

## Comparison of methods for the estimation of inert carbon suitable for initialisation of the CANDY model

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### Abstract

Almost all soil organic carbon turnover models rely on a partitioning of total organic carbon into an inert and a decomposable pool. The quantification of these pools has a large impact on modelling results. In this study several methods to estimate inert carbon in soils, based either on total soil organic matter or physical protection, were assessed with the objectives of (1) minimising errors in carbon and nitrogen dynamics and (2) ensuring usability for sites with marked differences in site conditions. CANDY simulations were carried out by varying solely the method for calculating the size of the inert carbon pool used to initialise the model. Experimental data from Bad Lauchstädt and Müncheberg were used for the simulation. The data were made available for modellers at a workshop held at Müncheberg (Germany) in 2004. The results concerning not only carbon but also nitrogen dynamics were analysed by applying selected statistical methods. It was shown that even in short-term simulations model initialisation procedure may influence the simulation results considerably. Three methods of estimating inert carbon were identified as being the most appropriate. These methods are either based on soil texture or pore-space classes and therefore account for the physical protection of soil organic matter. Thus, physical protection seems to be of major importance. By extending the scope of the investigation into nitrogen dynamics, additional support for the applicability of a selected method was obtained.

### Introduction

The simulation model CANDY (Carbon and Nitrogen Dynamics, Franko et al. 1995, 1997; Franko 1996, 1997) has been developed in order to provide information about carbon stocks in soils, organic matter turnover, N uptake by crops, leaching and water quality. A comparison of soil organic carbon models in 1997 showed CANDY

to be in the group with the best performance (Smith et al. 1997).

In most long-term organic matter models (Hansen et al. 1991; Franko et al. 1995; Coleman and Jenkinson 1996; Parton 1996, etc.), soil organic matter is partitioned in several pools with different turnover rates. In CANDY the decomposable soil organic matter can be subdivided into biologically active and stabilised soil organic

matter. The decomposable and the inert organic matter contribute to the total stock of carbon in the soil. The inert organic matter is considered to be stable and, therefore, does not participate in turnover processes.

As in other models (Falloon et al. 2000; Bruun and Jensen 2002) the manner in which CANDY is initialised influences the simulation results considerably. Model initialisation may be responsible for the behaviour of a soil as a source or sink of atmospheric CO<sub>2</sub> (Falloon and Smith 2000). In order to initialise the CANDY model, a value for decomposable carbon (C<sub>DEC</sub>) has to be specified by the user. Because it is not possible to measure the decomposable pool directly, in CANDY C<sub>DEC</sub> can be calculated from the history of the plot and the site-specific turnover conditions, or from the difference between an organic carbon (C<sub>ORG</sub>) measurement and the estimated inert carbon (C<sub>I</sub>). Thus, the amount of C<sub>DEC</sub> is affected by uncertainties in estimating C<sub>I</sub>. For example, if decomposable carbon is too high, the mineralisation of carbon and nitrogen may be overestimated, leading to a misinterpretation of organic matter dynamics and a surplus of mineral nitrogen in soil.

In the literature, several methods for calculating the amount of C<sub>I</sub> are described. They use either the relation between C<sub>I</sub> and soil texture (Körschens 1980; Körschens et al. 1998; Rühlmann 1999) or estimate C<sub>I</sub> as a part of the whole amount of soil organic carbon (Falloon et al. 1998, 2000). A new approach by Kuka et al. (2006), based on pore-space classes, shows that soil organic matter (SOM) localised in micro-pores is stabilised over a long time. Thus, this part of organic carbon should be very similar to the inert pool of the CANDY model.

In the investigation reported here, we tested all of these methods on their applicability for initialising the inert carbon pool in the CANDY model. Our objective was to find a method which fulfils the following criteria: (1) minimises errors in carbon and nitrogen dynamics and (2) provides usability for sites with marked differences in site conditions. In order to achieve our objective CANDY simulations were carried out by varying solely the method of estimating the initial value for C<sub>I</sub>. Simulation results for soil organic carbon and soil mineral nitrogen of the sites 'Bad Lauchstädt' and 'Müncheberg' were compared with observations. From among the huge number of statistical

methods that can be found in literature (Willmott and Wicks 1980; Fox 1981; Addiscott and Whitmore 1987; Loague and Green 1991; Smith et al. 1996, etc.) we used the mean, the root mean square error (RMSE; Fox 1981), the mean bias error (MBE; Addiscott and Whitmore 1987) and the index of agreement (IA; Willmott and Wicks 1980) for comparing predicted and observed values and assessing the C<sub>I</sub> estimations.

## Materials and methods

### *CANDY model*

CANDY consists of a modular system of sub-models and a data base system for model parameters, initial values, weather data, soil management data and measurement values. The submodels of CANDY are described briefly below and in detail by Franko et al. (1995).

