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

Joachim Post*, Fred F. Hattermann, Valentina Krysanova, Felicitas Suckow

Department of Global Change and Natural Systems, Potsdam Institute for Climate Impact Research, P.O. Box 60 12 03, 14412 Potsdam, Germany

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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 require 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 stem 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 (focusing 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 stemming from soil and climate input data variations are striking. At 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 (e.g. climate, land use and soil properties) 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 were identified: the mineralization rate coefficient, the carbon use efficiency parameter (synthesis coefficient) along with parameters determining the soil temperature influence on SOM turnover (mainly Q10 value) and the soil input related data (soil bulk density and initial soil C content) introduced the highest degree of model uncertainty. The here gained information can be transferred to other process-based SOM turnover models to consider stronger most crucial parameters introducing highest uncertainty contribution to soil C storage assessment under changing environmental conditions.

Keywords: Eco-hydrological modelling; Soil carbon; Uncertainty analysis; Sensitivity analysis; Model parameters; Input data

1. Introduction

Assessing changes of soil organic matter (SOM) due to land management practices, land use and climate change plays a crucial role in the fields of climate change mitigation (soil carbon sequestration), land–atmosphere interactions and soil fertility. Soil organic matter 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 (Lal, 2004).

Due to the complex interactions of processes affecting SOM dynamics, the use of integrated dynamic ecosystem models is seen as a useful tool to assess SOM dynamics.

* Corresponding author. Tel.: +49 (0)331 288 2417; fax: +49 (0)331 288 2695.
E-mail address: joachim.post@pik-potsdam.de (J. Post).

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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., 2005; Janssen et al., 1994; Saltelli et al., 2000a,b; 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 contribute most to this uncertainty (Janssen et al., 1994; Saltelli et al., 2004). Parameter uncertainty stems mainly 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). Besides parameter uncertainties, uncertainties related to input data (e.g. soil, land use, climate input data, land management practices) and scaling issues also have to be considered.

The aims 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, 2007a,b). Thereby the maximum 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.

2. Materials and methods

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 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 et al., 2000). The model is connected to meteorological, land use, soil and agricultural management data. Detailed process descriptions, validation studies and data requirements can be found in published literature (Hattermann et al., 2004, 2005; 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. (2007a,b).

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 CO_2 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; 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 are considered through reduction functions (Kartschall et al., 1990).

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; first-order 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., 2000a,b): (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 PDFs (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 Centre (JRC) in Ispra (Italy) has been used.

2.3.1. 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., 2005) also using Monte Carlo based global sensitivity and uncertainty analysis.

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 Distribution Functions (PDFs) 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 PDFs 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/Questionnaire.htm, as of 18/03/2007). 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 1). For example field soil respiration measurements in the study area suggest a Q10 value (Q10 is the value by which the respiration rate differs for a temperature interval of 10 °C) 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 PDFs 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 PDFs (through e.g. formal statistical procedures) is not feasible. Table 1 gives an overview of the input factors PDFs.

2.3.2. 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.

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

Table 1
Description of input factors (parameters, climate and soil input data and variations in agricultural management practices) used in the sensitivity and uncertainty assessment

Input factor	Description	Type	Distribution of PDF	Range (reference value)	References
k_{hum}	Turnover coefficient of active organic matter [d^{-1}] first soil layer (humus layer): k_{hum}, layers 2,…,n (mineral layers): k_{hum_r}	Parameter	Triangular	[0.0001: 0.0003]/[0.00015: 0.00025][a] (0.0002)	Bergmann et al., 1999; Klimanek and Schulz, 1997
k_{hum_r}		Parameter	Triangular	[0.00005: 0.0002]/[0.00005: 0.00015][a] (0.0001)	
k_{nit}	Nitrification coefficient [d^{-1}]	Parameter	Triangular	[0.001: 0.004] (0.0025)	
k_{syn}_ag	Synthesis coefficient of primary organic matter [d^{-1}], "carbon use efficiency parameter"	Parameter	Uniform	[0.55: 0.80]	Klimanek and Schulz, 1997; Lettau and Kuzyakov, 1999; Nicolardot, 2001
k_{syn}_ bg		Parameter	Uniform	[0.55: 0.80]	
k_{opm}_ag	Turnover coefficient of primary organic matter [d^{-1}]	Parameter	Uniform	[0.1: 0.45]	Klimanek and Schulz, 1997
k_{opm}_bg		Parameter	Uniform	[0.1: 0.45]	
frc_ag	Allocation of below and above-ground residuals	Parameter	Triangular	±20%	Klimanek, 1987; Klimanek and Schulz, 1997
frc_bg		Parameter	Relation	−1.0[a] frc_ag	
cnr_ag	Carbon/Nitrogen ratio	Parameter	Uniform	±20%	Klimanek and Schulz, 1997; Schulz, 1997
cnr_bg		Parameter	Uniform	±20%	
Q10	Q10 value of soil temp. reduction function	Parameter	Triangular	[1.5: 2.5]/[1.8: 2.2][a] (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][a] (35)	Kartschall et al., 1990; Rodrigo et al., 1997
wsat	Limit of saturated water content, part of soil water reduction function [Vol.%]	Parameter	Triangular	[0.4: 0.6] (0.5)	
temp.	Temperature [°C]	Climate	Normal	±2°C $\mu = 0$, $\sigma = 1.0$	Workshop Aberdeen
precip.	Precipitation [mm]	Climate	Normal	±10% $\mu = 0$, $\sigma = 0.05$	Workshop Aberdeen
radiation	Global radiation [MJ/m^2]	Climate	Normal	±30% $\mu = 0$, $\sigma = 0.15$	Workshop Aberdeen
fertinorg	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
harv_surp	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
initsoc	Initial soil carbon content [%]	Soil	Triangular	±10%	Workshop Aberdeen

