 27 years. Annual soil C losses derived from modelling studies are e.g. 89 g C m⁻² yr⁻¹ for Austria, 90 g C m⁻² yr⁻¹ for Belgium and 92 g C m⁻² yr⁻¹ for Europe (Janssens et al., 2003). Hence, values gained in this study are comparable to measurement based values cited in literature but lower compared to model based estimates.

Values reported based on model results generally overestimate net C losses in comparison to measured values. Up scaling (plot to regional scale) or using bulk regional assumptions of agricultural management and soil properties as in most models both imply disadvantages. For regional scale assessments of soil C changes an explicit consideration of local scale agricultural management properties like crop share distributions, harvest surplus management and fertilisation regimes seems necessary, which was tried to address in this study.

Regions contributing most to net annual C flux to atmosphere for the reference period could be identified based on the spatially distributed assessment (figure 5.6). Here the eastern loess regions and alluvial formed parts of the lowlands can be recognized. Soils in these regions possess highest soil C contents (figure 5.6) and are more vulnerable to changes than soils with low organic C. The fertile loess soils, the areas with highest NBE values, are dominated by intensive agricultural use. Alluvial soils in the lowland region are more affected by groundwater and can mainly be assigned to riparian zones of the Elbe River and contributories. These water influenced soils developed a high content of organic matter and act under cultivation as C sources. The mountain areas and periglacial formed parts of the lowlands (sandy soils) can most commonly be assigned as C sinks.

Under the assumed land management conditions and regionalized crop shares, the present-day dynamics of soil C storage was quantified. As observed climate possesses a trend in temperature and precipitation, one simulation using climatology of the year 1965 was done to approximately estimate effects of observed climate trend (1951 – 2000) on soil C storage. Climate conditions of 1965 representing mean climate properties (Krysanova et al., 2005) are applied for the period 1951 to 2000 to filter the observed climatic trend.

The increase in temperature (+0.8 K in the summer and +1.4 K in the winter period) causes an increase in turnover processes of soil C. Hence, due to climate change observed in the reference period, soil C storage for topsoil and for total soils decreased (figure 5.5). Net flux to atmosphere is approx. 7 g C m⁻² yr⁻¹ higher in the reference case (Ref07) than the "Ref07_1965" run (table 5.8). For total croplands this effect amounts to an increased flux to the atmosphere of about 0.28 Mt C per year (10¹² g). Although a more detailed assessment using statistically de-trended climatology instead an average year (1965) is needed for a robust assessment of observed climate change effects on soil C storage.

5.4.2 Scenario period, combined land use and climate effects

Climate change in the scenario period (2000 - 2055) leads to an enforcement of decreasing soil C content, especially for the topsoil C storage. Increase in mean temperature of 1.4 K until 2055 and CO₂ fertilisation effect on crop growth together with decrease in precipitation amounts (- 15%) for most of the study area lead to a decrease in crop yields (Hattermann et al., 2005a; Wechsung et al., 2005). This translates accordingly to a decrease in soil C input. An expected increase in crop growth due to higher temperatures and CO₂ fertilisation is not obtained in the study area (Hattermann et al., 2005a; Wechsung et al., 2005). Main reason for this is the decrease of precipitation and hence an alteration of hydrologic properties. (Hattermann et al., 2005a) investigated changes in water availability in the Elbe basin using the same simulation set up. Changes in temperature and precipitation led to an increase in evapotranspiration and a strong decrease in runoff properties, groundwater recharge and water resources. Climatic water balance (precipitation minus potential evapotranspiration) is negative and shows a clear decreasing trend for the period 1951 to 2055, with stronger decreases in the scenario period (2000 – 2055, -2.7 mm per year). The resulting decrease in soil water storage impacts soil organic matter turnover properties and counteracts the temperature effect on soil organic matter turnover. Hence the loss of soil C due to climate changes effects is less strong than reported in other studies. As example,

Bellamy et al. (2005) reported for England and Wales (based on soil measurements) largescale C losses from soils (0 - 15 cm soil depth) over the past 25 years under all land use conditions. Changes in climatic patterns (increase in temperature and decrease in precipitation) for this moist temperate region (with mostly wet soils) are seen as the main driver of the strong C losses. Although there is ongoing debate on temperature sensitivity on soil C turnover processes (e.g. Giardina and Ryan, 2000; Kirschbaum, 2000; Fang et al., 2005a; Knorr et al., 2005) there is meanwhile evidence for this feedback based on laboratory and field experiments, and modelling studies (Bellamy et al., 2005). The temperature effect on soil C turnover although weakens when soil moisture conditions inhibit soil C turnover as is most probable the case for parts of the Elbe basin. In contrary to Great Britain, where temperature effect on soil C turnover dominates, decreasing soil moisture effects on soil C turnover dominates for most of the Elbe basin (Jones et al., 2004). Nevertheless, climate change only significantly causes decline in soil C storage and increase in NBE. Additional C flux due to climate change only is 3.2 g C m⁻² yr⁻¹, which corresponds to an increase of 30% to the reference period with an additional flux of 0.13 Mt C per year (10^{12} g) in the scenario period.

The spatial pattern of change in topsoil C storage and NBE due to climate change only obtained in this study leads to an identification of regions with largest changes. Largest decreases in soil C storage are dominantly present for soils in the loess and alluvial formed lowland landscapes. Here soils with high soil C contents are present. It is obtained that soil C losses are proportional to soil C content, which also was observed for soil C losses in England and Wales (Bellamy et al., 2005). Most of the Elbe basin is characterised as C sources, with some regions acting as sink but becoming smaller under climate change impacts. Soils with low C content, dominating in the periglacial formed lowlands (sandy soils on groundmorains) and in the mountain regions delivered smallest soil C decreases for the set-aside case (as black fallow use) and climate change (CLC1).

Climate uncertainty derived through six realisation covering the precipitation range of all regionalized climate change scenarios, was low. Uncertainty ranges for NBE, topsoil and total soil C storage was obtained with +/- 0.8, +/-19 and +/-14.5 g C m⁻² respectively. The

5.4 Discussion

simulation results hence can be seen as stable related to climate change scenario uncertainty for the Elbe basin.

