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Transfer of carbon incubation parameters to model the SOC and SON dynamics of a field trial with energy crops applying digestates as organic fertilizers

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Abstract

The fertilization with organic amendments and digestates from biogas plants is increasingly used to increase carbon stock and to improve the soil quality, but little is still known about their long-term effects. A common method to analyse organic amendments and their mineralization is incubation experiments, where amendments get incubated with soil while CO_2 release is measured over time. In a previous study, carbon models have been applied to model the carbon dynamics of incubation experiments. The derived parameters describing the carbon turnover of the CCB model (CANDY Carbon Balance) are used to simulate the SOC and SON dynamics of a long-term field trial. The trial was conducted in Berge (Germany) where organic amendments like slurry, farmyard manure or digestates were systematically applied. To grant a higher model flexibility, the amounts of crop residues were calculated for roots and stubble separately. Furthermore, the mineralization dynamics of roots and stubble are considered by the model parameters for each crop. The model performance is compared when using the dry matter and carbon content received from the field trial and the incubation experiments, to evaluate the transferability. The results show that the incubation parameters are transferable to the field site, with rRMSE < 10% for the modelled SOC and rRMSE between 10% and 15% for the SON dynamics. This approach can help to analyse long-term effects of unexplored and unusual organic fertilizers under field conditions, whereat the model is used to upscale the C dynamics from incubation experiments, considering environmental conditions.

KEYWORDS
digestates, long-term field experiment, modelling carbon and nitrogen dynamics, parameter transfer, soil carbon incubation

1 | INTRODUCTION

With a rising demand of renewable energy, the number of biogas plants is growing continuously. The hereby accrued digestates are commonly applied to cropland to increase the carbon storage, recycle nutrients and improve soil fertility and soil quality. The long-term effects on soil properties are hard to determine, since the physical and chemical properties of digestates can vary significantly because of the substrates and their composition, the technical processing in the biogas plant, etc. (Barduca et al., 2020; Nielsen et al., 2020; Zirkler et al., 2014). Because of this variety, there is a need to evaluate the long-term behaviour of those substrates, whereat methods which are less time intense than long-term field experiments need to be developed.

Besides chemical properties of organic amendments, the soils to which they are applied can have a decisive impact on the carbon turnover, due to pH, soil texture, bulk density, etc. (Gami et al., 2009; Roy & Kashem, 2014). Incubation experiments are a common method to analyse the behaviour of organic amendments in soils under controlled conditions, with constant temperature and pre-defined water saturation. The CO_2 that is released during the microbial turnover is measured continuously. Commonly, several regression approaches or mineralization models are used to derive information from the incubation data, but the dynamics cannot be upscaled. The necessary transfer of that information to the field scale is quite difficult and not clear (Sleutel et al., 2005).

Long-term field experiments are conducted, amongst other things, to analyse organic amendments and their long-term behaviour, which are influenced by climate, field management, water supply, etc.; these experiments generate the most application-related data. However, those experiments are time- and cost-consuming and significant results cannot be retrieved until a certain time span is reached. Furthermore, the results of those experiments are site-specific, since they are influenced by climatic and soil-specific parameters.

The modelling of field experiments can be a possible approach to evaluate the soil organic carbon (SOC) and soil organic nitrogen (SON) dynamics of organic amendments. Still, the modelling poses a number of challenges for the operator. These include the choice of an appropriate model, which varies in complexity and scope. There are several models developed for arable lands like Century (Parton et al., 1987), RothC (Coleman & Jenkinson, 1999), ICBM (Andrén & Kätterer, 1997), C-TOOL (Taghizadeh-Toosi et al., 2014) and CCB (Franko et al., 2011), just to mention some. Further, the operator faces the collection of data, the parameterization of the model, the handling of changing measurement analytics, the choice of the initial value for the modelling, the validation of the model results and as well a method to determine the mineralization behaviour of organic substrates within the model concept.

Especially, new or seldom applied organic amendments cannot be explored within field experiments to their fullest extent. A plausible method to study the quality of organic substrates is the modelling of incubation, as shown by Gasser et al. (2021). The authors used the carbon turnover concepts of six mechanistic models to model the C dynamics of 72 incubated substrates. The hereby received parameters, which describe the mineralization, are assumed to be transferred to model the SOC and SON dynamics on field scale.

The hypothesis that the results from incubation experiments can be used to model the turnover of organic substrates on field scale is proposed. To validate this hypothesis, a result dataset from an incubation study (Gasser et al., 2021) is used to parameterize the CCB model accordingly and applied on a field experiment where the same organic materials that were studied during incubation are applied as organic amendments. The data of incubated roots and stubbles are used to parameterize the residues used to model the field trial. The implemented N turnover in the CCB model depends on the carbon turnover; therefore, the suitability of carbon incubation data is evaluated to calculate the N turnover of the field sites as well.

The following questions are addressed:

I Are the chemical properties required to characterize the organic substrates like C content, N content and dry matter content collected during incubation experiments, sufficient to cover the variability of those properties during a field trial?

II How to calculate the masses of roots and stubble in dependence of the main product, to evaluate the input in the SOC cycle?

III Are the parameters describing the mineralization, received from modelling incubated organic amendments, roots and stubble with the CCB model transferable to the field site?

2 | MATERIALS AND METHODS

2.1 | Field site of Berge

The field site was situated in Berge near Nauen, an agricultural experimental station of the Institute of Agricultural and Urban Ecological Projects at the Humboldt-Universität zu Berlin (IASP) (52°37′11″N and 12°47′16″E, and 51°49′N, 45 m above sea level), Germany.

The basic material for the soil generation of the site is glacial cover sand over boulder clay. The boulder clay on the trial area has different depths, which results in a heterogeneous soil texture from sand to loamy sand. The topsoil (0–20 cm) has a clay content of 1.1%, silt 9% and sand 88.9%. The bulk density is between 1.5 and 1.6 g/cm^3, while the pH value of the soil is 5.54.

The field trial was set up in March 2011 with a one-factorial randomized block design, with four replications. The crop rotation was winter rye as whole crop silage followed by maize and in the next year winter rye as whole crop and silage–sorghum. Fertilizers are applied twice a year before the sowing of either rye or maize/sorghum. Furthermore, it is to be noticed that all treatments have been cultivated with winter wheat and mustard as intercrop with an N fertilization of 100 kg N ha^{-1} as pre-management.

Five different digestates (DG) and farmyard manure (FYM) and cattle slurry (SLY) were used as organic fertilizers. In addition, there was also an unfertilized control (CRL) and one treatment receiving only mineral fertilizer (calcium ammonium nitrate [CAN]).

The fertilizer quantities are based on the amount of applied carbon of a standard farmyard manure (FYM) application of 12.5 t ha^{-1} a^{-1}. (7.5 t ha^{-1} before maize or sorghum and 5 t ha^{-1} before winter rye). The amount of the other organic fertilizers is determined by the amount of organic carbon (Corg) spread by the manure at every application date, so that the amount of Corg is the same for all applied organic fertilizers. The resulting differences in applied nitrogen are balanced by mineral fertilization (CAN). The treatments FYM and DG D-l start a year later compared with the other treatments (2012).