ag, above-ground; bg, below-ground.
[a] Ranges have been narrowed for the plot scale analysis as more detailed parameter information is available at the plot scale.

is made in each interval (Saltelli et al., 2000a,b). 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 1) PDFs 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 cobweb diagrams to get a first impression on single input sensitivity to model results.

2.3.3. 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. Furthermore we assessed the uncertainty at the plot scale at a certain time and the temporal course and on the spatial scale (river basin). Besides 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 1).

For the uncertainty assessment the coefficient of variation (deviation of a variable from its mean, ''standard error'', COV in %) was calculated according to eq. (1) to quantify the uncertainty to the mean value and to make a comparison between the different sources of possible uncertainty, with n = number of simulation runs, $\bar{x}$ = mean value of output, x_i = output value, sd = standard deviation:

$$\mathrm{COV}[\%] = \frac{1}{n-1}\sum_{i=1}^{n}\|(\bar{x}-x_i)\| * \frac{100}{\bar{x}} = \mathrm{sd} * \frac{100}{\bar{x}} \quad (1)$$

2.3.4. 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 one should refer to Helton (1993), Saltelli and Sobol (1995) and Saltelli et al. (2000a,b). 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., 2000a,b) 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; b_0, c_0, b_h, c_h are regression coefficients; j and h are respective input factors).

$$\hat{Y} = b_0 + \sum_{h\neq j} b_h x_h \quad \text{and} \quad \hat{X}_j = c_0 + \sum_{h\neq j} c_h x_h \quad (2)$$

The PCC is defined as the correlation coefficient between the terms $X_j - \hat{X}_j$ and $Y - \hat{Y}$ where X_j and Y are a particular parameter and output variable, respectively. $\hat{X}_j$ and $\hat{Y}$ are the estimated values of the linear regression.

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 behaviour 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).

Model outputs considered were the total soil carbon content (C_{tot}) and heterotrophic soil respiration (C_{resp}) for the respective areas under study (Table 2). Total soil carbon (C_{tot}) is referred to organic compounds only, not including inorganic content (carbonate). For plot scale assessment the C_{tot} and C_{resp} 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.

2.4. Data sets and study area for uncertainty analysis

For the plot 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., 2007; Körschens and Müller, 1996) for the Bad Lauchstädt site and (Mirschel et al., 2007; Rogasik and Schroetter, 1999; Rogasik et al., 2004) for the Müncheberg site and are shown in Table 2.

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 (Fig. 1). It covers an area of approximately 1900 km^2. 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%). The main agricultural area is in the southern region of the basin with mainly Luvic Arenosols on loess sediments (Fig. 1). Soils are mainly characterized by sandy to loamy soil texture (Cambic Arenosols, Podzols and Gleyic podzols) developed on glacial sediments.

3. Results and discussion

3.1. Factors sensitivity and importance

The PCC (partial Correlation Coefficient) was used in this study as sensitivity index because the 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. Factors are ranked according to their absolute values of PCC (|PCC|). Through interpretation of correlation plots between each of the input factors and the respective model output (C_{tot} and C_{resp}) a threshold of |PCC| = 0.20 could be identified. Input factors below this threshold do not show any notable impact to model output and are excluded from interpretation.

In general it can be stated that the model parameters describing the mineralisation dynamics of SOM (khum), the carbon use efficiency (synthesis parameter, ksyn) and the parameter regulating the influence of soil temperature on SOM (Q10), can be identified as most important factors (high |PCC| values, Table 3).