Future changes in agricultural land use yield to stronger effects on soil C storage than does climate change only. Regarding reference climate conditions and land use scenario with set-aside on surplus arable land (as black fallow, LCo) leads to a stronger decrease in soil C and leads to higher amounts of net annual C fluxes to atmosphere. Set-aside areas deliver considerably lower amounts of crop residuals, as the fields are kept open for potential future agricultural use. For this reason soil C reproduction through crop derived C inputs is lower putting the basin to a stronger future source of 23 g C m⁻² yr⁻¹. Large areas convert from C sinks to C sources. Under both climate and land use change conditions net C flux to atmosphere increases to 27 g C m⁻² yr⁻¹. For this case, croplands C emissions to the atmosphere for the entire basin are estimated with 1.13 Mt C per year. The management strategy to place set-aside on anticipated surplus arable land (with black fallow use as an extreme case) causes a strong increase in C emissions and is more than 3 times larger than the climate change effect. As noted by e.g. Rounsevell et al. (2005) or Schröter et al. (2005), surplus arable land area will increase considerable forming a relevant management opportunity to improve ecosystems services (e.g. C storage, water resources). Two management options proposed by e.g. (Smith et al., 2000; Lal, 2004b; Rounsevell et al., 2005) to enhance soil C storage or to substitute fossile fuel resources are extensification (ley-arable rotation) and bioenergy plants.

In terms of soil C storage both management options lead to increasing soil C and decreasing net flux to atmosphere in relation to the set-aside case (CLC1, table 5.5). Placing a ley-arable rotation (three years of field grass, sugar beet, winter wheat, summer barley rotation) on surplus arable (CLC1-Ley) land yields the strongest increase of soil C and converts the basin being a source of C in the set-aside case to a sink of C (- 3 g C m⁻² yr⁻¹, - 0.43 Mt C yr⁻¹ total croplands). This management option offers potential in terms of soil C sequestration and climate change mitigation. Interestingly surplus arable characterized by low fertile shows a strong increase in soil C content when placing a ley-arable rotation instead set-aside use. As noted by Sparling et al. (2003), regions with low C soils offer

potential for increasing soil C, which demonstrates the relevance of using surplus arable land (and low soil C status soils) properly.

Placing a typical bioenergy crops rotation instead of set aside (CLC1-Bio, table 5.5) leads to stabilization of soil C content and converts affected areas from C sources to C sinks. In terms of soil C storage both options (CLC1-Bio and CLC1-Ley) seem to be beneficial. This can also be seen considering selected regions, where ley-arable or bioenergy rotation leads to clear increases of soil C content.

Beside the impact on soil C storage, bioenergy crops (oilseed rape, winter rye for biofuel production and maize for biogas production as in our rotation scheme) can be used for energy generation. Furthermore, harvest by-products (e.g. grain straw) also offer the potential of being used as energy resource. As in our assessment of the latter case, the use of 80 % of harvest by-product although resulted in decreasing soil C storage. Harvest by-products potentially can be used either as energy resource, in livestock farming or can be incorporated into the soil. Incorporation into the soils is an important management strategy for soil C and humus reproduction, which is important to maintain or enhance soil fertility. Therefore the management option to use cereal straw as energy resource has to consider this effect (Lal, 2005). The energy gain through cereal straw may offset the loss of soil C (14.0 g C m⁻² yr⁻¹), but in terms of maintaining soil fertility exportation of 80% harvest by-products has to be seen critically.

Potentially, also cereal grains can be used for energy generation, but burning a food resource has to be seen critically concerning the world nutrition situation. Therefore this option was neglected in this assessment. Also neglected in this study are woody energy plants (e.g. poplar) or fast growing grasses. These fast growing plants consequently require more water and nutrients, which in respect to the anticipated water resource situation in the Elbe basin (Hattermann et al., 2005a) has to be considered critically. Although a detailed investigation seems necessary to quantify the impacts of these energy plants in respect to water availability, soil C storage and fossil fuel substitution potential.

The resulting energy gains through the use of bioenergy crops or harvest by-products are notable and up to 162796 TJ (10¹² Joule) substituting roughly 29393 10³ barrel oil. As the

CO₂ emission factor (European Commission, 1997) for biofuels is zero in relation to 57 kg CO₂ 10⁻⁹ J for natural gas, 74 kg CO₂ 10⁻⁹ J for diesel oil or 95 kg CO₂ 10⁻⁹ J for coal (Lal, 2005), the use of biofuels is beneficial in terms of reducing anthropogenic CO₂ emissions and states an important strategy mitigating the greenhouse effect. In relation to soil C storage effects, plantation of bioenergy crops on surplus arable land is a win-win strategy. Gains of soil C are obtained and biomass can be used as renewable energy resource.

Also a certain amount of harvest by-products offer a considerable potential for energy generation but has to be balanced out with soil C reproduction, which is an important factor to maintain soil C levels and soil fertility. Exporting a to high fraction of harvest by-products from the field may lead to soil erosion, deplete the soil C storage with an resulting increased C flux to the atmosphere (Lal, 2005). This fact has to be considered when using harvest by-products for energy generation. Compared to the CLC1-Bio case (see table 5.5), the use of harvest by-products (CLC1-Harv case) leads to an increased annual net C flux of 10. g C m⁻² yr⁻¹ which amounts to 0.41 Mt C yr⁻¹ or 1.44 Mt CO₂ yr⁻¹ respectively for the entire cropland area. The annual soil CO₂ loss of 1.44 Mt CO₂ is considerable lower than the potential CO₂ emission substitution effect by bioenergy of 11.43 Mt CO₂.

The here conducted assessment of potential energy generation by harvest by-products and bioenergy crops has to be seen with precaution because it neglects a full energy accounting in the life cycle. Here a detailed assessment would be necessary to come up with more accurate numbers. The presented values are biologically potential savings neglecting political and economic constraints. But the results obtained in this study highlight both the importance on how surplus arable land may be used and the potential of extensified agriculture or of bioenergy crop rotations in terms of soil C storage and climate change mitigation.

5.5 Conclusion

This study provides an assessment of present-day soil C dynamics and an analysis of effects of plausible regionalized climate and agro-economic change impacts on soil C storage and annual net C fluxes to the atmosphere for croplands in the German part of the Elbe river basin. The regionalized external driving forces climate and agro-economy allows spatially distributed assessments of combined and single relative contributions on soil C dynamics. Additionally the developed simulation setup allows quantifying feedbacks between trend in climate and its impact on land use. The spatial disaggregation of crop shares to the hydrotope level based on soil fertility characteristics was successful and helps to assess soil C dynamics at that scale.