In the soil temperature model the heat flow equation is solved based on a statistical approach for the calculation of the soil surface temperature.

The hydrological model is based on a capacity approach, and takes into consideration the draining of water by gravitation forces, interception of water by crops, potential and actual evapotranspiration, surface runoff and snow cover dynamics.

The crop model in its standard version consists of parameters describing the temporal development of crop height, soil cover and rooting depth as piecewise linear functions. Nitrate uptake by plants is calculated by a sigmoidal function for the distribution of the N demand over vegetation time. After harvest, a yield-dependent amount of organic matter from roots and plant residues is recycled to the soil as fresh organic matter with crop-specific quality parameters.

The organic matter turnover model includes the soil nitrogen model. Soil organic matter is subdivided in several compartments: up to six different pools of added organic matter, two pools of decomposable soil organic matter (one active and one stabilised) and an inert soil organic matter pool, which is independent from climate and agriculture and stays constant over time. Turnover dynamics of all degradable carbon pools follow first-order kinetics but are influenced by soil temperature, soil moisture and aeration conditions indicated by soil texture and depth of the soil

layer. Nitrogen dynamics are connected to the carbon fluxes via the C/N-ratio of the pools concerned. Mineral nitrogen is divided into a nitrate and an ammonium pool. The nitrogen-related processes are: plant uptake, mineral nitrogen input including atmospheric deposition, input of organic manure or plant residues, nitrate leaching, nitrification, denitrification and mineralisation of soil organic matter leading to nitrogen mineralisation or immobilisation.

The model inputs can be classified as parameters and scenario data. The parameters are:

- plant development characteristics (standard) – crop height, vegetation time, maximum root depth, etc.;
- soil data – soil density, particle density, field capacity, permanent wilting point, saturated hydraulic conductivity, amount of clay and silt;
- organic matter characteristics – C/N-ratio, dry matter content, turnover time, SOM reproduction coefficient.

The scenario data include:

- initial conditions for carbon, nitrogen and soil moisture;
- agricultural management data – emergence, harvesting, fertilisation, tillage, yield, N-uptake;
- weather data – precipitation, air temperature and global radiation preferably on a daily basis.

#### *Datasets from Bad Lauchstädt and Müncheberg and simulation with CANDY*

The datasets from Bad Lauchstädt (crop rotation) and Müncheberg (plot 1) used for the model simulation are described in detail in Franko et al. (2006) and Mirschel et al. (2006). In addition to these data we used the organic carbon measurements presented in Table 1. For Müncheberg no value at the beginning of the simulation was available. Therefore, the first value in Table 1 was estimated with a trend line using the four measured values. The simulation for both sites has been fitted to meet the starting  $C_{ORG}$  values. For the mineral nitrogen measurements the reader is referred to Franko et al. (2006) and Mirschel et al. (2006).

The simulation period for the Bad Lauchstädt crop rotation (BL) lasted from 1 September 1996 to 31 December 2003 and at Müncheberg plot 1 (MÜ) from 1 September 1992 to 31 December

*Table 1.* Measured soil organic carbon values for Bad Lauchstädt and Müncheberg.

Bad Lauchstädt		Müncheberg	
Date	$C_{ORG}$	Date	$C_{ORG}$
13 August 1997	2.13	01 September 1992	0.63 <sup>a</sup>
23 September 1999	2.14	03 May 1993	0.58
27 October 2000	2.19	21 September 1993	0.67
23 October 2001	2.03	17 July 1995	0.51
09 October 2002	2.07	01 October 1997	0.56
22 September 2003	2.06	–	–

<sup>a</sup>Estimated with a trend line using the four measured values

1998. Input data such as soil parameters, daily meteorological data and management information were taken from the datasets. In some cases data for the nitrogen uptake by crops, the vegetation time, the carbon input via straw and the C/N-ratio of straw were not specified but deducible from the datasets. If no data were available or deducible – for example, for C and N input with roots and crop residues – CANDY standard parameters (C/N-ratio, dry matter, rate and synthesis coefficients, etc.) were used. The soil parameters for wilting point and field capacity were adapted to measurements of soil moisture.

In order to initialise the CANDY model, a value for  $C_{DEC}$  in soil has to be specified. According to the equation

$$C_{DEC} = C_{ORG} - C_I, \quad (1)$$

with  $C_{ORG}$  = total organic carbon in soil and  $C_I$  = inert carbon.  $C_{DEC}$  were calculated using the starting  $C_{ORG}$  values from Table 1 and  $C_I$  values were calculated with the methods mentioned below. This procedure resulted in five initial values for  $C_{DEC}$ . With each initial value a CANDY simulation was started. No other parameters or scenario data were changed. Therefore, differences in simulated carbon and nitrogen dynamics came from the different initial values used.