The synthesis coefficients 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 with

Table 2
Description of experimental sites and study area used in this assessment

Process output	Location (simulation period)	Data provider (Reference)	Description	Fertilisation regime	Input data for model simulation
Long-term soil C dynamics	Bad Lauchstädt (1951–2002)	UFZ (Franko et al., 2007; Körschens and Müller, 1996)	Long-term static fertilizer experiment, soil organic carbon measurements in 0–20 cm soil depth, loess soil, flat	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)	Climate, soil, management data provided by data holder. Crop rotation: summer barley/ potatoes/winter wheat/sugar beet
	Müncheberg, fertilised plot (1963–2000)	ZALF (Rogasik and Schroetter, 1999; Rogasik et al., 2004)	Long-term field experiment V140, soil organic carbon measurements in 0–20 cm soil depth, sandy soil, flat	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)	Climate, soil, management data provided by data holder. Crop rotation: winter rye, potatoes, winter wheat, sugar beet, spring barley
	Nuthe river basin (1981–1997)	Land use: Corine data (Dollinger and Strobl, 1996)	Pleistocene lowland river	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)	Climate, soil, management data provided by data holders. Crop rotation for all agricultural sites: summer barley/ potatoes/winter wheat/sugar beet
		Soils: Buek 1000 (Hartwich et al., 1995)	Basin area: ~1900 km^2, 560 mm average Precipitation, 9°C average temp.		
		Climate: PIK database	Land use: 47% cropland, 42% forest Soils: mainly sand to (loamy) soils, *Cambic Arenosols* and *Gleyic podzol*s (FAO), mainly flat area		

ZALF: Leibniz-Centre for Agricultural Landscape and Land Use Research, Müncheberg, Germany; UFZ: Centre for Environmental Research, Leipzig/Halle, Germany.

the remaining part being 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. khum and khum_r in turn determine the mineralization rate and hence the turnover speed of active organic matter. The mineralization rate for humus layers (khum) and for the mineral layers (khumr) is of similar high importance. Higher mineralization rates (and hence higher khum and khum_r values) quicker decrease active organic carbon in soils and increase soil respiration rates.

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 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 (khum, khum_r and kopm) governing the SOM turnover. Consequently, for this case, the turnover of SOM is reduced. The positive sign of the PCC values (Table 3) for Q10 and topt for C_{tot} shows, that an increase of these two parameters leads to a relative increase of soil carbon and a decrease of soil respiration (C_{resp}, negative PCC values, Table 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 an accurate assessment is central in this approach. Bulk density (dens) is a key factor in determining the soil wilting point and field capacity and is used in the calculation of soil temperature. In the model, higher bulk densities in soils increase soils wilting point and reduce soils field capacity

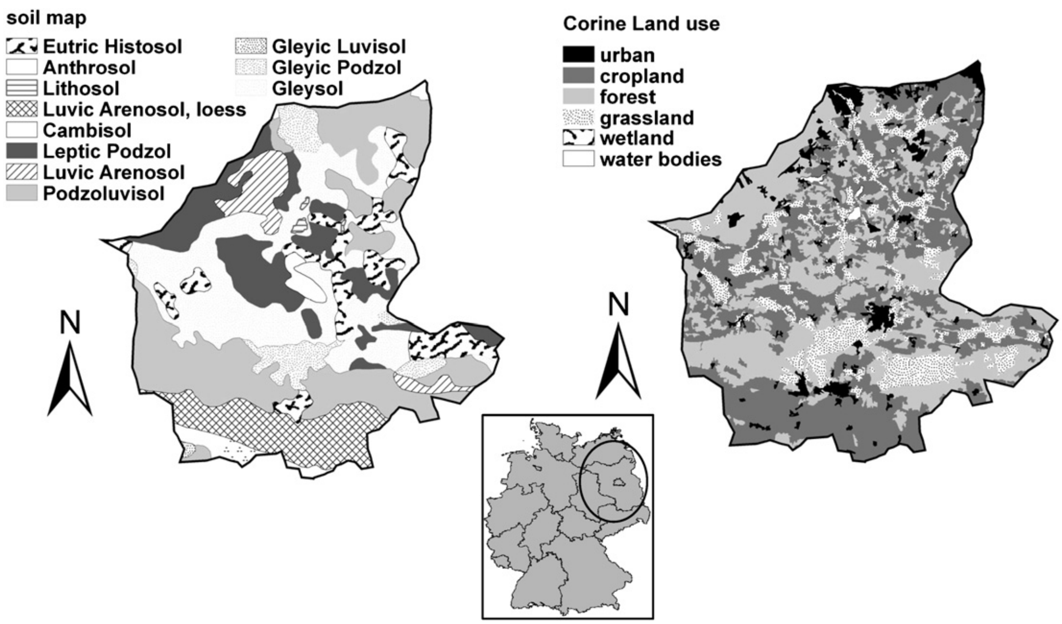

Fig. 1. Location of the Nuthe river basin and distribution of major soil types and land use classes based on BUEK1000 (soils, Hartwich et al., 1995) and CORINE data (land use, Dollinger and Strobl, 1996).