Simulated soil C dynamics for the reference period (1951 to 2000) considering local crop share distributions and observed climate deliver a slight decrease in soil C storage and a net annual flux of C to the atmosphere of ~11 g C m⁻² yr⁻¹. Impact of harvest by-product fractions remaining on the fields on soil C storage is high and highlights the importance of crop residuals for soil C reproduction. It is estimated that at least 50 % of harvest by-products should remain on fields for topsoil C reproduction at a basin scale average. This estimation is supported by field scale observations in the region (Zimmer and Roschke, 2001).

Determination of harvest by-product fraction incorporated into soils although remains uncertain with sparse information available to characterise this value. At least for the study area, an amount left on the fields between 70 and 80 % of total crop harvest by-products seems an appropriate assumption based on the information available. The estimation of this amount is highly influencing the assessment of soil C storage and net C fluxes.

Climate trend already present in the reference period causes an approximate net loss of C to the atmosphere of 7 g C m⁻² yr⁻¹ (0.28 Mt C for Elbe cropland area). Under anticipated future climate change this effect additionally amounts to about 4 g C m⁻² yr⁻¹. Increase of temperature (+1.4 K until 2055) results in an increase of soil C turnover which is inhibited by soil water storage. Soil water storage and water availability is lower than during the reference period due to decrease in precipitation amount in the river basin and other

alterations of the hydrologic cycle by vegetation and climate. Because of increasing atmospheric CO₂ contents and increase in temperature, crop growth is stimulated and growth period increases. Accordingly vegetation needs considerably more water, which states the limiting factor resulting in decreased crop yields under climate change conditions than obtained for the reference period. Hence soil C input derived from crop residuals decreases.

Anticipated agro-economic changes result in stronger alteration of soil C storage and annual net fluxes to the atmosphere than climate change only effects. Regionalized agroeconomic changes lead to an increase in surplus arable land to approx 30 % of cropland area. Possible future use of this area highly impact soil C balance.

Set-aside use (as black fallow, CLC1) results in an overall decrease of soil C storage and increase in net annual C flux to the atmosphere which is further accelerated by climate change. An extensified use with a ley-arable rotation (CLC1-Ley) converts the Elbe basin to a net C sink with increasing soil C contents. The latter effect was obtained when a bioenergy rotation is placed on surplus arable land (CLC1-Bio). Additionally bioenergy crops offer an energy generation potential of approx. 162 796 TJ per year. Considering the use of 80% harvest by-products as potential energy source would result in an annual gain of 125 492 TJ per year, but will also deplete soil C storage and increase net annual C fluxes to the atmosphere converting the Elbe croplands soils to C sources. Hence harvest by-products offer a noteable potential for energy generation but soil C reproduction has to be considered as well. The use of a bioenergy rotation on surplus arable land however is beneficial both in terms of soil C reproduction and substitution of fossil energy sources.

Regionally, areas suffering highest alterations and potential for soil C sequestration were identified based on the scenario assumptions used. Soils with high contents of C mainly in the eastern part of the loess area and in alluvial formed parts of the lowland landscape, deliver highest decrease of soil. For the loess area intensive agriculture is dominating with crop rotations and shares resulting in decreasing soil C, which already is visible for reference conditions. For soils influenced by water with high C content in the alluvial formed landscapes (riparian zones), climate change (increase in temperature and decrease in precipitation) causes strong decrease in soil C storage. This effect is amplified by crop share changes to set-aside with black fallow use and mitigated through e.g. extensified ley-arable rotation. Soils in periglacial formed lowlands and in the mountain landscapes (mainly less fertile soils with sandy to loamy soil texture and low soil C content) show weaker decrease due to climate change and set-aside use and deliver highest increases in soil C for crop rotations reproducing soil C (e.g. ley-arable, bioenergy, rotation with cover crops between cash crops).

Overall croplands in the Elbe basin are currently acting as C sources with increasing tendency under expected climate and agro-economic change assuming set-aside on surplus arable land. Agro-economic change alterations of soil C dynamics however are stronger than climate change and an appropriate use of surplus arable land determines whether the study area is a C source or a C sink in the future. Bioenergy and ley-arable rotations on surplus arable land deliver positive effects on total soil C balance with a considerable potential of bioenergy crops to substitute fossil fuel resources. Hence it offers one option to mitigate increasing CO₂ contents in the atmosphere. In contrast, using 80 % of harvest by-products of total croplands delivers a high energy generation potential, but is seen negative for soil C reproduction and maintaining soils fertility.

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Chapter 6

Summary, conclusion and perspectives

6.1 Model concept of SOM turnover and its integration in the ecohydrological model SWIM

Using simulation models to describe environmental processes or soil C and N turnover like in this case within an eco-hydrological modelling tool requires abstracting environmental processes into mathematical descriptions. These descriptions either try to represent the actual environmental process based on physical based laws or try to describe the process using empirical relationships. The latter one requires data and insights from laboratory or field scale investigations of certain processes.

Establishing or extending an existing modelling tool has to take into account the level of process abstraction and process detail necessary to account for an ecosystem reaction on environmental change at the scale considered and the research questions at hand. The model has to consider predefined and necessary process interactions (e.g. change in soil C turnover due to changing soil temperature) dependent on key questions to be answered and the target scale the model should operate on. When achieving these preconditions, modelling tools allow evaluating environmental change impacts on ecosystems, or in our case here, on soil C balance. But the question posed in chapter 1, namely "what kind of model concept is appropriate to describe soil organic matter turnover?" can only be answered taking into account the aims, the spatial scale and the time frame considered. Within this study the model SWIM was extended by a process-based soil C and N turnover description to investigate global change impacts in meso- to macro-scale river basins and for a time frame of approximately 100 years.

These circumstances were considered in the conceptualisation of the model extension, namely data availability to parameterise and run the model and to achieve certain model robustness. As noted recently by Ogle et al. (2006) the ideal case is that the scale in which model results are interpreted matches the scale of parameterization. Related to the scale considered here, organism oriented model descriptions of soil organic matter turnover are not applicable yet. Hence a process-based model concept was chosen.