Average inputs and operating parameters of the biogas plants providing the digestates are given in Table 1.

Biogas plant D uses liquid/solid separation of the digestate as a subsequent treatment. The cattle slurry that serves as substrate in plant A as well farmyard manure from plant D is used as a reference treatment in the field trial.

The climate data required for the modelling were obtained from a weather station of the German Meteorological Service which is located next to the experimental field.

2.2 | Soil sampling and analysis

At each plot, five soil samples were taken to a depth of 20 cm two times a year (2011–2020), once after the harvest of green rye in May and then after the harvest of either sorghum or maize in October. The soil was air-dried, sieved (<2 mm) and analysed for soil organic carbon (SOC) and nitrogen (Nt) content (Dumas method). From September 2015 on, the carrier gas in the analytics was changed from helium to argon. This leads to differences between the measurement results and a systematic offset for the Nt measurements. To correct this, a regression was calculated between comparative measurements with an adjusted R^2 = .9993 (Figure A1 in Appendix 1). This regression was used to convert the values carried out with helium to the values carried out with argon.

2.3 | CCB model description

The used CCB model, which is a simplified version of the carbon dynamic model in CANDY (Franko et al., 1995), is used. It describes the turnover of decomposable carbon in monthly time steps for average site conditions depending on crop yields and input rates of fresh organic matter (FOM). A specific characteristic of the CCB model is the handling of FOM as a list of specific pools from which the C is released to the atmosphere or used to build up new SOM. The decomposition is controlled by the FOM-specific parameters k_{fom} describing the breakdown of a specific FOM and eta (η) describing the part of carbon that is transferred to SOM. First, FOM is moved into the pool of active SOM (A-SOM), which is interacting with the pool of stabilized SOM (S-SOM). Additionally, the model concept includes the long-term stabilized pool (LTS-SOM) where SOM is considered as physically protected (Figure 1). The nitrogen turnover is linked to carbon turnover via the C/N ratio for each FOM pool, while the C/N ratio of A-SOM and S-SOM is set to 8.5 and the C/N ratio of the LTS pool is calculated with the initial Nt value and the carbon content of all SOM pools. The CCB does not consider a mineral N pool. The microbial-driven matter dynamics in the easily decomposable pools (A-SOM and S-SOM) are simulated in monthly time steps. This process, as well as the FOM turnover, is controlled by site conditions like soil texture, air temperature and rainfall. These conditions are aggregated into a Biologic Active Time (BAT in days [d]) expressing

TABLE 1 Input material and operating parameters of the four biogas plants included in the study

Plant	DG A		DG B		DG C		DG D-l; DG D-s	
Average Input	50%	Cattle slurry	43%	Pig slurry	86%	Con silage	30%	Cattle slurry
	30%	Corn silage	46%	Corn silage	14%	Rye silage	30%	Grass silage
	15%	Grass silage	10%	Grass silage			30%	Corn silage
	5%	Fodder remains	1%	Grain			10%	Farmyard manure
Operating temperature	Mesophile		Mesophile		Thermophile		Mesophile	
Retention time	70 days		60 days		50 days		80 days	

Abbreviation: DG, digestates, DG D is separated in liquid (l) and soil (s) components.

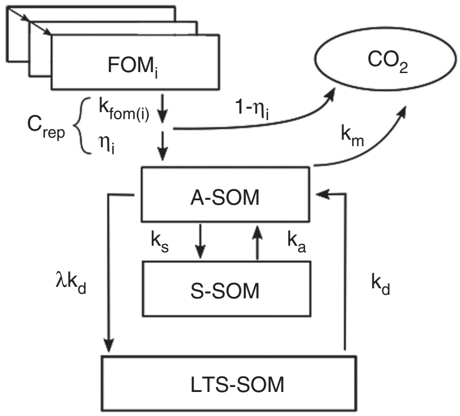

FIGURE 1 Scheme of the carbon turnover in CCB, organic matter in soil is subdivided into four compartments: (1) fresh organic matter (FOM) including roots, stubble and organic amendments, (2) biological active soil organic matter (A-SOM), (3) stabilized soil organic matter (S-SOM) and (4) long-term stabilized soil organic matter (LTS-SOM); the fluxes are indicated as lines with the corresponding parameters

the part time interval under the assumption that no environmental restrictions are in place. Additionally, a matter transfer between A-SOM and LTS pool is considered. A part of the newly built SOM (C_{rep}) is captured inside micropores and thus shielded from decomposition, whereas a part of C-LTS is released from protection and exposed to microbial turnover. Details about the CCB modelling approach and its applications to describe SOM topsoil dynamics were already published (Franko et al., 2011).

2.4 | Statistical analysis and model initialization

The yields, calculated stubble and root masses of the treatments, were tested for significant differences using the ANOVA, and in the case of significant differences, a post hoc Tukey test was performed. The normality of the data was tested with the Shapiro–Wilk test, in case of not normal distributed data the Kruskal–Wallis test was performed. The homogeneity of variances was tested with the Levene's test. The significance level was set to $\alpha = .05$.

The goodness of fit was compared by the root mean squared error (RMSE, Equation 1), and furthermore, the relative RMSE (rRMSE, Equation 2) was calculated to characterize the differences between observed values (O), $\overline{O}$ as mean of the observations and predicted values (P):

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

$$rRMSE = \frac{100}{\overline{O}}\sqrt{\frac{\sum_{i=1}^{n}(O_i - P_i)^2}{n}} \quad (2)$$

The choice of the appropriate starting value for modelling is not straightforward. There are different approaches that all show advantages and disadvantages. In this approach, the mean error (ME, Equation 3) was used to define the start value of each treatment.

$$ME = \frac{\sum_{i=1}^{i=n}(O_i - P_i)}{n} \quad (3)$$

All analyses were performed with R statistics (2019).

2.5 | Parametrization of the CCB model

Besides the climate data (air temperature [°C] and precipitation [mm]), the CCB model requires data on soil properties as well as k_{fom} and η values, which describe the mineralization for the organic amendments, roots and stubble. Furthermore, chemical properties, such as C, dry matter and N content of those substrates, have to be determined. Besides the quality parameters, the quantity of the organic substrates like organic fertilizers or roots and stubble is necessary to calculate the C and N input into the soil cycle.

2.5.1 | Root and stubble quantity parameters for Berge

The stubble and root mass in the CCB are calculated by a linear equation using the dry matter main product (MP_{dm}) to estimate either the root (RT_{dm}) or the stubble dry mass (ST_{dm}) (Franko et al., 2021):

$$RT_{dm} = FIX_r + BIX * MP_{dm} \quad (4)$$

$$ST_{dm} = FIX_s + RIX * STIX * MP_{dm} \quad (5)$$

The intercept of the linear equation describes a constant amount of root (FIX_r) or stubble mass (FIX_s) which is yield independent, while the slope describes a yield-dependent root (BIX) and stubble (RIX) factor. The part of stubble related to the above-ground crop residue, for example, straw, is expressed with STIX. Since all crops are harvested as whole plant, stubble is the only above-ground residues and, therefore, STIX is set to 1.