leading to higher soil water contents and a reduction of SOM turnover. Higher bulk densities increase the damping factor of soil temperature calculation (Krysanova et al., 2000). This effect tends to smooth and reduce soil temperature dynamics and may reduce turnover of SOM.

About eight factors (Q10, khum/k_humr, topt, ksyn_ag/ksyn_bg, init_soc, dens, Table 3) show 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. Under equilibrium conditions, the parameters driving biomass growth would dominate SOM turnover to a greater extend

Table 3
Sensitivity of input factors based on Partial Correlation Coefficient (PCC) calculated for soil carbon content (C_{tot}, 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 (Nuthe river basin, see Table 2) and for heterotrophic soil respiration (C_{resp}) 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

Rank	C_{tot} Bad Lauchstädt		C_{tot} Müncheberg		C_{tot} Nuthe river		C_{resp} Bad Lauchstädt		C_{resp} Müncheberg		C_{resp} Nuthe river	
	Factor	PCC ($R^2 = 0.99$)	Factor	PCC ($R^2 = 0.82$)	Factor	PCC ($R^2 = 0.96$)	Factor	PCC ($R^2 = 0.98$)	Factor	PCC ($R^2 = 0.62$)	Factor	PCC ($R^2 = 0.96$)
1	*khum*	−0.989	*init_soc*	0.762	*Q10*	0.938	*khumr*	0.982	*ksyn_ag*	−0.592	*Q10*	−0.953
2	*Q10*	0.986	*Q10*	0.653	*init_soc*	0.926	*Q10*	−0.960	*Q10*	−0.462	*khumr*	0.929
3	*ksyn_bg*	0.971	*khum*	−0.620	*khum*	−0.914	*dens*	0.945	*khum*	0.394	*topt*	−0.812
4	*temp*	−0.963	*ksyn_bg*	0.585	*topt*	0.776	*topt*	−0.884	*topt*	−0.337	*khum*	0.453
5	*topt*	0.962	*dens*	−0.538	*temp*	−0.340	*init_soc*	0.869	*harv_surp*	0.291	*init_soc*	0.306
6	*init_soc*	0.935	*topt*	0.406	*ksyn_ag*	0.299	*khum*	0.742	*dens*	0.283	*dens*	0.284
7	*dens*	−0.912	*ksyn_ag*	0.400	*ksyn_bg*	0.298	*temp*	0.697	*khumr*	0.250	*ksyn_bg*	−0.236
8	*ksyn_ag*	0.885	*glob*	0.334	*frc_bg*	−0.253	*harv_surp*	0.640	*temp*	0.222		
9	*fertorg*	0.880	*temp*	−0.282			*precip*	0.604	*glob*	0.204		
10	*harv_surp*	0.866	*harv_surp*	0.221			*kopm_bg*	−0.601				
11	*glob*	0.835	*fertorg*	0.200			*glob*	−0.502				
12	*precip*	0.505					*clay*	0.447				
13	*frc_bg*	−0.353					*fertorg*	0.383				
14							*ksyn_bg*	−0.293				
15							*frc_bg*	0.269				
							frc_ag=frc_bg					

Abbreviations of input factors are explained in Table 1. Ranking was performed based on the absolute PCC values. Only factors value greater than 0.2 are shown (for explanation see text). R^2, coefficient of determination; ag, above-ground; bg, below-ground.

(Zähle et al., 2005). The same holds for parameters determining soil temperature effect on SOM turnover constants (Q10 and topt).

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. Additionally it was distinguished between the inherent uncertainty at the plot scale and at the spatial (river basin) scale. Furthermore a quantification of land use and soil related uncertainty distribution is assessed.

3.2.1. 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 (Figs. 2 and 3b) with a range of 0.55% C_{org} ($\pm$0.275% C_{org}, $\pm$0.13 t C ha^{-1} yr^{-1} Bad Lauchstädt) and 0.11% C_{org} ($\pm$0.055% C_{org}, 0.05 t C ha^{-1} yr^{-1} Müncheberg, Table 4) at the end of the simulation period. Overall uncertainty introduced when considering variations of all input factors is for the Bad Lauchstädt site 0.63% C_{org} ($\pm$0.315% Corg, $\pm$0.15 t C ha^{-1} yr^{-1}) and 0.13% C_{org} ($\pm$0.065% Corg, $\pm$0.06 t C ha^{-1} yr^{-1}) for the Müncheberg site (Table 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 (Fig. 3c–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). 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).