As mentioned in chapter 1 and 2, classic soil organic matter models of the processbased type using first order rate kinetics like in CANDY (Franko et al., 1997b), DAISY (Jensen et al., 1997), CENTURY (Parton et al., 1987) or RothC (Coleman et al., 1997) partition the soil organic C to conceptual pools with intrinsic mean residence / turnover times. These models distinguish mostly between three soil C pools, for instance active, slow and passive pools as in CENTURY or biomass, humus and inert soil C pools as in RothC. Plant derived primary organic matter pools are most often separated in decomposable and resistant pools as in the RothC model or in structural and metabolic pools as in the CENTURY model.

The more soil C pools or compartments are distinguished, the more the fact that organic matter is transformed in continuum is accounted for. But the central point here is first to initially allocate these pools and find relationships of C fluxes between them. Magnitudes of these pools of course vary considerable depending on environmental conditions but most models are using static allocation schemes. Additionally, most models divide organic matter into a number of pools using data-fitting techniques. But it is not often possible to measure the properties of each pool of soil C, e.g. there is no analytical method available to determine the number or size of the various pools to be simulated (Fang et al., 2005b). This problem refers to the fact that transformations of organic matter and analytical determination of the transformation status (by e.g. laboratory methods) does commonly not match to the soil C pools assigned in simulation models. Hence the choice of approaches is more or less either to model the measurable or measuring the modelable as discussed in an article by Elliott et al. (1996). Referring to the scale the model should operate on it was decided for the first choice ("model the measurable") in this study.

To minimise this source of model uncertainties one has to acknowledge that number of parameters and environmental information increases with a growing amount of distinguished soil C pools. For instance, most models (e.g. CANDY, RothC) consider a so called "inert" or "refractory" soil C pool, which is believed to be physically and chemically stable and features turnover times greater than 1000 years. Again the initialisation of the magnitude of this pool depends on environmental conditions, mainly on clay content, and many others beside that. Although empirically gained relationships to initialize this pool do exist, the discrepancies of results obtained are considerable and hence the uncertainty in initialising this pool is very high. Of course there is no doubt that chemical and physical protected carbon compounds in soils (e.g. charcoal or black carbon, lower limit of soil C content) exist. But when considering land use and climate impacts in time frames of about 100 years it is assumed here that it is not necessary to account for an inert pool.

Most models consider an inert pool to guarantee that soil C storage does not undergo a certain lower threshold over time, but this effect may become relevant when considering simulation times of several centuries. Additionally, recent work by Skjemstad (2001) and Gleixner et al. (2002) suggest that it is not necessary to consider an inert C pool, and their investigations provide evidence that the total organic carbon content should be considered in the turnover cycle. Hence neglecting a physical and chemical protected soil C pool for the purposes of this study seems justifiable. Consequently, the amount of parameters is already reduced compared to other process-based soil organic matter models.

Furthermore, the SOM turnover concept proposed in this study does not distinguish between active, slow and passive soil C pools. Instead, only one soil C pool is present (beside the primary organic matter pools), but with different turnover properties depending on soil depth. As noted above, recent work states that all soil organic C is subject to turn over. It is argued here that a conceptualisation into e.g. three soil C pools (active, passive and stable) is only necessary if there is evidence that these pools show different sensitivities under changing environmental conditions, e.g. soil temperature changes. In the case of temperature sensitivity there is an ongoing intense debate whether different soil C pools show different sensitivities to temperature change (see chapter 4 for a discussion on that issue). It is assumed in this study that different soil C pools do not show different sensitivities to environmental changes. There is no clear evidence yet, gained through field or laboratory experiments, or through simulation studies, that different soil C pools could respond differently on soil temperature changes. This assumption can be supported with findings by e.g. (Fang et al., 2005a; Fang et al., 2006a), but is currently controversially discussed (Giardina and Ryan, 2000; Knorr et al., 2005; Reichstein et al., 2005a; Fang et al., 2006a) and needs further research. In this study it is assumed that turnover sensitivity is not different for different soil C pools, but depends on soil depth. The appropriateness of the assumption to assign only one heterogeneous soil C pool to reflect soil C changes due to changes in quality and quantity of soil C input and turnover properties in soils (through e.g. land use change or climate change) is also supported in recent work by Fang et al. (2005b). A major advantage is less data and parameter necessary to run the model and the availability of direct measurements of soil C carbon contents to test and validate the model.

The same argumentation as above can be stated for primary organic matter (plant debris and animal residues). Again, initialisation and allocation of several pools for primary organic matter showing intrinsic turnover times is linked with uncertainties. The same holds true with fluxes between different primary organic matter pools and soil organic matter pools. In this case, the fact that different plant parts have different turnover properties is accounted for through partitioning up to five plant parts (as dead fine roots, coarse roots, foliage, twigs and branches, and stems) and in intrinsic turnover properties of each plant species distinguished. Relevant studies to parameterise the turnover properties of these fractions for the plants distinguished in this study are provided through numerous studies relating to laboratory and field investigations (see chapter 2 to 4 for details).

Hence the process-based descriptions adopted here can be seen as robust in terms of data needed for parameterisation and the fact that it has to operate in meso to macro scale, and for a time span of about 100 years. It also provides the opportunity to test and validate the model extension with readily available field scale observations (e.g. from long-term experiments). Additionally, it was achieved that the model extension for soil C and N turnover possesses the same level of process complexity as other descriptions in SWIM and the overall process detail was maintained.

The adopted description of soil C and N turnover (for details see chapters 1 and 2) was integrated into the eco-hydrological river basin model SWIM. This ensures that the relevant processes are connected and are linked with each other. The soil C and N turnover model therefore is linked to basin and soil hydrology and nutrient dynamics, soil temperature dynamics, and plant growth, including plant nutrients and water demands. Furthermore soil C and N turnover is linked so soil C turnover is reduced if inorganic soil N status (Nitrate and Ammonia) is too low. Additionally, soil C turnover directly affects soil N processes by providing energy for this process. A combined simulation of soil C and N processes is necessary, and one process can not be described correctly without the other. Soil temperature and soil water dynamics are directly impacting these processes, which is considered in the extended SWIM version. The strength of SWIM to adequately represent soil water and nutrient processes in river basins under present environmental conditions and potential future changes is an important feature to properly reflect soil organic C dynamics.