#### *Calculation of inert carbon ( $C_I$ )*

Körschens (1980) and Körschens et al. (1998) found a relationship between  $C_I$  and the content of clay and fine silt which can be described with the equation:

$$C_{I-K\ddot{O}} = a \cdot b \quad (2)$$

where  $b$  is the percentage of soil particles  $< 6 \mu\text{m}$  and  $a$  is usually taken as 0.04. According to Schulz (1997) the regression coefficient  $a$  has a range from 0.04 to 0.05. In our investigation we used both 0.04 ( $C_{I-K\ddot{O}I}$ ) and 0.05 ( $C_{I-K\ddot{O}II}$ ) to define the possible range of  $C_I$ .

Rühlmann (1999) suggested an equation to describe the influence of soil texture on the carbon content of long-term bare fallow soils:

$$C_{I-R\ddot{U}} = 0.017 \cdot c - 0.001 \cdot \exp(0.075 \cdot c) \quad (3)$$

where  $c$  is the percentage of soil particles  $< 20 \mu\text{m}$  and  $C_{I-R\ddot{U}}$  (%) is the soil organic carbon content of long-term bare fallow soils which were assumed to be similar to the size of the inert organic carbon pool.

Based on Falloon et al. (1998, 2000)  $C_I$  (tonne C per hectare) can be estimated from the total stock of carbon using the following equation (Eq. 4) and its upper (Eq. 5) and lower (Eq. 6) confidence levels:

$$C_{I-FAL} = 0.049 \cdot C_{ORG}^{1.139} \quad (4)$$

$$C_{I-FAL(+95)} = 0.1733 \cdot C_{ORG}^{1.4624} \quad (5)$$

$$C_{I-FAL(-95)} = 0.01384 \cdot C_{ORG}^{0.8156} \quad (6)$$

where  $C_{ORG}$  (in tonnes C per hectare) is the total amount of organic C in the soil.

An approach to estimate organic carbon in micro-pores based on the hypothesis that the stabilisation of soil organic matter is a result of its location at places with low biological activity, which in turn is caused by a limitation of oxygen, was suggested by Kuka et al. (2006). In our investigation with the CANDY model the organic carbon in micro-pores is considered to be inert.

The total organic carbon is distributed to the different pore-space classes – micro-, meso- and macro-pores – according to their surface area. The pore-space classes used (micro, meso and macro) are related to wilting point (WP), field capacity (FC) and pore volume (PV), respectively. The inner surface area of each pore class is calculated from the volume of the considered pore-space class  $V_m$  [WP, FC–WP, PV–FC (in cubic metres)] and

the equivalent pore radius  $R_m$  (in metres).  $R_m$  for the micro-, meso- and macro-pores was set to  $5 \times 10^{-8}$ ,  $10 \times 10^{-8}$  and  $500 \times 10^{-8}$  m, respectively.

$$A_m = 2 \cdot \frac{V_m}{R_m}, \quad m \in \{\text{micro; meso; macro}\}. \quad (7)$$

Considering organic carbon in micro-pores ( $C_{I-MIP}$ ) as ‘inert’, its amount can be calculated according to the equation:

$$C_{I-MIP} = C_{ORG} \cdot \frac{A_{\text{micro}}}{A_{\text{micro}} + A_{\text{meso}} + A_{\text{macro}}}, \quad (8)$$

with  $C_{I-MIP}$  (M.%) mass of carbon in micro-pores,  $C_{ORG}$  (M.%) mass of total organic carbon in soil and  $A_{\text{micro, meso, macro}}$  (in square metres) inner surface of pore class.

### Statistical methods

For this investigation we selected the following statistical methods to obtain information about differences deriving from varying  $C_I$  initial values.

The root mean square error (RMSE; Fox 1981) and the mean bias error (MBE; Addiscott and Whitmore 1987) provide information about the average difference between predicted ( $P_i$ ) and observed ( $O_i$ ) values.

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (P_i - O_i)^2}{n}} \quad (9)$$

$$MBE = \sum_{i=1}^n \frac{P_i - O_i}{n}, n = \text{number of samples}. \quad (10)$$

A lower RMSE indicates a more accurate simulation. The lower limit of RMSE is 0. MBE can take positive or negative values. Its calculation does not include a square term, thus, predicted values below and above the observed values cancel out, and the result gives an indication of the bias error.

The ‘index of agreement’ (IA) suggested by Willmott and Wicks (1980) is intended to be descriptive and is both a relative and a bounded measure.

$$IA = 1 - \frac{\sum_{i=1}^n (P_i - O_i)^2}{\sum_{i=1}^n (|P_i - \bar{O}| + |O_i - \bar{O}|)^2},$$

$$0 \leq IA \leq 1, \quad (11)$$

with  $n$  = number of samples and  $\bar{O}$  = mean of the observed data.