Besides 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 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 (Fig. 3a), whereas the simulation was conducted with 1.2 t ha^{-1} yr^{-1} organic fertilisation to ensure

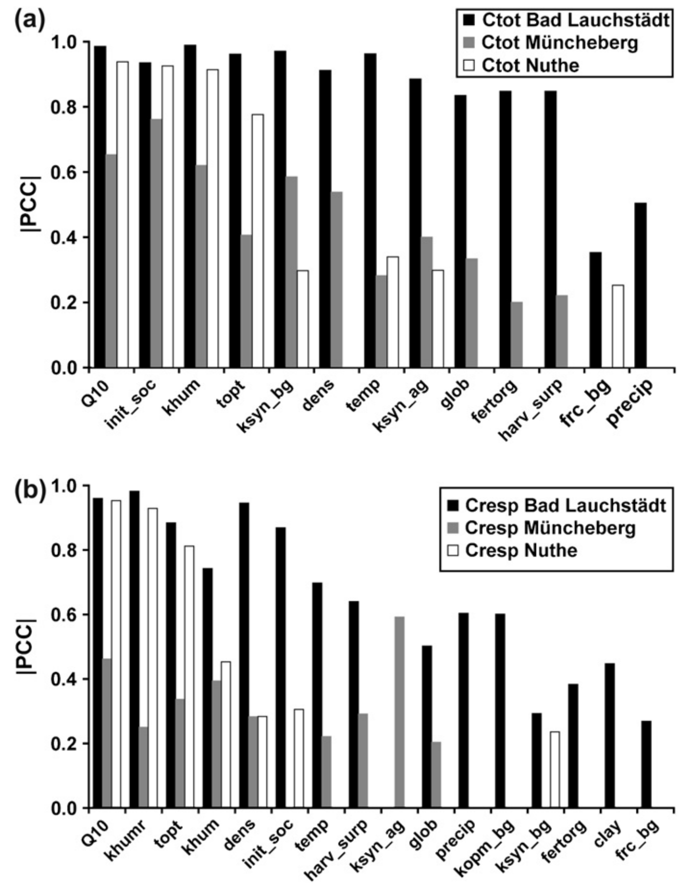

Fig. 2. Input factors with |PCC| values above the threshold of 0.2 for C_{tot} (a) and C_{resp} (b) and all cases (Bad Lauchstädt, Müncheberg and Nuthe river basin).

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.

Furthermore the absolute range of uncertainty is lower for the Müncheberg case possessing low soil organic carbon content which is independent from the different simulation times. This suggests that poor soils (with generally low soil organic matter contents) are less sensitive to variations in model parameter than soils with high fertility (generally featuring 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).

3.2.2. Spatial scale assessment

For comparison of the variability between the different sources of uncertainty the coefficient of variation (COV%, see equation 1) was used. 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.