6.2 Process interactions and key environmental drivers of soil C dynamics

Relevant process interactions and the ability of the extended model to reflect impacts of different land management practices were demonstrated in chapters 2 and 3. For soil-crop systems a successful evaluation of water and nutrient dynamics could be demonstrated for

various climatic, edaphic and land management properties in eastern Germany. Soil temperature, soil water, soil nitrogen, soil carbon dynamics and crop growth were represented reasonably well in comparison to field scale measurements for these processes. Some problems were also identified. For example, soil temperature simulation did not completely reflect land cover influences, which could be attributed to the simple empirical process formulation adopted. In addition plot scale simulation of crop yields showed certain discrepancies to measurements which can also be explained by a process description designed for regional scale crop yield assessments, where SWIM was evaluated successfully (Krysanova et al., 1998, 1999; Hattermann et al., 2005a). It must be stated that especially agro-technological change as sort improvement is not implemented in SWIM. SWIM simulates crop growth sensitive to climate and soil properties but not to technological impacts. Although nutrients and water uptake by crops, and soil water and soil Nitrogen dynamics were successfully simulated under different soil conditions and climate in comparison to measurements.

It was be demonstrated for long-term soil C dynamics that the model is able to successfully reflect impacts of crop types, crop rotations and different organic and inorganic fertilisation regimes for two long-term field experimental sites. The results obtained using the extended SWIM model for soil C dynamics at these sites are of similar goodness as other process-based soil organic matter models (e.g. CENTURY, CANDY, RothC) as demonstrated in a model intercomparison study (Powlson et al., 1996; Smith et al., 1997b). Dynamics of soil C storage were checked using measured and cited values for soil heterotrophic respiration, which generally agree with the simulations (see chapter 2). This exercise of evaluating relevant processes under different environmental conditions states a necessary precondition for assessment studies.

In a next step it was important to evaluate model sensitivities to changing external drivers. This was done for selected agricultural management practices, like for different amounts and types of fertilisation, different crop rotational types, cover crops impacts and effects of harvest by-products remaining on the fields on soil C storage for two experimental field sites. The obtained results generally agreed with comparable findings cited in literature

and measurements, and proved the model's ability to reflect selected management impacts on long-term soil C storage (see chapter2).

Organic and inorganic fertilisation effects on SOC storage were estimated between - 0.13 t C ha⁻¹ yr⁻¹ and +0.1 t C ha⁻¹ yr⁻¹, which correspond to observations made for the same field sites. Impacts of different crop shares and crop rotations with and without including cover crops led to simulated changes of -0.13 t C ha⁻¹ yr⁻¹ and +0.07 t C ha⁻¹ yr⁻¹. Simulated C storage impacts of crop types and crop shares correspond to values cited in literature and with accounting schemes developed for on farm soil C reproduction screening necessary under a national regulation (German Soil Law, BBodSchGes, UmwR, 2005). Soil C changes due to incorporating grain straw to the soil, an important measure for soil C reproduction, was calculated for different amounts left on the fields and resulted in soil C changes between -0.1 t C ha⁻¹ yr⁻¹ and 0.027 t C ha⁻¹ yr⁻¹. These simulation exercises demonstrate successfully the ability to quantify selected managements impact on soil C storage and offer the potential to explore their regional or river basin scale impacts.

6.3 Uncertainty and sensitivity

An aspect that has become necessary when applying simulations models in environmental impact studies, delivering information for e.g. decision making or about how a region's soil C properties might develop under future environmental conditions, is a detailed uncertainty analysis. The method of uncertainty analysis applied here (Monte Carlo based uncertainty assessment using latin hypercube stratified sampling, see chapter 4) also results in information about which factors and parameters are most important and which ones can be left out. This information is crucial, for instance for determining these factors and for process understanding.

In this study an important issue was to not only incorporate model related parameters in the uncertainty analysis, but also factors relating to model input data as soil properties, climate and land management factors. This allows ranking by importance of model parameters along with external driving forces derived from generalized and regionalized information sources (e.g. land use map derived from satellite information, climate observations interpolated to a certain spatial scale and so on). In addition to the factor sensitivities, the magnitude of change in soil C storage delivers important information when interpreting results from assessment studies using a simulation model. But the magnitude not only depends on input factor's variation ranges but also on the temporal evolution of uncertainty and the spatial distribution of uncertainty. Therefore and a step that is not performed commonly is an assessment of spatial and temporal development of uncertainty.

Attached to all these input factors is a typical error range. This error range is very difficult to estimate because detailed information on these ranges is very seldom available. Information was taken from e.g. literature sources where possible. For others, input factors ranges were derived from expert judging (field scientists and modellers) based on questionnaires, but also by subjective estimation.

The most important parameters, contributing most to uncertainty at the same time, were identified as soil carbon turnover related parameters: the carbon synthesis parameter ("determining the carbon use efficiency"), soil carbon mineralization parameter (k_{aom}) and the temperature dependence of soil C turnover (Q10 factor). These model parameters clearly contribute most to uncertainty at the field scale. But for regional scale assessments it is demonstrated that input data related uncertainties gain in magnitude. It is here that soil input data (soils bulk density and initial soil C content) and second climate input data (air temperature) have considerable impact on model uncertainty. It was also shown that model uncertainty increases with simulation time (chapter 4).

Magnitudes of uncertainty related to regional soil and land use characteristics were disclosed next to a quantification of uncertainty in simulating long-term soil C dynamics and the identification of key sensitive factors contributing most to that uncertainty. In this finding soil influenced by anaerobic soil conditions either temporally or permanently, for instance Gleyic soils (Gleysols), show highest uncertainty values after soils with high loess substrate contents. As for the broad land use types grassland, forest and croplands it was found that croplands deliver the highest magnitudes of uncertainty. Overall uncertainty accounts for $\pm - 0.065$ to $\pm - 0.3$ % soil carbon content which corresponds to a rate of about 0.06 to 0.15 t C per hectare and year. In terms of the field scale uncertainty assessments the model uncertainty is still within soil C measurements variability.

As shown in chapter 4, the quantified uncertainty does not interfere with simulated long-term trends of crop rotation impacts on soil C dynamics. Hence the model structure is adequate and the model is capable to assess land management impacts on long-term soil C storage under the quantified uncertainty. The uncertainty assessment conducted in this study considers all relevant sources of uncertainty for the temporal and spatial domain and not just model parameters like in most studies reported. The derived information here from is relevant for interpreting results from assessment studies. Furthermore the uncertainty assessment conducted for this type of simulation model is transferable to other process-based soil organic matter models and therefore provides useful information on attached uncertainties when simulating regional scale long-term soil organic C dynamics.

