Modelling soil organic matter dynamics on a bare fallow Chernozem soil in Central Germany

Uwe Franko\textsuperscript{a,⁎}, Ines Merbach\textsuperscript{b}

\textsuperscript{a} UFZ – Helmholtz Centre for Environmental Research, Department of Soil Physics, Halle, Germany
\textsuperscript{b} UFZ – Helmholtz Centre for Environmental Research, Department of Community Ecology, Halle, Germany

\textbf{A B S T R A C T}

Soil organic matter (SOM) can be characterised by soil organic carbon (SOC) and/or total nitrogen (TN). The observed dynamics of SOC and TN in the topsoil of a 28-year-old fallow experiment on Haplic Chernozem was modelled using the Candy Carbon Balance (CCB) model. This study selected two treatments from this experiment where the soil was kept bare with mechanical or chemical (herbicides) treatments. The CCB model was improved to include the SOC related change of soil physical parameters and dynamic handling of the physically stabilised SOM pool. Over 28 years of bare fallow the top soil lost about 10 t/ha of SOC and > 1 t/ha of TN. The results from observation and modelling reflected the increased SOM turnover due to soil tillage. The modelled size of the physically stabilised SOC pool was about 55% of total SOC and only reduced slowly during the almost three decades, but the implementation of this effect improved simulation results and reduced the relative RMSD (unitless) from 0.051 to 0.044 for SOC and from 0.053 to 0.049 for TN error level. From these results we conclude that the larger the SOM change the more important is the integration of the turnover of physically stabilised SOM within the modelling approach.

1. Introduction

Soil and soil functions are gaining increasing attention because healthy soil is a fundamental requirement for sustainable development. As the largest terrestrial biotic carbon pool (Stockmann et al., 2013), SOM is a particular focus of the global change debate. SOM is a driver for important soil functions like carbon storage and nutrient release. However, SOM is affected by global change due to the interactions with climate conditions and changes of land management. Therefore, modelling is widely used to predict possible impacts of land use changes on SOM storage in search for carbon sequestration strategies or adaptation measures, especially regarding agroecosystems.

Most SOM models distribute the organic matter (OM) of the soil between several conceptual pools with specific turnover times to reflect the observed SOM dynamics on long-term experiments where, in most cases only SOC is used to indicate the quantitative changes while the N component of SOM is not considered. If the turnover time of a pool is very high or tending to infinity, it may be considered as inert or more generally, as being stabilised long-term. In common agricultural systems this long-term stabilised SOC represents the basic level above which the SOC observations fluctuate, representing the dynamics of the more labile pools. On a bare fallow treatment these more labile SOM pools are continuously depleted, and the observable SOC dynamics are increasingly dominated by the properties of the stabilised SOM pools. Hence, SOC dynamics on bare fallow treatments are considered suitable to analyse the behaviour of the long-term stabilised SOM pool (Barré et al., 2010; Menichetti et al., 2015).

A special fallow experiment on a Chernozem soil was started in 1988 in Bad Lauchstädt, Germany including treatments to study the effects of keeping the soil bare by either tillage or herbicide application. The SOM data from this experiment were used to model the behaviour of stabilised SOM on these bare fallow treatments and to review the assumptions about the tillage effect on SOM turnover already implemented in the CCB model (Franko and Spiegel, 2016).

In general, the CCB model (Franko et al., 2011) considers three pools of SOM: active SOM (ASOM), stabilised SOM (SSOM), and long-term stabilised SOM (LTS). These SOM pools can be combined with different pools of fresh organic matter according to the land use. Site-specific turnover is simulated using the concept of Biologic Active Time (Franko and Oelschlägel, 1995), which is similar to the use of the site-specific rate modifier within ICBM (Introductory Carbon Balance Model) of Andrén and Kätterer (1997).

So far, the CCB model concept has considered the LTS pool as not taking part in the turnover processes. Following the concept of Kuka...
et al. (2007), the calculation of the LTS pool size is based on indicators of soil structure given by the hydrological soil characteristics such as pore volume, field capacity, and permanent wilting point ($\Theta_{pwp}$) as reported by Puhlmann et al. (2006). These hydrological soil characteristics are influenced by soil texture, SOC concentration, and bulk density (BD). We therefore hypothesise that BD and $\Theta_{pwp}$, which depend on soil texture and SOC, are the main drivers for changes in the LTS pool size. In many cases, these physical soil properties are handled as parameters that don’t change over the investigated time. This might be reasonable when looking at short time scales and moderate SOC changes that are typical for many agroecosystems. However, this assumption is not reasonable in case of an extraordinary SOC variation after land use changes from normal agriculture to bare fallow. Despite the known dependence of BD and $\Theta_{pwp}$ from SOC (e.g. Körschens et al., 1995), it remains an open question to what degree a change of soil physical properties influences the observable SOM dynamics in terms of SOC and TN. Therefore, we included both elements (C and N) in the assessment of the model results and implemented an additional sub model in CCB that adapts BD and $\Theta_{pwp}$ to the current SOC level and changes the LTS pool size according to the actual soil physical parameters.