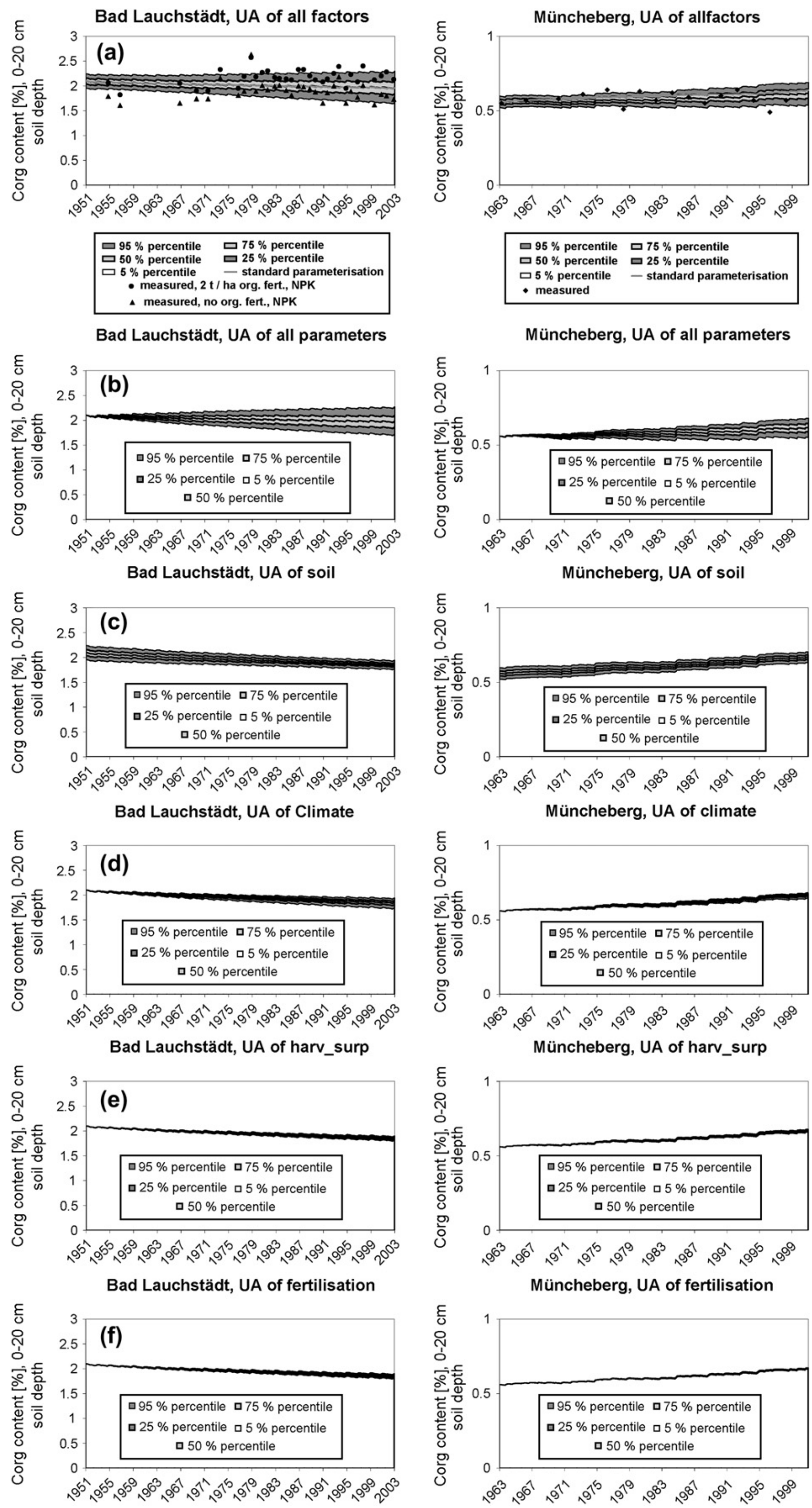

Fig. 3. Temporal development of uncertainty for experimental sites Bad Lauchstädt (right) and Müncheberg (left) for 51 and 37 years simulation period respectively considering (a) all factors, (b) parameters, (c) soil, (d) climate, (e) crop harvest management (harv_surp) and (f) fertilisation. Results 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 2) and measurements representing 2 t C ha^{-1} yr^{-1} (black circles) and no organic fertilisation (black rhombic sign) are shown.

Table 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}]

Input factors	Bad Lauchstädt [% C_{org}]		Müncheberg [% C_{org}]		Bad Lauchstädt	Müncheberg	Difference (95–5 percentile value) Bad Lauchstädt		Difference (95–5 percentile value) Müncheberg	
	Mean start	Mean end	Mean start	Mean end	90% confidence range of uncertainty [% C_{org}]		[% C_{org}]	t C ha^{-2}/ t C ha^{-2} yr^{-1}	[% C_{org}]	t C ha^{-2}/ t C ha^{-2} yr^{-1}
(a) All factors	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
(b) Parameters	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
(c) Soil	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
(d) Climate	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
(e) harv_surp	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
(f) Fertilisation	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

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 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 5). The same can also be stated for climate input variations, but there it is less pronounced. In terms of mean COV values (Fig. 5), soil input derived uncertainty (mainly through init_soc, see Section 3.1) is even higher than the parameter contribution.

The pattern of the spatial uncertainty distribution regarding the investigated sources is similar with clearly distinguishable areas of high and lower uncertainty (Fig. 4a–f). 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 developed on loess deposits and croplands with Cambisols are dominating (see Fig. 1).