6.4 Regionalising external driving forces and regional impacts study

As demonstrated in chapters 2, 3 and 4 the extended model is capable of quantifying selected environmental change impacts on soil C storage and the attached model uncertainty. As stated before, climate and land use (land cover and land management) are the key external drives impacting soil C storage after other ecosystem functions. For meso- to macro-scale impact studies these external driving forces need to be regionalized accordingly, in addition to determining spatially distributed soil properties.

Chapter 5 proposes a conceptualization of regionalized land use and climate properties for the recent past and present situation in combination with a regionalization of anticipated climate and land use changes. This was performed for agriculturally used areas in the German part of the Elbe river basin, as croplands face significant future changes. Also agriculture is the dominating land use in the Elbe basin and agriculture led and most probably will lead to the most pronounced changes in soil C storage.

In chapter 5 an algorithm for generating spatial crop cover patterns on arable land (described in detail in Wechsung et al., 2005) and its application in a modelling framework for assessing impacts of land use and climate change on soil C balance is proposed. Complementary to other studies, which use a lumped characterisation of crop shares, a consideration of local crop share information in accordance with county based crop statistics was included. This constitutes an important step towards enhanced accounting of regional scale crop cover effects on soil C storage. Besides characterising reference conditions, the algorithm was also used for regionalising global agro-economic change expected in the future. For the study area (Elbe river basin), the anticipated change results in an decrease of arable land by 30 % due to areas dropping out of economic use and becoming abandoned. A land use change scenario which is consistent in terms of its climate and socio-economic boundary conditions taking feedbacks into account was established along with the regionalisation of global climate change scenario developed in the GLOWA (GLObal WAter) Elbe project (Gerstengarbe and Werner, 2005; Hattermann et al., 2005a; Wechsung et al., 2005).

The basin scale assessment study of regionalized global change impacts on soil C storage estimates present day and future soil C storage and characterises land-atmosphere fluxes of carbon for croplands. Currently croplands in the Elbe basin can be attributed as source for soil C denoting a net C flux of 11 g C m⁻² yr⁻¹. But the fraction of harvest by-products remaining on the field is substantially influencing soil C storage. This confirms the importance of harvest by-products for soil C reproduction. Additionally, a net annual flux of 7 g C m⁻² yr⁻¹ to the atmosphere could be estimated due to the climate trend of + 0.8 K already present for the period 1951 to 2000. Furthermore, single and combined effects of climate and agro-economic change impacts on soil C storage were derived. Climate change for the scenario period from 2001 to 2055 alone accounted for an extra flux of 4 g C m⁻² yr⁻¹, and land use change (assuming black fallow on croplands falling out of economic use) yielded an extra of 12 g C m⁻² yr⁻¹. Hence anticipated agro-economic changes result in stronger alteration of soil C storage and net annual fluxes to the atmosphere than climate change effects alone. Thereby, estimated climate change scenario uncertainty on soil C storage and fluxes are low.

As concluded in chapter 5, future use of agricultural land anticipated to fall out of use ("surplus arable land") is of paramount importance for soil C balance. Soil C balance of the Elbe basin is considerably affected by the decision on how to use this land. I investigated three potential uses, namely (1) setting aside (black fallow use), (2) a typical bioenergy rotation, (3) and extensified use as ley-arable land. Using a ley-arable or bioenergy rotation converts the basin croplands to an overall sink of soil C and increases soil C storage.

Besides using harvest by-products, bioenergy crops additionally offer, the potential for energy generation and hence a substitution of fossil fuel sources. One more simulation run was established using 80% of harvest by-products on total cropland exploring the biological potential of harvest by-products as energy source. An energy potential of 37 000 TJ per year $(1TJ = 10^{12} \text{ Joule})$ equalling a substitution of approximately 7000 10³ barrels of oil (1 barrel = 159 litre) per year could be estimated using only the biomass derived from the bioenergy rotation on surplus arable land. Using harvest by-products yields an extra 125 000 TJ per year for potentially substituting 22 000 10³ barrel of oil annually. The total gross energy equivalent of 162 000 TJ per year is roughly 1% of total German primary energy consumption (~ 14 500 000 TJ) per year. However, these numbers have to be interpreted cautiously as they state the biological potential with no consideration of economical and political factors. In addition a full energy balance accounting for the production scheme has to be performed to obtain a sounder picture. The use of harvest by-products furthermore is also an important factor for soil C reproduction. The export of 80% harvest by-products for energy generation led to a significant decrease of soil C storage and increase of net C flux from soils to the atmosphere in the Elbe basin. Hence both effects, soil C reproduction to maintain soil fertility, and energy generation from biomass to substitute fossil fuel sources important in terms of climate change mitigation, have to be balanced out.

6.5 Key achievements and findings

With this study a comprehensive modelling approach is proposed to estimate present-day and future soil organic matter dynamics and their alteration under land use and climate change. The study provides an extensive evaluation of the model's appropriateness to simulate soil organic matter changes and related processes. An uncertainty assessment of model estimates on soil C storage is provided for the established modelling tool. An exemplary assessment study of possible soil C changes for croplands is demonstrated based on regionalized climate and socio-economic changes taking feedbacks into account. The extended model is capable of quantifying selected land management practices, land use and climate impacts on soil C storage beside impacts on water quantity, water quality and vegetation growth properties within meso- to macro-scale river basins. The major achievements and findings of this study are:

- For the basin scale assessments it is estimated that croplands in the Elbe basin currently act as a net source of carbon. Although this highly depends on the amount of harvest by-products remaining on the fields. Future anticipated climate change and observed climate change in the basin already accelerates soil C loss and increases source strengths. But changing agro-economic conditions, translating to altered crop share distributions, display stronger effects on soil C storage than climate change.
- Depending on future use of land expected to fall out of agricultural use (~ 30 % of croplands as "surplus" land), the basin either considerably looses soil C and the net annual C flux to the atmosphere increases (surplus used as black fallow) or the basin converts to a net sink of C (under extensified use as ley-arable) or reacts with decrease in C source strength when using bioenergy crops. Bioenergy crops additionally offer a considerable potential for fossil fuel substitution, whereas the basin wide use of harvest by-products for energy generation has to be seen

critically. Harvest by-products play a central role in soil C reproduction and a percentage between 50 and 80 % should remain on the fields in order to maintain soil quality and fertility.