The root and stubble masses that are needed for the parametrization are derived from Höcker (2017), who analysed these masses for different crops under different N supply in field trials. The retrieved masses of yield, stubble and roots are used to calculate the parameters, which describe the quantity dependency of roots and stubble on the yield of the main product.

The parametrization of the root and stubbles quantity is evaluated, by comparing two approaches. The first method (R1) includes a yield-independent part, FIX_r and FIX_s unequal to 0 (Figure 2 R1) with a lower sensitivity to the yield, while for the second method (R2), FIX_r and FIX_s are set to 0 assuming the stubble and root masses are proportional to the yield (Figure 2 R2). The control (CRL) and the mineral fertilized plot (CAN) are used to compare and evaluate both approaches.

It should be noted that the regression describing the amount of sorghum roots is strongly influenced by one data point, which causes a negative intercept (Figure 2, R1 stubble). In this case, the intercept (FIX_r) was forced through 0 and, therefore, there is no yield-independent part for the sorghum roots. The parameters are displayed in Table 2.

2.5.2 | FOM quality parameters from incubation data

The CCB model distinguishes between FOM inputs as organic amendments (in this case organic fertilizers), the incorporation of by-products and the remaining of stubble and roots after the harvest. Those inputs have substrate-specific mineralization behaviour, which are received in this context from incubation experiments.

Incubation experiments

The organic fertilizers were incubated at 20°C and one batch over a period of 139.7 days while the second batch was incubated over 251.7 days, each with 6 replicates. They were incubated in 40 g soil with a clay content of 1%, loam 9% and 90% sand with a water saturation of 60%.

The plant roots and stubble were incubated for 165 (3 replicates) and 300 (5 replicates) days at 22°C in 100 g soil (7% clay, 21% loam and 72% sand) with a water saturation of 50%. Detailed information about the experimental set-up and procedure can be found in Appendix 2.

Gasser et al. (2021) demonstrated in a model ensemble approach amongst other models, the application of the CCB to incubation data. In this context, k_{10} and k_{12} were fitted to the mineralization of 72 different organic substrates. Those substrates include the organic amendments, which are applied on the field experiment in Berge, as well as roots and stubble substrates of the same crops as grown in Berge. In the approach by Gasser et al. (2021), the parameters k_{fom} and η of the CCB model had been transformed to k_{10} and k_{12} to unitize the pool flows, which can be retransformed by the following equations:

$$k_{fom} = k_{10} + k_{12} \tag{6}$$

$$\eta = \frac{k_{12}}{k_{fom}} \tag{7}$$

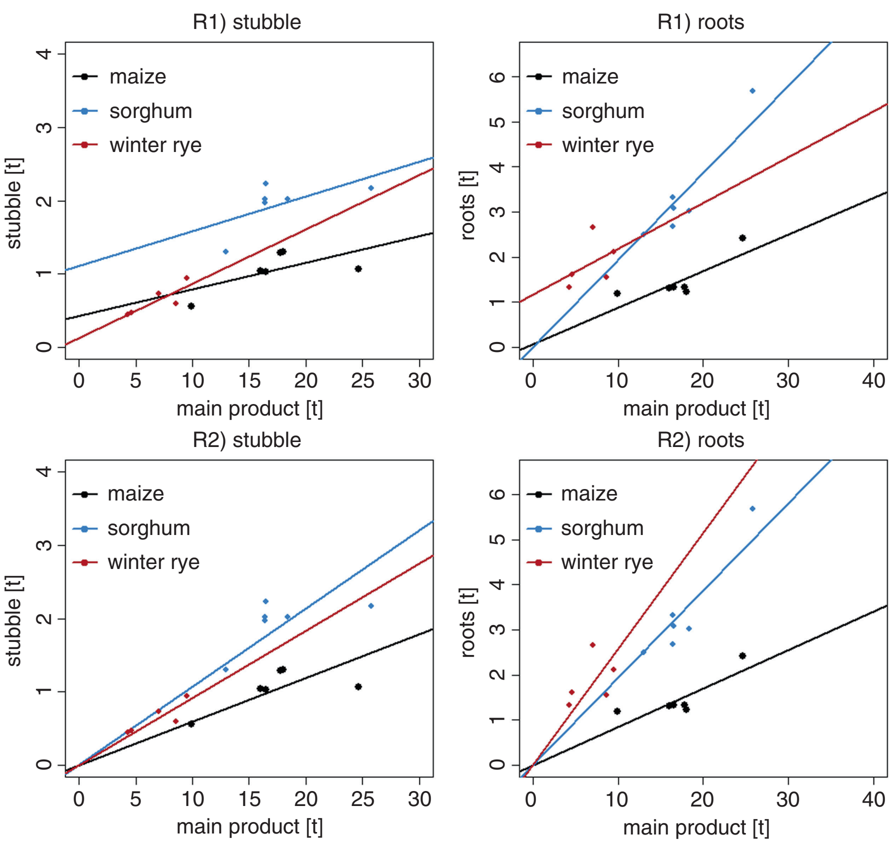

FIGURE 2 Linear regression of main product dry matter and the stubble or root dry matter of crops; (a) linear regression with yield-independent part (intercept) and yield-dependent part (slope)(*R1*); (b) linear regression with solely yield-dependent part (intercept = 0)(*R2*); data (Höcker, 2017)

The parameters (k_{10} and k_{12}) were optimized to the incubation curves, using the *Levenberg–Marquardt* algorithm; an example is shown in Figure 3. The hereby achieved model accuracy varied between a RMSE [%] of 0.6 and 3.5 for the organic fertilizer and between 1.5 and 6.7 for the plant residues (roots and stubble). The parameters have been retransformed to k_{fom} and η as required by the CCB model and are now labelled as such. The incubation experiments were carried out with different temperatures and soils textures, those were considered accordingly by the model, while the water saturation was assumed to be optimal.

Quality parameters for organic fertilizers

During optimization for some organic fertilizers, the algorithm reached the parameter limits of the CCB model for k_{fom} and η resulting in no valid solution of k_{fom} and η predicting the incubation trend. In this case, only the valid parameters of the batch ($N = 2$) where the limits were not reached are used. This accounts for FYM and DG D-s ($N = 1$). The C/N ratio, dry mass, k_{fom} and η values of the organic amendments, which result from the analysis of the incubated organic fertilizer, are presented in Table 3.

When transferring the incubation results to field scale, the question arises how comparable the laboratory results are with those measured in the field trial. The CCB model calculates the amount of added carbon by multiplying the dry matter with the carbon content of organic amendments. Both properties vary over time and different batches of organic amendments. Figure 4 shows the carbon concentration of the organic amendments on the field trial (C1) and the carbon concentration of the incubation experiment (C2). Both values are tested for the SOC modelling, and the results are compared in a later section (3.2).