Table 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 eq. 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

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 (Fig. 5a). 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, Fig. 5b). 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., 2005). Soil physical properties of loess soils (driving the soil water dynamics) are difficult to characterise as loess soils possess an inherent high variability of soil physical properties like available field capacity or soil porosity (Post et al., 2007a,b). 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 Gleysol 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 3.1) and climate variations change the temperature sensitivity of SOM turnover and deliver 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 (Fig. 5a 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 3.1) and parameters (mainly khum and ksyn, see Section 3.1) are increased or decreased. As noted for the

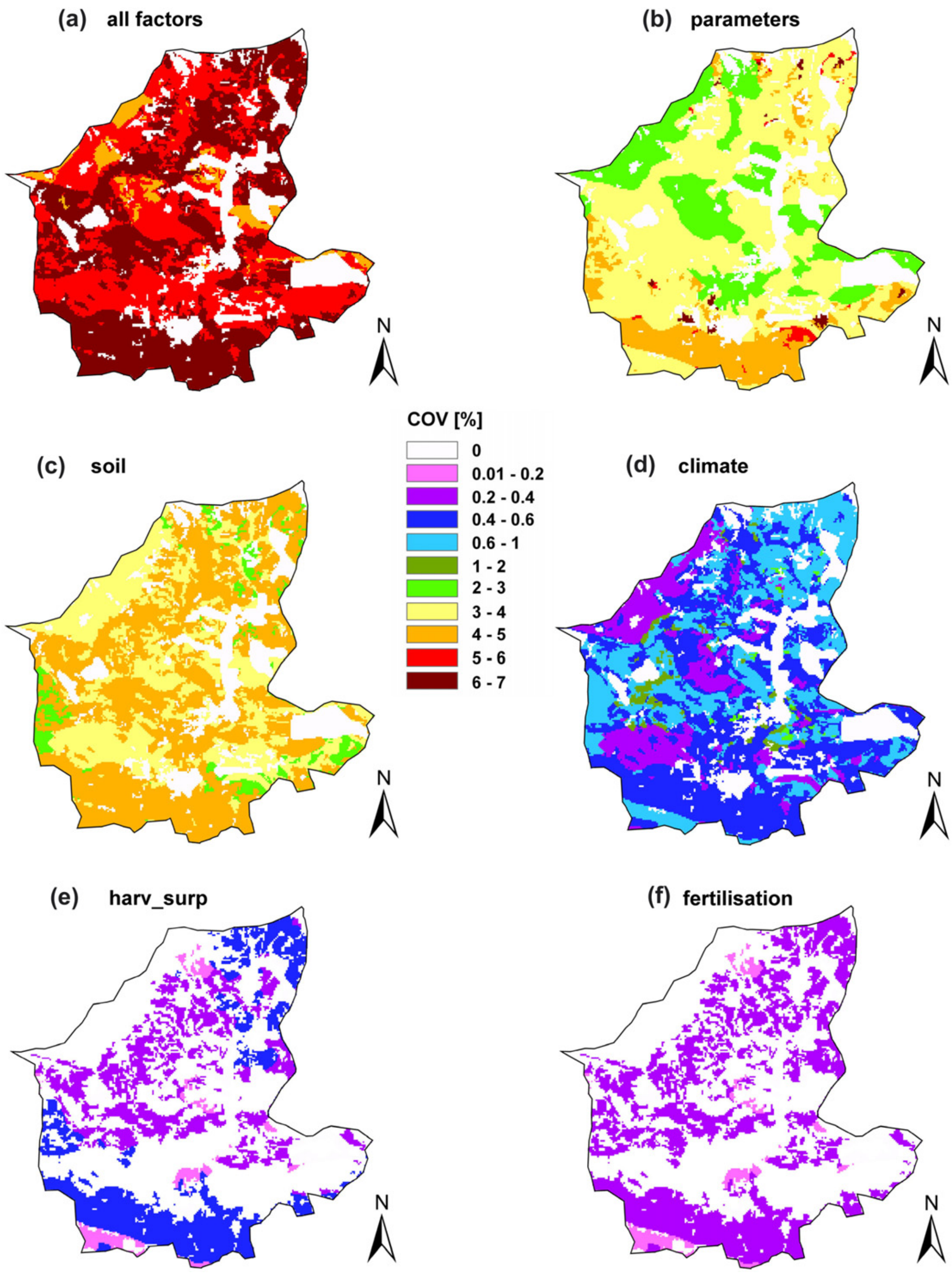

Fig. 4. Spatial distribution of uncertainty for the Nuthe river basin expressed as coefficients of variation values (COV in %, see eq. 1) for (a) all factors, (b) parameters, (c) soil, (d) climate, (e) crop harvest management (harv_surp) and (f) fertilisation.

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.