- Simulated impacts of external driving forces (climate, soil and land use) on soil C storage correspond to observations of soil C changes and allows quantifying soil C dynamics under altered environmental conditions. Recommended agricultural management practices effects on soil C storage (for example different fertilisation amounts, crop rotation and crop shares effects, effects of cover crops and harvest surplus management) can especially be assessed. As example, root crops and silage maize decreases soil C content over time, while ley-arable rotations and the inclusion of cover crops increase soil C storage.
- Compared to other process-based soil organic matter models, the descriptions proposed here relate SOM pools and turnover properties to readily measurable quantities. This reduces the number of model parameters, enhances the comparability of model results to observations, and delivers same performance simulating long-term soil C dynamics as other models.
- Magnitudes of uncertainty, in their temporal and spatial characteristics, and related to model parameters and model input data (for example soil information, climate, agricultural management assumptions) are disclosed. Importance ranking (sensitivity analysis) yielded that the soil organic C mineralization rate constant, the synthesis coefficient (determining the amount of C and N being respired or stored in the soils) together with Q10 parameter for soil temperature sensitivity on soil C and N turnover are introducing the highest degree of uncertainty. At the river basin scale, soil and climate input factors gain importance. Further on, soils influenced by anaerobic conditions and loess soils together with croplands are estimated as areas showing highest uncertainty values. But overall uncertainty attached to soil C

storage simulations does not interfere with model's responses to changing environmental conditions.

• New is that the SOM turnover description is embedded in an eco-hydrological river basin model, allowing an integrated consideration of water quantity, water quality, vegetation growth and soil organic matter changes under different environmental conditions. SOM turnover is considered as coupled soil C and N turnover.

6.6 Perspectives

The established modelling tool facilitates integrated consideration of different ecosystem services. Hattermann et al. (2005a) recently demonstrated an integrated assessment of global change impacts on water resources and crop yields in the Elbe basin, using the same simulation set-up as described in chapter 5. Hattermann et al. (2005a) concluded that anticipated climate change leads to severe impacts on groundwater recharge and river flow. Consequently the natural environment and communities in parts of the Elbe basin will have considerably lower water resources under expected climate change. Hence a combined analysis of land use change and climate change impacts on water availability, crop yields and soil C storage would provide useful information for decision making or for planning adaptation measures to encounter environmental problems. For example, woody or fast growing energy plants like poplar plants or elephant grass offer the potential for energy generation but possess a high water and nutrient demand for growth. For regions facing water deficit problems in the future, as it is the case for some parts in the Elbe basin, encouraging fast growing plants may lead to harmful effects. Same causality can be attributed to e.g. land use conversions from croplands to forest. In terms of soil C storage this measure is beneficial, but in terms of water availability, large scale afforestation in a water stressed region is disadvantageous. In a recent work using SWIM within the Elbe basin, Wattenbach et al. (submitted) suggest a negative impact of afforestation of abandoned arable land on the regional water balance. The established model offers the perspective to conduct integrated impact studies taking environmental interactions into account. Preparation of response curves for e.g. soil water availability or soil C storage to changing environmental components or measurements adopted would provide useful insights on ecosystem behaviour and information for decision making.

In terms of land use conversions accountable under the Kyoto protocol (Article 3.4, e.g. conversion of croplands to forest), the proposed model extension may be used to assess impacts on soil C storage. Although, for long-sighted time frames, C saturation effects and lower C limit of soils becomes relevant beside impacts of land use history. But information on the latter for the considered scale is still sparse. Together with the recently implemented approach for an enhanced forest dynamics representation in SWIM (Wattenbach et al., 2005), soil C dynamics in mineral soils may be estimated and land use conversion effects could be investigated in the future.

Wetland and riparian zone impacts on soil C dynamics are also relevant. (Hattermann et al., 2004, 2005a) established improved descriptions of groundwater and riparian zones processes in SWIM and demonstrated their relevance in terms of diffuse nutrient input into rivers and lakes and for the water and nutrient balance of river basins. As was identified in chapter 5, soils with high C content are more susceptible to expected climate change than soils with a low soil C content. Hence wetland and riparian zone soils may be important sources of C fluxes to the atmosphere in the future, which could be addressed in further research work. Future development of lateral transport and retention processes of dissolved organic carbon and nitrogen (especially in riparian zones) and linking the erosion submodel of SWIM to translocations of particle bounded organic C, would constitute a further step towards complete C cycling between hydrosphere, pedosphere, biosphere and atmosphere. Furthermore, information on the largely unknown flux of dissolved C from land to oceans under changing environmental conditions would contribute to further understanding.

Up to now, socio-economic changes are considered in climate and land use change scenarios. In terms of regional C emission estimation the natural science part addressed here should be linked to socio-economic processes. Neither economic nor ecosystem models alone can provide an integrated estimate of the economic and environmental effects of different mitigation options. Linking socio-economic and natural science aspects would constitute an important step towards achieving climate change mitigation.

However, the methodology and assessment presented here demonstrates the potential for integrated assessment of soil C change alongside with other ecosystem services (soil fertility, water quality and availability, and agricultural productivity) under global change impacts and provides information on the potentials of soils for climate change mitigation and on their soil fertility status.

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List of Figures

- Fig. 2.1: Schematic representation of the SOM model extension (SWIM –SCN)24

- **Fig. 4.3**: Temporal development of uncertainty for experimental sites Bad Lauchstädt (right) and Müncheberg (left) for 51 and 37 years simulation period respectively considering a) all factors, b) parameters, c) soil, d) climate, e) crop harvest management (harv_surp) and f) fertilisation. Results shown are 5, 25, 50, 75, 95 percentile values based on 500 model runs expressed in percent of soil organic carbon content (Corg, 0-20 cm soil depth). In a) simulation using standard parameterisation (grey line) and measurements at the respective sites are shown. Please note that for Bad Lauchstädt no measurement were conducted for the fertilisation scheme used in this study (1.2 t C ha⁻¹ yr⁻¹, various amount of NPK, see table 4.2) and measurements representing 2 t C ha⁻¹ yr⁻¹ (black circles) and no organic fertilisation (black rhombic sign) are shown.
- **Fig. 4.4**: Spatial distribution of uncertainty for the Nuthe river basin expressed as coefficients of variation values (COV in %, see equation 4.1) for a) all factors, b) parameters, c) soil, d) climate, e) crop harvest management (harv_surp) and f) fertilisation......112