The objective of this study was to assess the performance of the extended CCB model to predict the dynamics of SOC and TN in general, to analyse the dimension of the modelled LTS pool change and the tillage impact on SOM dynamics under bare fallow. Furthermore, we compared our results with results from Barré et al. (2010) where the SOC under bare fallow at several sites was described by an exponential function.

2. Material and methods

2.1. Experimental design

In this study data from a field experiment situated on a Haplic Chernozem soil in Bad Lauchstädt, Central Germany (51°24’N, 11°53’E) was used. The climate is semi-humid with a mean annual air temperature of 8.9 °C and 481 mm mean annual precipitation for the last three decades.

The experiment was started in 1988 to study different fallow treatments: mechanical bare fallow (MBF) keeping the soil bare by tillage, chemical bare fallow (CBF) keeping the soil bare by herbicide application, the combination of mechanical and herbicide treatment to keep soil bare, and a zero treatment leading to a succession of weed flora. Every treatment consists of four replicated plots on a previously topsoiled area of 42 m². For this study, only the MBF and CBF treatment were selected. The MBF was grubbed with a field cultivator several times throughout a year and ploughed every autumn to a depth of 28 cm. CBF was sprayed with herbicides (mainly triazines and glyphosate) several times a year with a knapsack sprayer to prevent any greening.

The soil texture of the experimental area was analysed in 1988 by using the Köhn pipette method in accordance with DIN ISO 11277: 2002–08 (2002) to determine the soil particles < 6.3 μm, resulting in an average value of 24.3 ± 1.1 M%. The clay content of the top soil (21 M%) was resumed from a more general soil description of the Haplic Chernozem at the Bad Lauchstädt site (Altermann et al., 2005).

Soil samples were taken separately from all four replications every autumn with an auger from a depth of 0–30 cm. A mixed sample from 20 randomly chosen points per replication was analysed for SOC and TN by dry combustion using a C/H/N analyser (Vario El III, Elementar, Hanau, Germany).

2.2. Dynamics of the physically stabilised SOM

According to the CIPS (Carbon In Pore Space) model (Kuka et al., 2007) a highly stabilised SOC pool is closely associated with the inner surface of micro pores ($r < 0.05 \mu m$) in soil. Until now, CCB and its ancestor CANDY (Carbon And Nitrogen Dynamics, Franko and Oelschlägel, 1995) have addressed this pool as being stable over long-term, assuming it as constant since change in size with time was expected to be insignificant. It is likely that this postulate is not reasonable for the time after conversion from a cropped soil with sufficient supply of organic matter into a bare fallow treatment. Thus, we considered a dynamic approach for the LTS pool in our modelling study.

Assuming that the LTS dynamics is controlled by soil physical properties, the pool size can be calculated by:

$$\text{SOC} = \alpha(A_p + A_m + A_b)$$  \hspace{1cm} (1)

where $\alpha$ is an areal specific carbon concentration, $A$ is the inner area of micro ($\mu$), meso ($m$), and macro ($M$) pores in soil. The size of the LTS pool is given by:

$$C_{LTS} = \alpha \Lambda_p$$  \hspace{1cm} (2)

Using our approach, a change of the LTS pool size will be triggered by a volume change of micro pores $V_p$. Like described in the CIPS model (Kuka et al., 2007), we associate $V_p$ with soil moisture at wilting point ($\Theta_{pwp}$). Assuming cylindrical pores, the volume of the micro pores is related via the (virtual) radius $r_p$ and the total length $l_p$ to the inner area $A_p$ of all micro pores:

$$V_p = \Theta_{pwp} \pi r_p^2 l_p$$  \hspace{1cm} (3)

$$A_p = 2\pi r_p l_p = 2\Theta_{pwp}$$  \hspace{1cm} (4)