3.3. Implications for long-term soil organic carbon dynamics

The quantified uncertainty provides useful information to interpret simulation experiments and to assess for example 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). Besides other studies, crop rotation impacts on long-term SOC contents

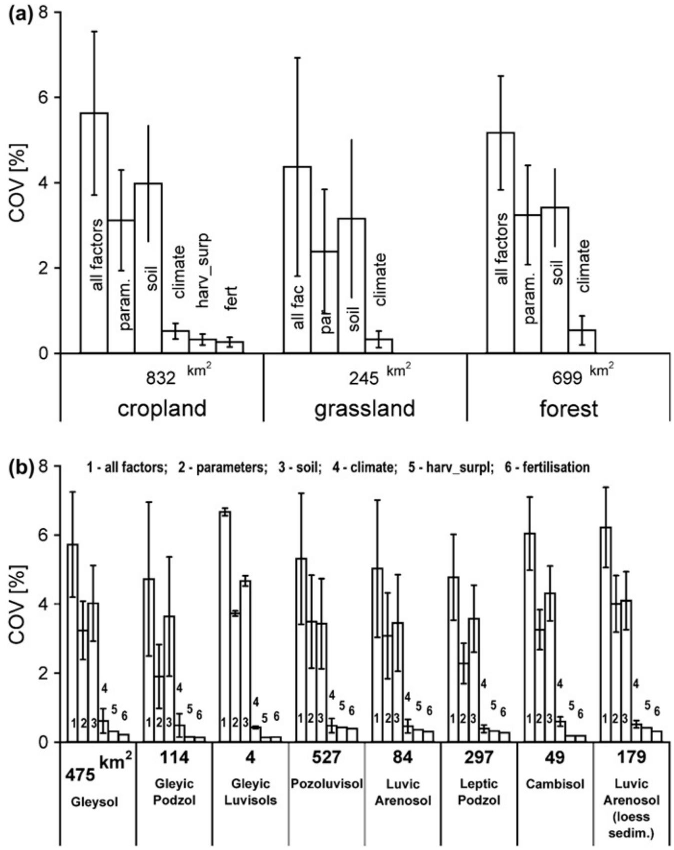

Fig. 5. Contributions of broad land use types (a) and major soil types (b) in the Nuthe river basin expressed by zonal mean values and standard variations (black lines) of coefficient of variation (COV in %, see eq. 1) considering (1) all factors, (2) parameters, (3) soil, (4) climate, (5) crop harvest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

are estimated around -0.078 to $+0.36$ t C ha^{-1} yr^{-1} in Norway (Singh and Lal, 2005) and -0.13 to $+0.1$ t C ha^{-1} yr^{-1} for the study area (Post et al., 2007b) using the described modelling tool. As noted by Freibauer et al. (2004) and Smith (2004) the related uncertainty of crop rotation impact is very high but was not quantified. Relating here the 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 (Fig. 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 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. The example shows that the presented study allows specifying the 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 and different

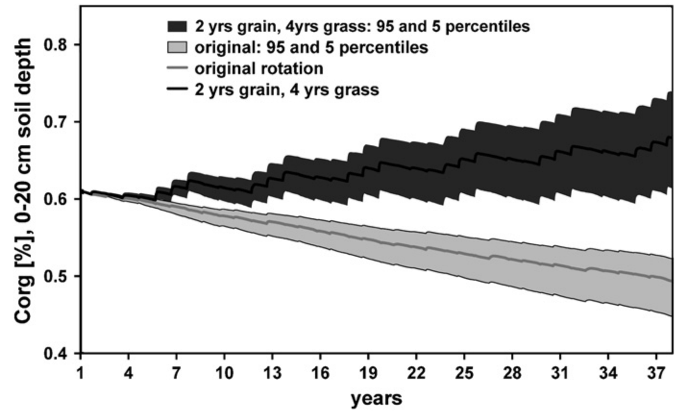

Fig. 6. Parameter based uncertainty related to crop rotational impacts on long-term soil organic carbon dynamics (Post et al., 2007a,b) for the Müncheberg site considering the original rotation (see Table 2) and a lay arable use (2 years grain crops and 4 years grass) under unfertilised conditions.

scales lead to different characteristics of uncertainty magnitudes and that a temporally and spatially quantification of model parameters and input data derived uncertainty is necessary.

Soils with high SOC content (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 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 5, Fig. 4a).

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 2.3.1). 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.

4. Conclusion

The assessment reveals that model parameters describing the mineralisation rate 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. This is an important finding transferable to other SOM models of this kind.

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., 2005; Hyvonen et al., 2005; Reichstein et al., 2005b) and needs further research efforts. 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., 2005; 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., 2005; Knorr et al., 2005; Reichstein et al., 2005b).

The rate of soil organic matter mineralisation has 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 the carbon use efficiency parameter (synthesis parameter). 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. This underlines the relevance of soil mapping and long-term soil surveys 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 most important input factors can also be transferred to other model of this kind, as these parameters are central also for other process-based SOM models (Bergmann et al., 1999; Lettau and Kuzyakov, 1999).

Besides 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.

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 soil physical properties parameterisation for 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 PDFs 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. 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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