- Fig. 5.7: Basin scale average for croplands only for four scenario assumptions (land use reference and climate reference Ref07 as black line, land use scenario and climate scenario CLC1 as black line and rectangles, land use reference and climate scenario CCo as bright grey with triangles, land use scenario and climate reference LCo as dark grey with circles) for topsoil C storage (g C m⁻², a), total soil C storage (g C m⁻², b) and Net Biome Exchange (g C m⁻², c).
- Fig. 5.8: Difference map for mean topsoil C storage (g C m⁻²) for a) Climate Change only (CCo) minus reference condition (ref07), c) Land use change only (LCo) minus reference condition and qualitative illustration in changes of Net Biome Exchange (NBE) for b) Climate Change only (CCo) minus reference condition and d) Land Use change only (LCo) minus reference condition. Please note that averaged values of the periods 1991 to 2000 for the reference conditions and 2046 to 2055 for the scenario conditions are used. Topsoil C storage values below zero denote a loss of C under scenario conditions compared to reference conditions. Abbreviations are explained in table 5.5.
- Fig. 5.10: Maps of topsoil C storage difference (g C m⁻², left) and qualitative expressions for Net Biome Exchange (NBE, right) for a) CLC1 minus Ref07, b) CLC1-Bio minus Ref07, c) CLC1-Ley minus Ref07 and d) CLC1-Harv minus Ref07. Please note that averaged values of the periods 1991 to 2000 for the reference conditions and 2046 to 2055 for the scenario conditions are used. Topsoil C storage values below zero denote a loss of C under scenario conditions compared to reference conditions. Scenario acronyms are explained in table 5.5).

List of Tables

Table	2.1 : Description of experimental sites used for testing SOM model extension	
Table	2.2 : Description of crop rotation types, fertilisation regimes and crop residue management practices considered in the simulation exercise	
Table	2.3 : Representation of statistics describing the model performance of POM decomposition	
Table	2.4 : Simulated yearly soil respiration (SR) values for three land cover types compared with literature cited values and measurements	
Table	2.5 : Representation of statistics describing the model performance in simulating soil carbon dynamics for the Müncheberg experimental site (a) and Bad Lauchstädt long-term static fertilisation experiment (b)	
Table	2.6 : Changes in SOC content for the simulation period (cumulative) and the yearly increment of change for the different crop rotations, grain straw additions and different fertilisations at the Müncheberg and Bad Lauchstädt sites	
Table	3.1 : Overview of simulated sites and processes used for model evaluation	
Table	3.2 : Description and site conditions of experimental sites used for model evaluation.59	
Table	3.3 : Overview of statistics used in the model evaluation procedure	
Table	3.4 : Representation of statistics describing the model performance in simulating soil temperature for a) Müncheberg, plot 3, 20 cm, b) Müncheberg, plot 3, 50 cm, c) Bad Lauchstädt, crop rotation, 5 cm, d) Bad Lauchstädt, crop rotation, 20 cm soil depth68	
Table	3.5 : Representation of statistics describing the model performance in simulating soil water contents for a) Müncheberg Plot 3 with respective soil depths, b) Bad Lauchstädt crop rotation with respective soil depths, c) Berlin Lysimeter 9,10 (135 cm	
	groundwater depth) and 11,12 (210 cm groundwater depth), <i>Cambisol</i> soil73	
Table	groundwater depth) and 11,12 (210 cm groundwater depth), <i>Cambisol</i> soil73 3.6 : Representation of statistics describing the model performance in simulating crop yield for a) Müncheberg plot 3, b) Bad Lauchstädt long-term plot only for winter wheat yields, c) Bad Lauchstädt, short-term crop rotation plot76	
Table Table	groundwater depth) and 11,12 (210 cm groundwater depth), <i>Cambisol</i> soil	

VI

- Table 4.4: Uncertainty ranges for the plot scale assessment (Bad Lauchstädt and Müncheberg experimental sites) of all considered sources a) all factors, b) parameters, c) soil, d) climate, e) crop harvest management and f) fertilisation expressed in percentage changes in soil organic carbon content (0-20 cm soil depth) of the 5 and 95 percentile values of 500 simulation runs and the respective mass changes of soil organic carbon [t C ha⁻¹] and the yearly increment [t C ha⁻¹ yr⁻¹].
- Table 4.5: Comparison of uncertainty for the plot scale assessment (Bad Lauchstädt and Müncheberg sites) and river basin scale assessment (Nuthe river basin) expressed as coefficient of variation values (COV in %, see equation 4.1) for all considered sources a) all factors, b) parameters, c) soil, d) climate, e) crop harvest management and f) fertilisation.
- Table5.1: Overview of crop rotations and crop sequences used for regionalization of county
level crop shares based on soil fertility (7 classes). Crop type acronyms are explained
in table 5.2.134

- Table5.4: Description of simulation assumptions during the reference period (1951 to 2000)
for the parameterisation of harvest by-product percentage remaining on the fields.
Please note that Ref07 assumptions are used also for future scenario cases (2001 to
2055).139
- Table 5.5: Characterisation of reference case and climate and land use change scenario assumptions considered in this study.
 141
- **Table** 5.6: Selected hydrotopes to exemplary describe local effects of climate and land use
change on soil C storage and fluxes.143
- Table5.7: Correlation between original and re-allocated crop shares for the Elbe basin per
state and across crops (1996 1999)146

Table 5.8: Over the respective simulation period averaged results of main components for
the investigated simulation cases. Acronyms in the table are explained in table 5.5

Curriculum vitae and Publications

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Publications

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- **Post, J.** 2002. Diploma Thesis: Auswirkungen von Landnutzungsänderungen auf den Wasserhaushalt des oberen Rio Guadalentin (Südost Spanien) - Anwendung eines flächendifferenzierten Wasserhaushalts-Simulations-Models. Diplomarbeit, Universität Trier.

Erklärung

Hiermit erkläre ich, dass die Arbeit an keiner anderen Hochschule eingereicht sowie selbstständig und nur mit den angegebenen Mitteln angefertigt wurde.

Berlin am 23.04.2006

(Joachim Post)

Jedem Anfang wohnt ein Zauber inne (Hermann Hesse)