Additionally, it is assumed, that the long-term (physically) stabilised carbon is evenly distributed over the inner surface of the micro pores:

$$C_{LTS} = \alpha A_p = 2 \alpha r_p l_p$$  \hspace{1cm} (5)

$$\Delta C_{LTS} = \beta \Lambda \Theta_{pwp}$$  \hspace{1cm} (6)

where $\beta$ is a variable factor relating the LTS carbon to the volume of micro pores. Following Eq. (6), the changes of $C_{LTS}$ are related to the changes of $\Theta_{pwp}$:

$$\Delta C_{LTS} = \beta \Lambda \Theta_{pwp}$$  \hspace{1cm} (7)

The value of $\beta$ in Eq. (7) is calculated during the model initialisation by:

$$\beta = \frac{\text{SOC}\cdot F_{LTS}}{\Lambda \Theta_{pwp}}$$  \hspace{1cm} (8)

The implementation of this sub-routine includes the modelling of the soil physical parameters with respect to SOC changes. Therefore, we first calculated BD dynamics using the model of Rühlmann and Körschens (2009) and used the pedotransfer function of Vereecken et al. (1989) to find the parameters for the widely used water retention model of Van Genuchten (1980). This way it was possible to adapt the extension of micro pores according to the actual BD and SOC values.

2.3. Implementation of carbon and nitrogen fluxes

In the CIPS model, the carbon flux into the micro pore space is restricted to dissolved organic carbon (DOC). Any DOC production or consumption is closely related to microbial activity. The ASOM pool of the CCB model behaves very similarly to soil microbial biomass. Therefore, we assume that the flux between time step $t_i$ and $t_{i+1}$ to/ from the LTS pool only affects the ASOM pool and hypothesise that:
\[ \Delta C_{\text{LTS}} = -\Delta C_{\text{ASOM}} = C_{\text{LTS}}(t_{i+1}) - C_{\text{LTS}}(t_i) \]  

Both LTS and ASOM pools have a different C/N ratio (\( \gamma \)), meaning that a flux (\( N_{\text{flx}} \)) between the mineral nitrogen and an organic N pool also has to be considered:

\[ N_{\text{flx}} = \Delta C_{\text{ASOM}} \gamma_{\text{ASOM}} - \Delta C_{\text{LTS}} \gamma_{\text{LTS}} \]

A growing LTS pool (N-poor) will withdraw C from the N-rich ASOM pool and set mineral nitrogen free (which means prevention of the mineral nitrogen from being immobilised during the decomposition of fresh organic matter). A decreasing LTS pool leads to nitrogen immobilisation due to the ASOM growth and has to be considered as N-sink.

### 2.4. Calibration and model assessment

According to the experimental design, the MBF treatment was modelled with the standard assumption of a tilled soil, while for the CBF treatment, we applied the model adaptation for non-tilled soil as described by Franko and Spiegel (2016) where the non-tillage impact is modelled as reduction of turnover activity in dependence of site conditions. Furthermore, we assumed an initially homogeneous top soil in the experimental area concerning SOC concentration and soil texture. Altogether, three parameters had to be calibrated by model inversion using root mean square deviation (RMSD) as error function. In a first step, we calibrated the carbon dynamics determining the initial SOC concentration and the structure factor \( F_{\text{flts}} \) that were taken to be identical for both treatments. As second step the initial nitrogen concentration was determined in an analogue way by using TN data. CCB considers the carbon dynamics independent from nitrogen but connects the nitrogen turnover to the carbon via the C/N ratio.

In addition to the CCB model, we applied an empirical approach to have an extra benchmark for the assessment of the CCB results. In the same way as Barré et al. (2010), we applied a combination of an exponential decrease from an initial SOC level \( C_{\text{ini}} \) to a final constant \( C_{\infty} \) that was identified as the stable pool by Barré et al. (2010):

\[ \text{SOC}(t) = (C_{\text{ini}} - C_{\text{tri}}) e^{\exp(-k_i t)} + C_{\text{tri}} \]  

where \( t \) is the time in years, \( k_i \) is the turnover coefficient. The model was fitted to the observations using the Levenberg-Marquardt algorithm (Moré, 1978) from the nls.lm function in the minpack.lm R package (Elzhov et al., 2015). According to the experimental design, we added the constraint for both treatments to start with an identical \( C_{\text{ini}} \) value, while the parameters \( k_i \) and \( C_{\infty} \) where determined individually for each treatment in order to reflect the soil tillage effect.