## Results and discussion

### Calculated inert carbon

The  $C_I$  values used to calculate initial  $C_{DEC}$  values for the simulation of the Bad Lauchstädt and Müncheberg sites and the total organic carbon content are shown in Figure 1. Apart from the remarkable differences in total organic carbon between the two sites, Figure 1 shows that with the  $C_{I-FAL}$  method, which is simply based on total  $C_{ORG}$ , the lowest  $C_I$  values are obtained. However, the lower and upper confidence levels of  $C_{I-FAL}$  cover nearly the whole range of possible inert carbon. This is in complete agreement with the statement of Falloon et al. (1998) 'that the confidence limits of the model are wide'. For the methods  $C_{I-KÖI}$ ,  $C_{I-KÖII}$  and  $C_{I-RÜ}$ , which are all based on soil texture and suggest a kind of physical protection of soil organic matter, the following order for both sites was found:  $C_{I-RÜ} < C_{I-KÖI} < C_{I-KÖII}$ . Whereas, with the new  $C_{I-MIP}$  approach the highest inert carbon value of all methods was calculated in the case of the Bad Lauchstädt site. With respect to the Müncheberg site  $C_{I-MIP}$  is located between  $C_{I-RÜ}$  and  $C_{I-KÖI}$ . Thus, a clear ranking of the  $C_{I-MIP}$  method with respect to the amount of calculated inert carbon is not possible. Similar to the  $C_{I-KÖI}$ ,  $C_{I-KÖII}$  and  $C_{I-RÜ}$  approaches, the  $C_{I-MIP}$  approach is suggesting physical protection, but the latter uses pore-space classes instead of soil texture and is also dependent on the total amount of  $C_{ORG}$ . Therefore, it shows a more dynamic behaviour. For example, changes in pore-space class distribution because of a modified tillage regime result in a different  $C_{I-MIP}$  value.

### Simulation results and statistics

To give the reader an impression of the model outputs produced with different initial  $C_I$  values,

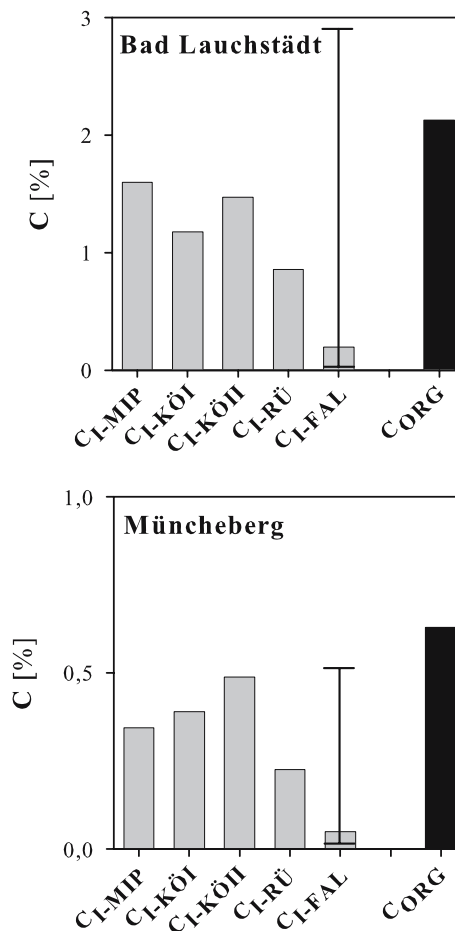


Figure 1. Calculated inert carbon ( $C_I$ ) and total soil organic carbon ( $C_{ORG}$ ) for Bad Lauchstädt and Müncheberg.  $C_{I-MIP}$  = Kuka et al. 2006;  $C_{I-KÖI}$  and  $C_{I-KÖII}$  = Körschens 1980 and Körschens et al. 1998 with  $a = 0.04$  and  $0.05$ , respectively;  $C_{I-RÜ}$  = Rühlmann 1999;  $C_{I-FAL}$  = Falloon et al. 1998, 2000. I = Confidence interval for  $C_{I-FAL}$ .

the simulation results for  $C_{ORG}$  and  $N_{MIN}$  are presented in Figures 2 and 3, respectively. In the case of  $C_{ORG}$  there is a clear differentiation – increasing with time – between the model runs. The distinct influence of different initial  $C_I$  values on  $N_{MIN}$  in soil, especially for the Bad Lauchstädt site, emphasises the importance of a careful model initialisation even for short simulation periods.