Quality parameter for plant residues (roots and stubble)

The values for k_{fom} and η (k_{10} & k_{12}) for the plant residues were also obtained from Gasser et al. (2021), whereby the analysed incubation experiments were conducted for fine and coarse roots separately. Owing to the different mineralization behaviour of coarse roots (relatively fast) and fine root (relatively stable)(Gasser et al., 2021), k_{fom} and η were weighted according to their ratio, derived from Höcker (2017) (see Table A1 in Appendix 3). For green rye, no incubation data were available; therefore, the incubation data of winter wheat were used instead. The k_{fom} and η values of roots and stubble used for the simulation of the field site in Berge are shown in Table 3.

The C/N ratio of the plant material was taken from Mewes (2017) who conducted the incubation experiments for the plant residues.

TABLE 2 Parameters used to calculate the carbon input of plant residues (roots and stubble) in the CCB for the method R1 with a yield-independent part and R2 with solely yield dependency, describing the relation between the main product and either stubble or root mass

Plant residues	RIX (R1)	FIX_s (R1)	BIX (R1)	FIX_r (R1)	RIX (R2)	FIX_s (R2)	BIX (R2)	FIX_r (R2)
Maize	0.0364	0.42	0.081	0.07	0.059	0	0.085	0
Sorghum	0.0475	1.1	0.194	0	0.107	0	0.194	0
Winter rye	0.074	0.13	0.102	1.16	0.092	0	0.258	0

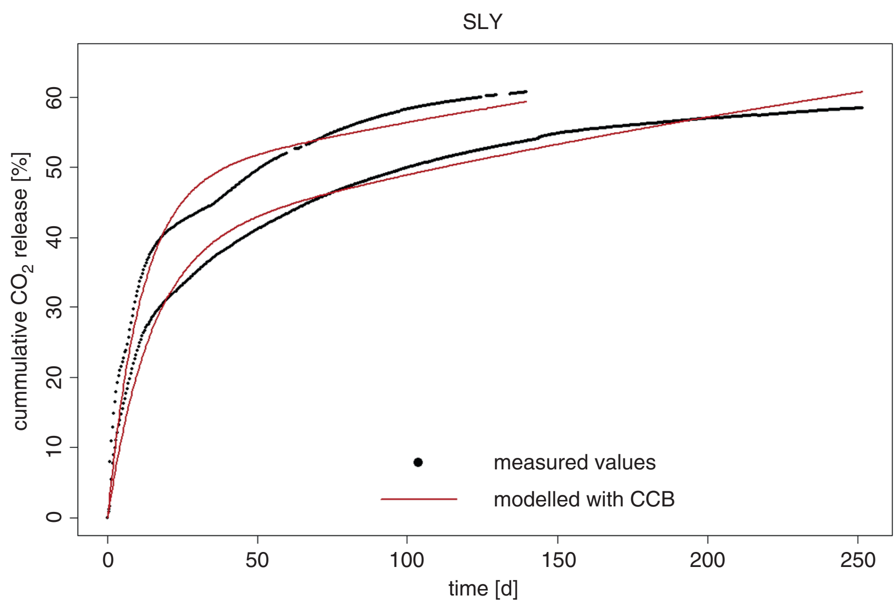

FIGURE 3 Optimization of the CCB model to the mean respiration curves of the organic amendment slurry (SLY) with the Levenberg–Marquardt algorithm (k_{10} & k_{12}), for two batches with 6 replicates, with a period of 140 days (RMSE = 2.38) and 252 days (RMSE = 1.45); the measured respiration (black) and the model prediction (red)

TABLE 3 k_{fom} and η values, as well as chemical properties like C/N ratio, dry matter content and C content of the organic amendments, roots and stubble, derived from the incubation experiment ($N = 2$, $*N = 1$) and the mean RMSE [%] of the model fit to the respiration curves of the organic substrates

Organic substrates	k_{fom} [d^{-1}]	η [−]	C/N [−]	Dry matter [%]	C content [%]	Mean RMSE [%]
SLY	0.2445	0.55403	10.4	9.2	41.5	1.91
FYM	0.0951*	0.67062*	12.8	23.7	32.1	0.68*
DG A	0.32917	0.81297	5.8	6.7	37.7	1.68
DG B	0.10606	0.5913	5.6	4.1	39.6	2.14
DG C	0.33322	0.74272	5.4	6.7	47.4	2.67
DG D-l	0.26218	0.76117	5.2	7.1	39	1.65
DG D-s	0.2146*	0.80332*	13.5	21.3	40.3	1.16*
Maize stubble	0.067	0.313	73.0	–	42.0	3.78*
Maize roots	0.124	0.418	55.7	–	37.8	2.86
Sorghum stubble	0.073	0.258	57.0	–	41.0	6.13
Sorghum roots	0.112	0.456	43.4	–	33.4	2.72
Winter wheat stubble	0.070	0.258	86.0	–	42.0	5.2
Winter wheat roots	0.139	0.579	34.7	–	35.6	2.14

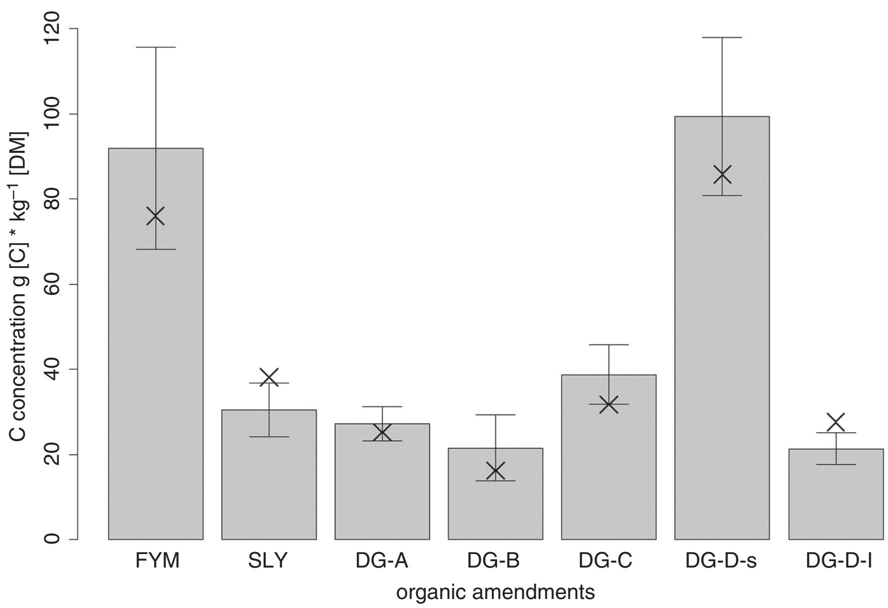

FIGURE 4 Carbon concentration of the organic amendments from the field trial (histogram) and incubation experiment (X) ($N = 2$); bars represent standard deviation ($N = 9$)

3 | RESULTS

3.1 | Analysis of the field experiment

The mean yields for each treatment are displayed in Table 4. Yields for winter rye have a normal distribution, whereas yields for maize and sorghum are not normally distributed. Hence, the Kruskal–Wallis test was performed, which shows no significant differences between yields and treatments, maize *p*-value = .6186 and sorghum *p*-value = .8446. The analysis of variance homogeneity showed that the variances are homogeneous for all crops. For winter rye, the ANOVA showed significant differences between the treatments (*p*-value = .0003), which is why the post hoc Tukey test was performed. The CRL treatment was significantly different from CAN (*p*-value = .0004), SLY (*p*-value = .0011), DG A (*p*-value = .0356) and DG C (*p*-value = DG D-s; *p*-value = .0026), while all other treatments showed no significant differences.