For the model assessment of each treatment, we also calculated the relative RMSD (RMSDrel) using the observed values (\( O \)), their arithmetic mean (\( \bar{O} \)) and the model predictions (\( P \)):

\[ \text{RMSD} = \sqrt{\frac{\sum_{i=1}^{n} (O_i - P_i)^2}{n}} \]

\[ \text{RMSD}_{\text{rel}} = \frac{1}{\bar{O}} \sqrt{\frac{\sum_{i=1}^{n} (O_i - P_i)^2}{n}} \]

For a comparative evaluation of the CCB results with the exponential approach (Eq. 11), we calculated the corrected Akaike’s Information Criterion (AICc) according to Burnham and Anderson (2002). For the SOC prediction the CCB modelling was based on the adaptation of two parameters (SOC for \( t = 0 \) and \( F_{\text{flts}} \)) that where assumed identical for both treatments. With the exponential approach we calibrated five parameters: the initial SOC value identical for both treatments and the parameters \( k_i \) and \( C_{\infty} \) separately for each treatment. The model assessment was related to the experiment as union of both treatments

\[ \text{AICc} = 2k + n \ln \left( \frac{\sum_{i=1}^{n} (O_i - P_i)^2}{n} \right) + \frac{2k(k + 1)}{n - k - 1} \]

where \( k \) is the number of calibrated parameters and \( n \) the number of observations.

All error analyses including ANOVA and graphics were done with R software (R core team, 2014) using the packages ggplot2 (Wickham, 2009) and RODBC (Ripley and Lapsley, 2014).

### 3. Results

#### 3.1. Performance of the CCB model

The results showed that the extended CCB model was able to reproduce the observed dynamics for both elements SOC and TN (Fig. 1). In average of both treatments, the relative error RMSDrel was 0.044 and 0.049 for SOC and TN, respectively. Without consideration of LTS dynamics (not shown), the relative error was 0.051 and 0.053 for SOC and TN, respectively. Furthermore, the now improved model reproduced the observations with an error near to the relative observation error (coefficient of variation) was for SOC 0.026 (MBF) and 0.028 (CBF) and for TN 0.044 (MBF) and 0.041 (CBF).
3.2. Comparing CCB with an exponential function

To compare the modelling procedure with CCB, the initial SOC concentration for both treatments was forced to the same value and resulted in $2.004 \pm 0.052$ M%. The $k_\text{t}$-value representing the turnover time and the prediction of the final SOC concentration reflected the expectations for each treatment (MBF: $C_\infty = 1.605 \pm 0.040$ M%, $k_\text{t} = -0.1286 \pm 0.0463 \text{ yr}^{-1}$; CBF: $C_\infty = 1.639 \pm 0.049$ M%, $k_\text{t} = -0.1112 \pm 0.0481 \text{ yr}^{-1}$).

Both models (CCB vs. exponential function) generally represent a good fit to the SOC data. The adaptation to the observations is a little better for the exponential approach (RMSD = 0.074 M%) compared with the CCB model (RMSD = 0.078 M%). However, this reduced error is based on the calibration of five parameters, while the CCB approach required the calibration of only two parameters. Therefore, we found in our case the CCB model (AICc = −272.2) to be preferable to the application of an exponential function (AICc = −271.6). While the performance differs only marginally, the process based explanation brings an obvious benefit.

3.3. Development of LTS pool size

From the initial LTS pool (44,319 kg/ha), CCB calculated a carbon loss of 1554 and 1232 kg/ha for the MBF and CBF treatment, respectively. This loss is lower than 2% of the initial SOC stock of 80,157 kg/ha, which is a small effect considering the extreme change of land use from an arable soil to bare fallow. The model results suggest that the physical protection is so efficient through the first years of this experiment that the overwhelming part of decomposed SOM comes from the easily accessible pools.

4. Model performance

We discuss the model performance first in comparison to the observations using absolute error measures and second in comparison to other modelling studies for bare fallow soils using relative errors because of the different SOC levels.

The results of the improved CCB model on the bare fallow land use as shown in Figs. 1 and 2 were satisfactory. The average RMSE value for both treatments was 0.078 M% SOC and 0.0075 M% TN. The SOC error is lower than in a former CCB application from Franko et al. (2011) for the Bad Lauchstädt site with cropped soil (RMSD = 0.115 M% SOC) and in the same order of magnitude as the mean standard deviation of the observed data (0.056 M% SOC and 0.0085 M% TN).

In our study, we presented for the first time modelling results from CCB for TN, therefore, the model performance can only be assessed in comparison with the observations. The results are promising because in both treatments the model error (Fig. 2) is lower than the mean standard deviation of the measurement.