For Bad Lauchstädt the carbon and nitrogen dynamics and the differences between the simulations are higher than for Müncheberg. In addition to mineralisation, this may be due to other processes such as leaching or denitrification. In fact, nitrogen leaching is very low at the Bad Lauchstädt

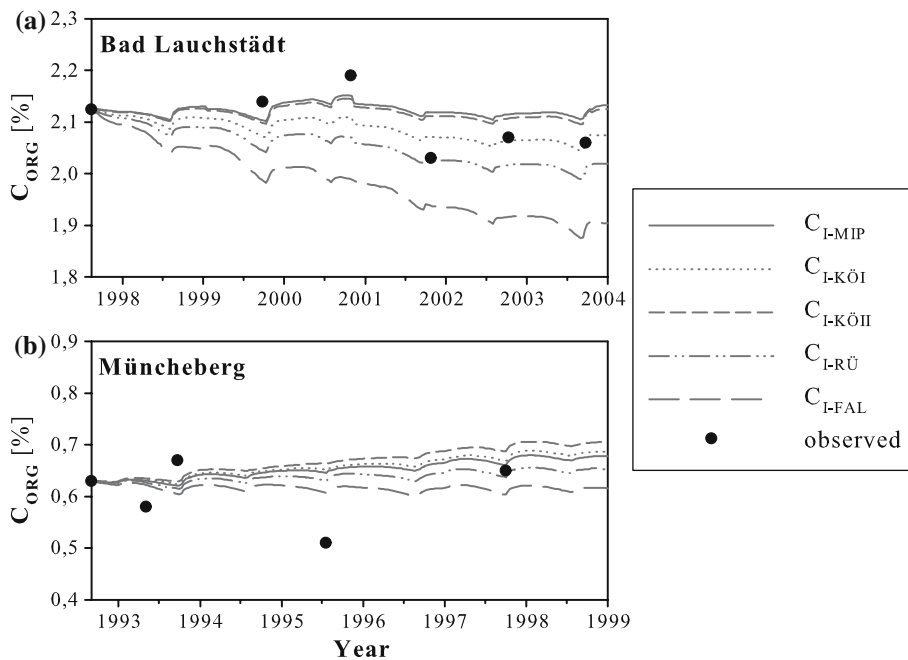


Figure 2. Simulation results for organic carbon ( $C_{ORG}$ ) dynamics using different initial  $C_I$  values for Bad Lauchstädt (a) and Müncheberg (b).  $C_{I-MIP}$  = Kuka et al. 2006;  $C_{I-KÖI}$  and  $C_{I-KÖII}$  = Körschens 1980 and Körschens et al. 1998 with  $a=0.04$  and  $0.05$ , respectively;  $C_{I-RÜ}$  = Rühlmann 1999;  $C_{I-FAL}$  = Falloon et al. 1998, 2000.

site (see Kersebaum et al. 2006) due to a high water storage capacity and low precipitation (see Franko et al. 2006). Thus, the other nitrogen-related processes have to be adequately taken into account for an assessment of model initialisation.

The examination of the mean ( $m_C$ ,  $m_N$ ) and the mean bias error ( $MBE_C$ ,  $MBE_N$ ) for carbon and nitrogen, respectively (Tables 2, 3), indicates that in most cases the observed values are exceeded by the corresponding predicted values. Only for organic carbon and  $C_{I-KÖI}$ ,  $C_{I-RÜ}$  and  $C_{I-FAL}$  of the Bad Lauchstädt site an underestimation can be found. For the Müncheberg site, the  $MBE_C$  and  $MBE_N$  are the lowest for  $C_{I-FAL}$  and  $C_{I-KÖII}$ , respectively. For Bad Lauchstädt, the lowest mean bias errors are obtained for  $C_{I-KÖI}$  and  $C_{I-MIP}$ . Consequently, no method seems to be clearly better than the others in predicting initial values for  $C_I$ .

Looking at the carbon root mean square error (RMSE, Figure 4) for Bad Lauchstädt, the method for estimating  $C_I$  proposed by Falloon et al. (1998, 2000) differs clearly from the other  $C_I$  methods, which account for physical protection of soil organic matter. Obviously, the  $C_{I-FAL}$  method

underestimates the inert part of soil organic matter for Bad Lauchstädt (see Figure 1), leading to an overestimation of the decomposable part, followed by a fast decline in soil organic matter and a surplus of mineral nitrogen (see Figure 2). For Müncheberg there is no substantial difference in  $RMSE_C$  between any of the methods used in this investigation. In the case of mineral nitrogen, greater differences in the root mean square error can be found.  $C_{I-MIP}$  and  $C_{I-KÖII}$  are in the leading group for the Bad Lauchstädt site and, accompanied by  $C_{I-KÖI}$ , in the leading group for the Müncheberg site.

The index of agreement (IA, Figure 5) more precisely suggests that for both sites the  $C_{I-FAL}$  method decreases in accuracy compared to the others with respect to predict  $C_I$  in the initialisation of the CANDY model. Falloon et al. (2000) pointed out that their  $C_I$  method was not expected to be valid for soils with a large  $C_I$  content. The 'Haplic Chernozem' (FAO 1994) of Bad Lauchstädt may belong to that category. However, Schmidt et al. (1999) detected charred organic carbon (up to 45% of the bulk organic carbon) in German chernozemic soils.