3.2 | Root and stubble quantity parametrization

The two methods R1 and R2, which describe the quantity parametrization for roots and stubble, are compared

TABLE 4 Mean yields [t*ha^{-1}] and standard deviation for crops and treatments, within the year 2011 (*2012)–2020

Treatment	Winter rye	Sorghum	Maize
CRL	8.436 ± 7.75	19.644 ± 9.44	24.600 ± 11.96
CAN	26.426 ± 9.25	33.084 ± 17.51	33.587 ± 17.05
FYM*	20.964 ± 8.35	28.699 ± 16.38	33.653 ± 13.52
SLY	25.443 ± 8.54	32.642 ± 17.39	39.673 ± 16.36
DG A	21.237 ± 8.06	27.520 ± 14.66	38.246 ± 14.73
DG B	18.748 ± 7.88	28.920 ± 14.69	37.599 ± 16.06
DG C	21.426 ± 7.68	29.137 ± 16.24	41.492 ± 11.51
DG D-s	24.515 ± 6.91	32.295 ± 18.27	38.562 ± 11.55
DG D-l*	15.090 ± 8.89	22.893 ± 9.49	34.167 ± 8.28

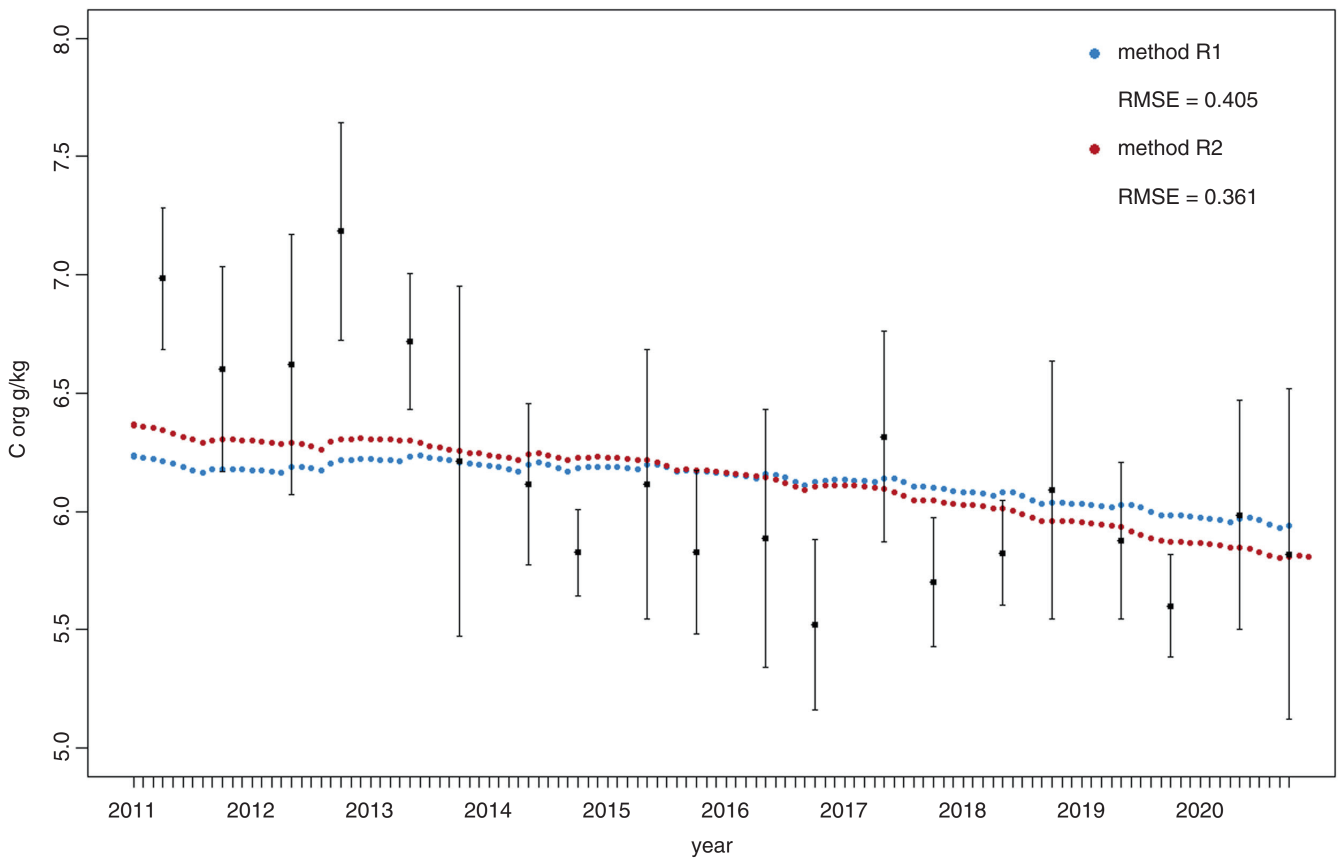

FIGURE 5 Mean measured Corg (markers) and *SD* (*N* = 4) for CRL treatment, output of the model with parametrization of root and stubble dry mass from linear equation considering yield-dependent and yield-independent part (blue, R1) vs. equation considering only yield-independent part (red, R2), initialized with ME

in Figure 5. R1 with a yield-independent part and, therefore, a lower yield dependency and R2 without a yield-independent part and a higher yield dependency were tested at the CRL plot.

The model fit can be improved with method R2, with a reduction in the RMSE by 0.045 g/kg (for the CAN treatment the RMSE gets reduced by 0.004 g/kg). Thus, method R2 has been used for further calculations.

The resulting masses of stubble and roots which were calculated with the R2 method are displayed in Table A2 in Appendix 4. No significant differences between the treatments and corresponding stubble or root masses of the crops have been detected after the described procedure in section 2.4, except for the control treatment of winter rye roots and winter rye stubble.

3.3 | Organic amendments quality parametrization

The comparison of the model results, using the carbon concentration measured during the field trial C1 and for the incubation experiments C2, shows no superior performance for one of the applied methods. For FYM, SLY, DG B and DG D-s, the used dry matter and carbon concentration measured in the field improve the RMSE [g/kg], while for DG C and DG D-l, the properties measured for incubation experiment reduce the RMSE (Table 5). The difference between the two methods is very small that it does not lead to a clear preference of one method over the other.