The quality of the CCB predictions for SOC dynamics was comparable to other studies. The CCB performance after calibration of initial SOC and the structure parameter $F_{\text{ini}}$ (RMSD$_{\text{rel}}$ = 0.044) for SOC is similar to the bare fallow modelling with Yasso07 where RMSD$_{\text{rel}}$ = 0.045 after calibration of initial C stock (Karhu et al., 2012). Better results were reported by Saffih-Hdadi and Mary (2008), using the AMG model (RMSD$_{\text{rel}}$ = 0.0036) but only after fitting of four parameters.

The empirical approach of an exponential SOC decrease down to an inert level (Eq. 11) was easy to fit to the observed SOC data and resulted in a lower RMSD than CCB. Nevertheless, the application of the mechanistic model is preferable not only because of the better AICc value but also because of its potential to explain the system behaviour.

4.4. Representation of stabilised SOM

Following the exponential approach, the stable pool at the study site was 1.6 M% SOC (MBF) and 1.64 M% SOC (CBF) which is more than double in size compared with the results from Barré et al. (2010) for a set of bare fallow experiments throughout Europe ranging from 0.25 to 0.68 M$\%$ SOC. Related to the initial SOC stocks the calculated stable pool ranged from 0.084 to 0.54 according to Barré et al. (2010) and from 0.1 to 0.49 following a different study from Petersen et al. (2005). The share of the stable pool in the initial SOC at our study site accounted for 0.80 (MBF) to 0.81 (CBF). Obviously, in both cases (absolute and relative) our results don’t fit in the range from both other studies. That might be a consequence of the duration of the experiment for only 28 years or related to the special character of the Haplic Chernozem soil at the Bad Lauchstädt site.
The share of LTS pool in the initial SOC at the beginning of the experiment calculated of the CCB model with respect to soil structure amounted only to 0.55 which is lower than identified with the exponential approach and close to value of 0.54 for the Grignon bare fallow experiment (Barré et al., 2010) but still above the range given by Petersen et al. (2005).

4.4. Tillage effect

The experimental results confirm the tillage impact for both SOC and TN. The impact of a different rooting system is excluded on bare fallow. Thus, this result provides clear evidence of a more intensive decomposition of SOM due to a more intensive tillage of the soil on the MBF treatment, which is also reflected by the CCB model.

The applied pedotransfer functions provide a reasonable sensitivity of BD and \( \theta_{\text{pwp}} \) to SOC changes. BD is reduced with increasing SOC concentration with 0.108 g cm\(^{-3} \) per 1 M\% SOC, which is the same value published by Körschens et al. (1995). \( \theta_{\text{pwp}} \) is increased with 1.56 VOL\% per 1 M\% SOC. This is equivalent to a \( \theta_{\text{pwp}} \) change of 1.96 M\% per 1 M\% SOC and a change of hygroscopicity of 1.1 M\% per 1% SOC assuming the conversion factor of 1.785 given in Verstraeten et al. (1971). This is higher than the maximum sensitivity of − 0.08 g cm\(^{-3} \) per 1 M\% SOC reported by Körschens and Waldschmidt (1995) but still of a similar order. In the general site description Altermann et al. (2005) identified values of BD = 1.4 g/cm\(^3 \) and \( \theta_{\text{pwp}} = 15.5 \) VOL\% with 2.05 M\% SOC. This is comparable to the model predictions in this case (BD = 1.359 g/cm\(^3 \); \( \theta_{\text{pwp}} = 16.46 \) vol\%).

5. Conclusions

The fitting results underline that the model was successfully applied to bare fallow treatments on Haplic Chernozem to represent the dynamics of SOC and TN in topsoil, including the effect of different soil management (MBF vs. CBF). The results confirm that the model concept to represent tillage effects (Franko and Spiegel, 2016) that was validated at the Fuchsenbigl tillage experiment in Austria is also applicable to different site conditions. The handling of physical soil properties as dynamic variables depending on SOC was the precondition to overcome the static character of the LTS pool in CCB. The results showed that in the case of a degrading Haplic Chernozem soil, the changes of the LTS pool itself are moderate. Despite this, considering the dynamics of physically stabilised SOM resulted in an improvement of modelling results for the bare fallow treatments of this study, but may be less important for scenarios with moderate SOC changes. The detected size of the stabilised pool in the experimental and modelling results was outside the limits of other studies. It will require more research to decide whether the comparably large LTS pool is a distinctive property of this Haplic Chernozem soil.
References


R Core Team, 2014. RODBC: ODBC Database Access. (R package version 1.3-10). http://CRAN.R-project.org/package=RODBC.