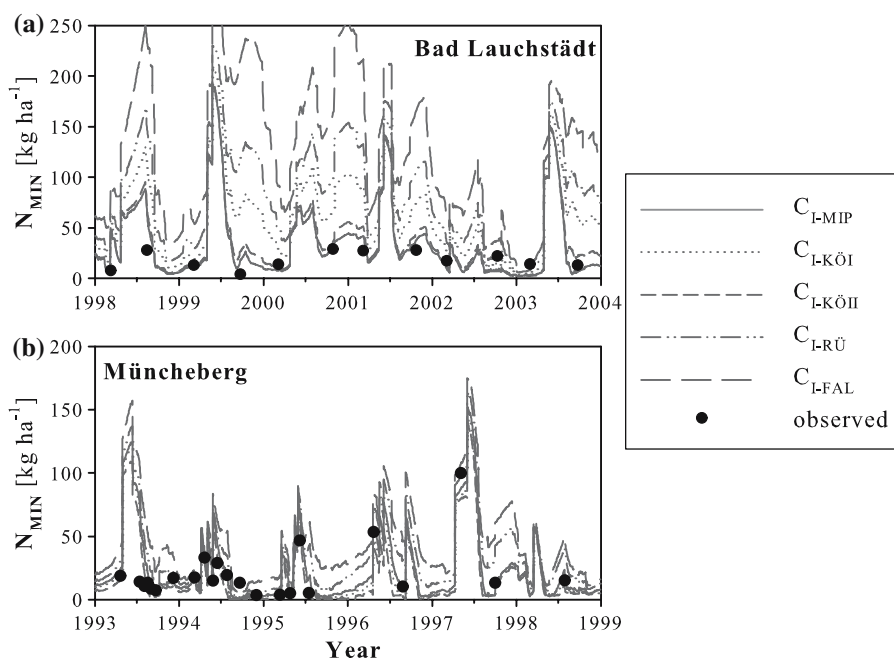


Figure 3. Simulation results for mineral nitrogen ( $N_{\text{MIN}}$ ) dynamics using different initial  $C_I$  values for Bad Lauchstädt (a) and Müncheberg (b).  $C_{I\text{-MIP}}$  = Kuka et al. 2006;  $C_{I\text{-KÖI}}$  and  $C_{I\text{-KÖII}}$  = Körschens 1980 and Körschens et al. 1998 with  $a=0.04$  and  $0.05$ , respectively;  $C_{I\text{-RÜ}}$  = Rühlmann 1999;  $C_{I\text{-FAL}}$  = Falloon et al. 1998, 2000.

Table 2. Quantitative statistical measures for simulations with different initial inert carbon ( $C_I$ ) values for the Bad Lauchstädt site.  $C_{I\text{-MIP}}$  = Kuka et al. 2006;  $C_{I\text{-KÖI}}$  and  $C_{I\text{-KÖII}}$  = Körschens 1980 and Körschens et al. 1998 with  $a=0.04$  and  $0.05$ , respectively;  $C_{I\text{-RÜ}}$  = Rühlmann 1999;  $C_{I\text{-FAL}}$  = Falloon et al. 1998, 2000

Bad Lauchstädt <sup>a</sup>	$m_C^b$	$\text{MBE}_C^b$	$m_N^b$	$\text{MBE}_N^b$
$C_{I\text{-MIP}}$	2.12	0.027	23.6	5.49
$C_{I\text{-KÖI}}$	2.08	-0.018	51.6	33.5
$C_{I\text{-KÖII}}$	2.11	0.021	28.8	10.7
$C_{I\text{-RÜ}}$	2.03	-0.060	75.8	57.7
$C_{I\text{-FAL}}$	1.94	-0.149	124	106
O <sup>c</sup>	2.09	—	18.1	—

<sup>a</sup> $n_C=5$ ;  $n_N=12$ .

<sup>b</sup>m, Mean; MBE, mean bias error; subscript C, carbon (%); subscript N, mineral nitrogen ( $\text{kg ha}^{-1}$ ).

<sup>c</sup>O, Observed.

Table 3. Quantitative statistical measures of simulations with different initial inert carbon ( $C_I$ ) values for the Müncheberg site.  $C_{I\text{-MIP}}$  = Kuka et al. 2006;  $C_{I\text{-KÖI}}$  and  $C_{I\text{-KÖII}}$  = Körschens 1980 and Körschens et al. 1998 with  $a=0.04$  and  $0.05$ , respectively;  $C_{I\text{-RÜ}}$  = Rühlmann 1999;  $C_{I\text{-FAL}}$  = Falloon et al. 1998, 2000

Müncheberg <sup>a</sup>	$m_C^b$	$\text{MBE}_C^b$	$m_N^b$	$\text{MBE}_N^b$
$C_{I\text{-MIP}}$	0.64	0.036	28.5	8.07
$C_{I\text{-KÖI}}$	0.64	0.040	25.3	4.86
$C_{I\text{-KÖII}}$	0.65	0.050	20.9	0.53
$C_{I\text{-RÜ}}$	0.63	0.024	38.8	18.4
$C_{I\text{-FAL}}$	0.61	0.006	50.8	30.4
O <sup>c</sup>	0.60	—	20.4	—

<sup>a</sup> $n_C=4$ ;  $n_N=23$ .