3.4 | CCB model results and validation

The final modelling of the field trial was conducted with the FOM quantities of stubble and roots calculated with the method R2, and the C concentrations of the organic amendments are taken from the incubation experiments (C2). Figure 6 shows the mean values with standard deviation for the Corg measurements, the corresponding regression and the results of the CCB model for all treatments. The corresponding RMSE, rRMSE and *SD* of the observed Corg values are displayed in Table 6. The CRL and the CAN treatments show a negative trend over the observed period; this trend is captured by the regression and by the CCB model. Nevertheless, the CCB model overestimates and shows a much smaller decrease in Corg for CRL and CAN treatments compared with the regression. In contrast, the regression and the CCB model display an increase in SOC for the other treatments. The CCB model estimates a smaller increase in Corg for the FYM treatment compared with the regression; this accounts especially for later years.

Figure 7 shows the Nt turnover of Berge. The regression indicates a negative trend of Nt for the CRL and CAN treatment, while the CCB model predicts a slight decrease for Nt in the CTL treatment and stable Nt dynamics in the CAN treatment for the given period. For all treatments with organic amendments, the data show stable or slightly increasing Nt concentration. The CCB prediction indicates a slight increase for those treatments.

4 | DISCUSSION

In mechanistic carbon models, commonly at least one parameter describing the carbon turnover or the pool sizes gets calibrated to fit the field measurements (Benbi & Richter, 2002). In this study, no model parameter was optimized to the field data except for the initial value, instead the CCB model was fitted to the carbon turnover of incubation experiments, including organic amendments, roots and stubbles, with substrate-specific k_{fom} and η values. The modelling of the respiration curves showed overall good results (Table 3) only for sorghum stubble and winter wheat stubble the RMSE was slightly higher, which can be caused by fluctuating respiration curves. Uncertainties arise from the incubation data for green rye, since it is sowed every year on the field site but no incubation data for the stubble and roots of green rye were available. Instead, the incubation results of winter wheat were used, which are assumed to be the most similar to green rye and do not differ in chemical properties vital from green rye (Edmisten et al., 2008).

Further uncertainty can arise from the variability of the organic amendments applied on the field site. The physical and chemical properties for the organic amendments vary over the time, depending on the batch, while the CCB model uses constant parameters, which can lead to an over or underestimation of dry mass, C and N content. The comparison of the average chemical parameters of the organic amendments applied to the field (C1) and those derived from the laboratory (C2) vary only slightly. Moreover, for two treatments the chemical parameters derived from incubation are not within the standard deviation of the field values (Figure 4). Also, the RMSE for the modelled SOC values does not show big differences between methods C1 and C2, and for the here considered field trial the chemical properties of the organic substrates received from the incubation experiments can be used to model the field trial with good results.

The model outcome of the CCB slightly underestimates the SOC loss of the control treatment, but the results are still within the standard deviation of the observed Corg values and the rRMSE with 5.87 is in a good range. The separate implementation of roots and stubble in the CCB and the parameterization of their dynamics in the laboratory enable the observation of the influence of roots, stubble and organic fertilizers on the SOC dynamics in the field in much greater detail. Levavasseur et al. (2020) used I_{ROC} values to parametrize the AMG model, with overall good results except for the control treatment, their explanation is the inappropriate allometric coefficients for roots. The here presented methods R1 & R2 were explicitly tested on treatments

TABLE 5 RMSE [g/kg] of the CCB output (Corg) using the mean dry matter content and carbon content of organic amendments from the field trial (C1) and the incubation experiment (C2), residual mass calculate with method R2, initialization with ME

	FYM	SLY	DG A	DG B	DGC	DG D-s	DG D-l
RMSE C1	0.584	0.401	0.401	0.366	0.429	0.446	0.511
RMSE C2	0.600	0.409	0.406	0.375	0.425	0.456	0.503

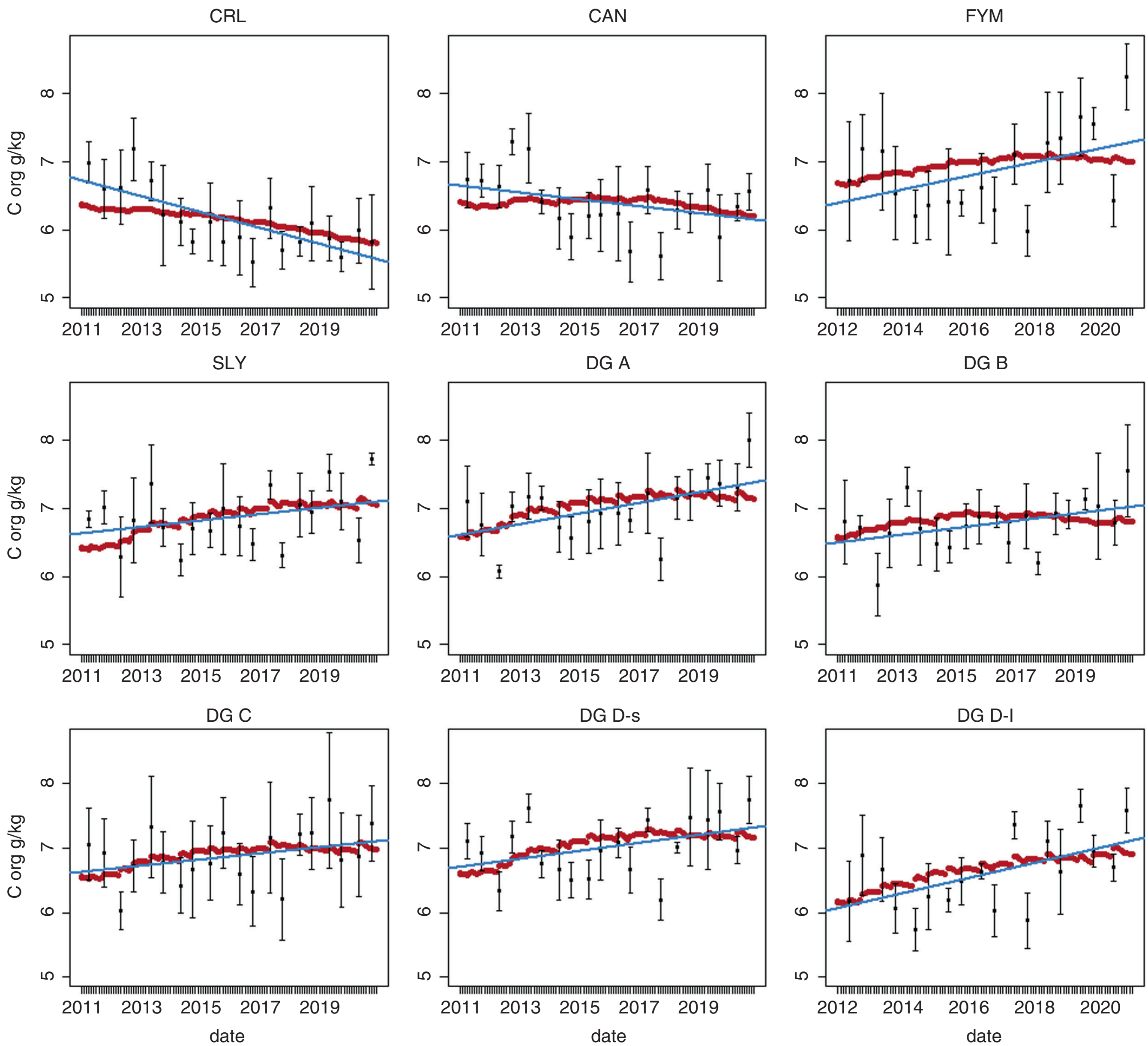

FIGURE 6 Mean measured Cog (markers) with *SD* ($N = 4$, 0–30 cm), CCB simulation (red line), CCB initialized with ME for each treatment, parametrization of residues R2 and chemical properties from incubation experiments (C2), regression (blue line). CAN, mineral fertilizer; CRL, control; DG, digestates; FYM, farm yard manure; l, liquid fraction; s, solid fraction; SLY, slurry

without the influence of organic amendments, which lead to an improved model accuracy and RMSE values which are smaller than the *SD* of the observed Corg values. Nevertheless, the observed data still indicate a linear trend, which is because the short period of the field trial and a longer period would lead to more pronounced dynamics. The CRL and the CAN treatments receive no addition of organic amendments, and both treatments show a decrease in Corg and Nt. The calculated amounts of stubble and roots do not vary significantly across treatments. Hence, rise in Corg for the treatments with the addition of organic amendments depends mainly on the input of Corg throughout the amendments and is not caused by the increase in net primary production and, therefore, more residues. The CAN treatment has the highest yields amongst others but still shows a decrease in Corg; Maltas et al. (2018) found similar results in their research, where the increase in crop does not induce a significant increase in Corg. Furthermore, the statistical analysis of the yields shows that there are only significant differences in the yield between the treatments, of winter rye between the CRL and some treatments with organic

Treatment	RMSE SOC	*SD* Corg	rRMSE SOC	RMSE SON	*SD* Nt	rRMSE SON
CTR	0.361	0.416	5.87	0.077	0.054	13.35
CAN	0.422	0.359	6.62	0.073	0.053	12.25
FYM	0.600	0.537	8.76	0.98	0.064	14.96
SLY	0.409	0.345	5.96	0.081	0.048	12.52
DG A	0.406	0.349	5.81	0.077	0.048	11.64
DG B	0.375	0.375	5.54	0.074	0.063	11.66
DG C	0.425	0.587	6.17	0.065	0.059	10.12
DG D-s	0.456	0.350	6.48	0.072	0.053	10.90
DG D-l	0.503	0.371	7.61	0.095	0.043	14.99

TABLE 6 RMSE [g/kg] and rRMSE (%) for the modelled treatments with CCB and the mean (*N* = 4) observation of the treatments, mean standard deviation (*SD*) for Corg and Nt measurements (*N* = 4)

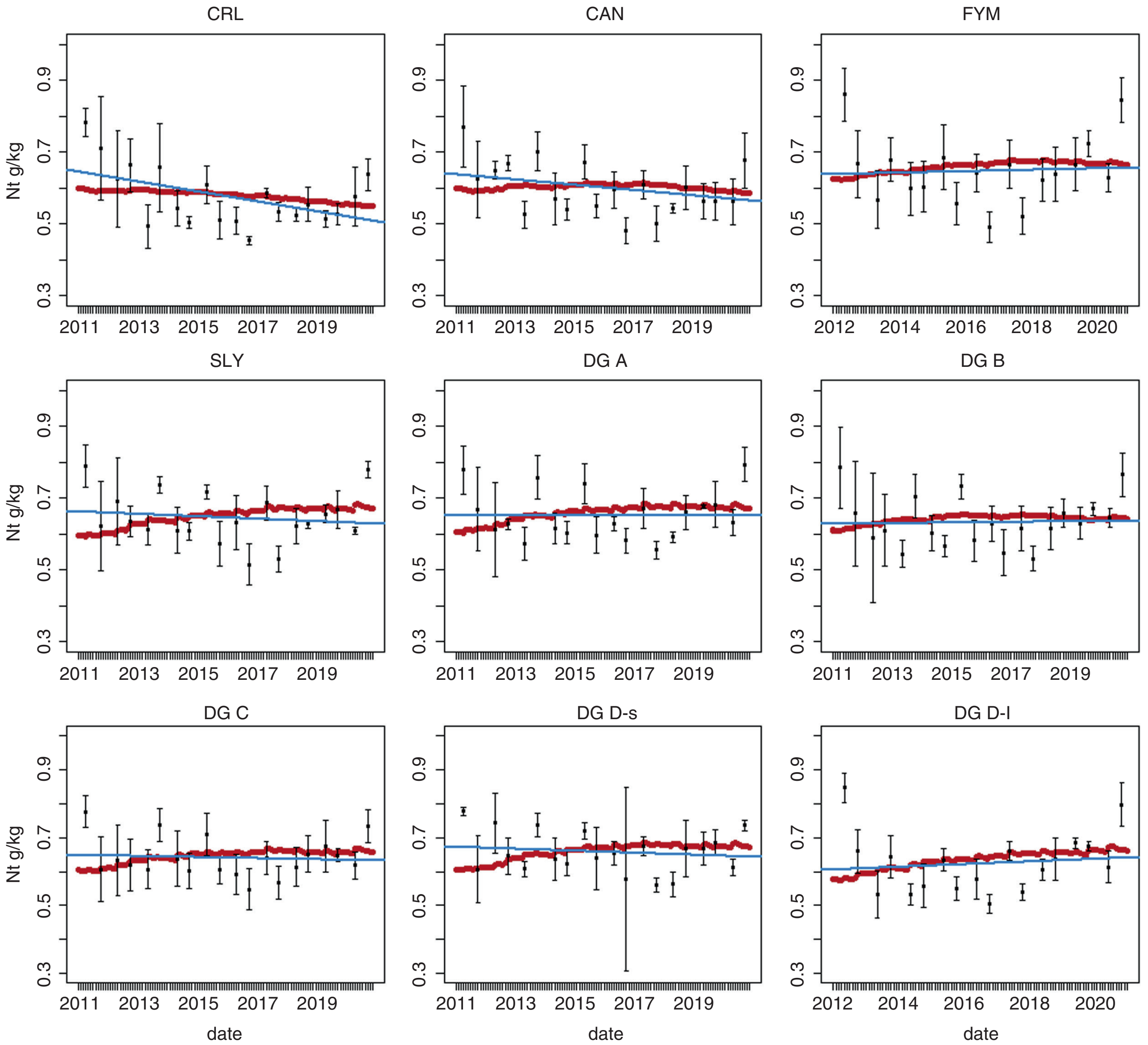

FIGURE 7 Mean measured Nt (markers) with *SD* (*N* = 4, 0-30 cm), CCB simulation (red line), initialized with ME for each treatment, parametrization of residues with R2, and chemical properties from incubation experiments (C2), regression (blue line). CAN, mineral fertilizer; CRL, control; DG, digestates; FYM, farm yard manure; l, liquid fraction; s, solid fraction; SLY, slurry

amendments. Most likely, the field trial needs to be continued for several years to observe significant effects.