<sup>b</sup>m, Mean; MBE, mean bias error; subscript C, carbon (%); subscript N, mineral nitrogen ( $\text{kg ha}^{-1}$ ).

<sup>c</sup>O, Observed.

The new  $C_{I\text{-MIP}}$  approach proves to be as good as  $C_{I\text{-KÖI}}$  and  $C_{I\text{-KÖII}}$ .  $C_{I\text{-RÜ}}$  is located between the leading group and  $C_{I\text{-FAL}}$ . The usefulness of the approach by Körschens (1980) and Körschens et al. (1998) was also pointed out by Ludwig et al. (2003), however there are some indications that

this method is not generally applicable. Problems arise particularly for soils with a very high content of fine particles (FP = clay + fine silt) and low  $C_{\text{ORG}}$  content, a situation that can be found in the long-term experiment from Prague-Ruzyně with FP=41.2% (J. Klir, personal communication) and

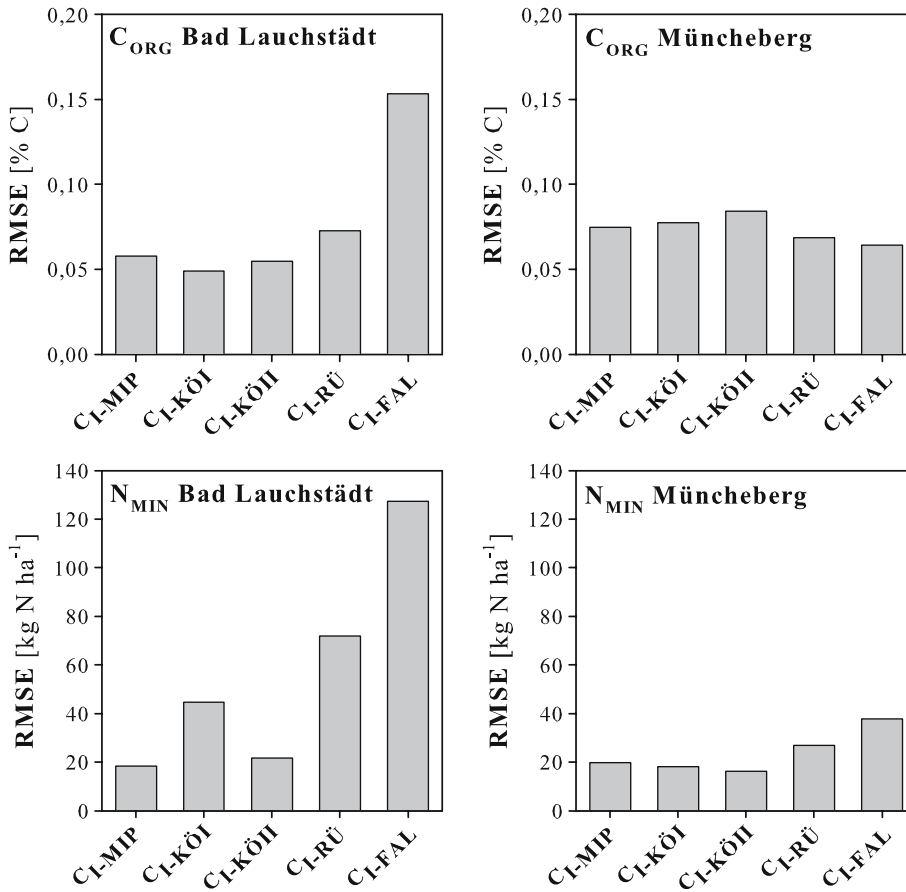


Figure 4. Root mean square error (RMSE) for organic carbon (%) and mineral nitrogen (kg ha<sup>-1</sup>) of simulations with different initial  $C_I$  values for the sites Bad Lauchstädt and Müncheberg.  $C_{I-MIP}$  = Kuka et al. 2006;  $C_{I-KOI}$  and  $C_{I-KOII}$  = Körschens 1980 and Körschens et al. 1998 with  $a=0.04$  and  $0.05$ , respectively;  $C_{I-RÜ}$  = Rühlmann 1999;  $C_{I-FAL}$  = Falloon et al. 1998, 2000).

$C_{ORG}$  values from 1.1 to 1.4% (Kubat et al. 2003). Other examples are the long-term experiments of Giessen with  $C_{ORG}=0.99\%$  and  $FP=25\%$  (Boguslawski and Debruck 1976) and Gembloux with  $C_{ORG}=0.92\%$  and  $FAT=24\%$  (Droeven et al. 1982). In all these cases the approach by Körschens (1980) and Körschens et al. (1998) leads to an overestimation of  $C_I$ .

## Conclusion

Our results show that an important factor in the CANDY model initialisation procedure is the method chosen for the calculation of  $C_I$  as this will have a strong influence on modelling results, even in short-term simulations. The coupled investigation of carbon and nitrogen dynamics leads to a more secure decision on the applicability of a  $C_I$

method than simply looking at carbon dynamics because an underestimation of inert carbon causes an overestimation of decomposable carbon and a surplus of mineral nitrogen in the soil (or vice versa).

Of the  $C_I$  methods considered, the  $C_{I-FAL}$  method, based simply on total soil organic carbon, is shown to be the least appropriate for a soil with a high amount of inert carbon, such as the Bad Lauchstädt 'Haplic Chernozem', whereas the  $C_{I-KOI}$  and  $C_{I-KOII}$  methods as well as the new  $C_{I-MIP}$  approach, all of which allow for the effects of physical protection of soil organic matter, proved to be successful in estimating the inert organic carbon pool in soils of both of the sites investigated. Hence, physical protection seemed to be of major importance for simulating carbon and nitrogen dynamics.



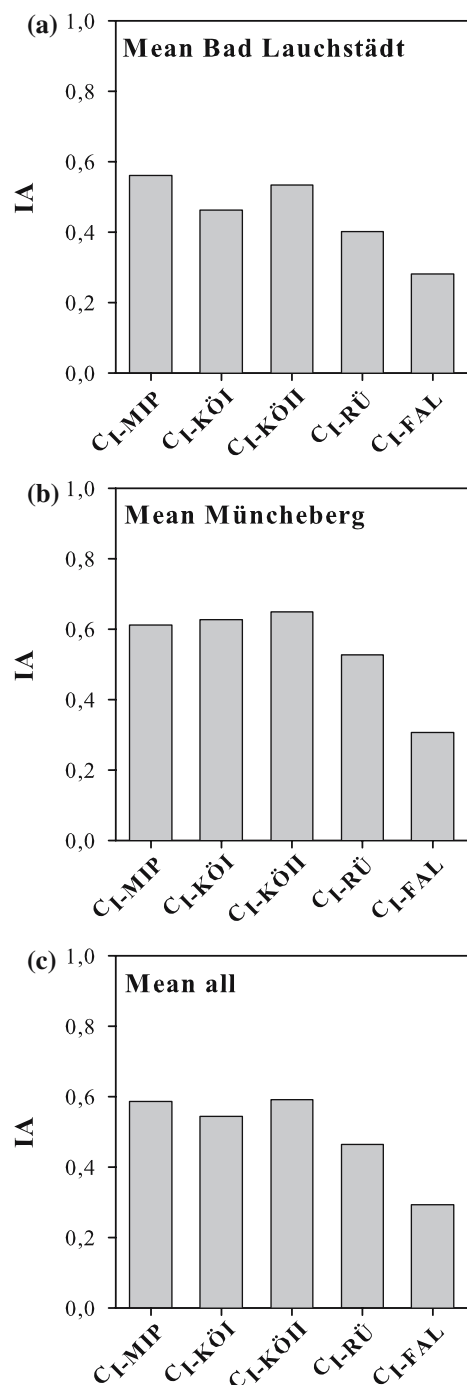


Figure 5. Mean index of agreement (IA) of simulations with different initial  $C_I$  values for the sites Bad Lauchstädt (a) and Müncheberg (b) (in each case: mean of organic carbon and mineral nitrogen) and for both sites (c) (mean of organic carbon and mineral nitrogen and sites).  $C_{I-MIP}$  = Kuka et al. 2006;  $C_{I-KÖI}$  and  $C_{I-KÖII}$  = Körschens 1980 and Körschens et al. 1998 with  $\alpha=0.04$  and  $0.05$ , respectively;  $C_{I-RÜ}$  = Rühlmann 1999;  $C_{I-FAL}$  = Falloon et al. 1998, 2000.

In contrast to the methods which primarily consider soil texture ( $C_{I-KÖI}$ ,  $C_{I-KÖII}$  and  $C_{I-RÜ}$ ) the  $C_{I-MIP}$  approach uses pore-space classes and also includes the total amount of  $C_{ORG}$ . Changes in pore-space class distribution of one soil, because of a modified tillage or a changed organic manure regime, would result in a different  $C_{I-MIP}$  value for the soil. Consequently, this  $C_{I-MIP}$  method is able to express differences in soil structure and organic matter supply at one site. Further studies, with a wider range of soil types and soils with different tillage regimes and soil organic matter levels, are required to see whether the new  $C_{I-MIP}$  approach is generally applicable.

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