Overall, the modelled SOC values show a good fit (Figure 6) with rRMSE between 5.8% and 8.7%, which is comparable to other studies (Begum et al., 2017; Franko et al., 2021; Levavasseur et al., 2020). Furthermore, the RMSE and the mean *SD* of the observed Corg values are in a comparable range; thus, the measuring errors and the variability of the plots are in the same scale as the model error. The reason why the FYM and DG C-l treatment shows a higher rRMSE compared with other treatments could be because of the optimization to the incubation data where one incubation batch could not be modelled because the CCB model reached its parameter limits since its mineralization was too low. Therefore, incubation experiments should be conducted on different batches of organic material to cover their variability, owing to the composition of parent material, the processes in gas plants and other influencing factors. Furthermore, the parameter limits could be extended to model more resilient substrates in the incubation experiment. While for the modelled SON values the rRMSE is above 10% and the RMSE ≈ 0.01 [g/kg] for each treatment, the parameters might not be as easy transferable, since the SON calculation in the CCB model depends on the dynamics of carbon turnover and the mineral nitrogen pool is not considered. Furthermore, the Nt data show high variability; the first data points had to be adjusted due to the change in analytics, which can lead to inaccuracies. Further studies with N incubations as a basis could be a solution to improve the model accuracy.

5 | CONCLUSIONS

This study successfully demonstrated how model parameters and chemical properties derived from incubation experiments can be transferred to model field experiments without many adaptations or optimization of parameters to the field site. Those site-independent parameters are particularly important for scenario calculations and regionalization and can help to predict the behaviour of organic amendments under field conditions. They are transferable to other sites with different environmental conditions, because the climate and soil functions implemented in the model can be adapted to the new sites. Also, more uncommon substrates could be analysed with incubation experiments and combined with model predictions, be a cheaper and less time intense approach to evaluate the long-term behaviour of selected substrates compared with field experiments, while the N dynamics which rely on the C dynamics are not as easily transferable to the field site and need further investigation.

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DATA AVAILABILITY STATEMENT

Data available on request from the authors

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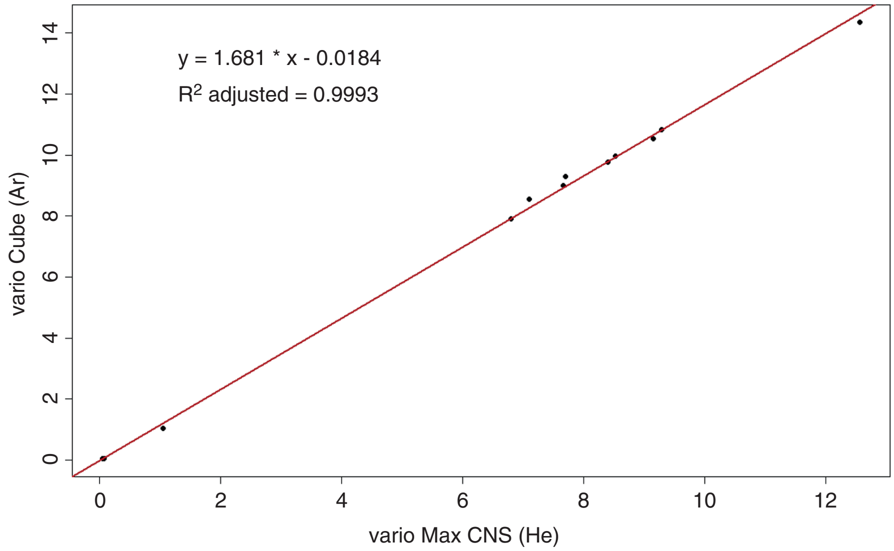
APPENDIX 1

FIGURE A1 Regression between the two carrier gases (Helium and Argon) used to analyse the total Nitrogen content



APPENDIX 2

Experimental set-up for the organic fertilizers

Chemical analysis

Bulk soil was collected from the upper layer of an arable loamy sand at Berge (Germany, Brandenburg). Before use, the soil was air-dried and sieved <2 mm. The C and N contents of the soil were 0.71% and 0.06% of dry matter (DM), respectively. The pH value (determined in 0.01 mol CaCl2) was 5.7. Digestates were taken from several agricultural biogas plants in the Brandenburg area. Dry matter (DM) content was determined gravimetrically after drying the soil at 105°C, and organic dry matter (ODM) content was calculated as the loss of weight between 105 and 550°C. The concentration of total nitrogen in the fresh material was determined using the Kjeldahl method. The Corg content was measured in lyophilized grounded samples using an elemental analyser (Elementaranalysator vario C, Elementar Analysensysteme GmbH, Hanau, Germany).

Experimental design

40 g of soil were mixed with digestate, in a quantity to add 140 mg of Corg. Mixtures of soil and substrate were placed in 100 ml incubation vessels, and moisture content was adjusted to 60% maximum water-holding capacity (WHC). The CO_2 production was determined using a respirometer (CarbO2Bot, prw electronics, Germany). Hourly respiration was measured by the change in conductivity as a result of CO_2 absorption in 0.6 M KOH. During incubation, vessels were opened regularly in order to maintain adequate oxygen concentrations. Empty vessels were used as blanks. Vessels filled with soil only served as a control variant. The experiment was conducted for 140 & 252 days at a temperature of 20 ± 1°C. All variants were replicated sixfold. Based on the amount of CO_2 C evolved in each substrate, the cumulative amount of total evolved C was calculated for the entire incubation period. In order to calculate the CO_2 C release out of the organic substrates, the CO_2 C values of the control soil were subtracted from the mixed soil sample CO_2 C values.

Experimental set-up for the roots and stubbles

The description of the experimental set-up was taken from Mewes (2017).

Set-up of the incubation study

Apparent course of EOC-induced CO2 release of 40 plant residues was measured in two incubation experiments under controlled laboratory conditions. The second incubation experiment contained pea residues and all fine roots. In both experiments, straw was included as standard residue. This should allow comparing the results obtained by the two separate experiments. The plant residues were homogenously mixed at a rate of 400 mg EOC per 100 g soil. Then, the soil was filled into small tubes (soil columns) at a bulk density of 1.1 g cm-3. Soil columns with and without plant residues were prepared with 3 and 5 replications, respectively. Contrary to previous investigations, no mineral N was added, taking limited nitrogen availability into account. Incubation temperature was 22°C. At the start of incubation, soil water content was adjusted to 20.8 ml H_2O per 100 g soil, expressing 50% of water-holding capacity (ISO 16072). After 301 days of incubation, the mineral N concentration in each soil column was determined in an extract by spectrometric measurement (DIN 19746).

Measurement of CO_2 release during the incubation study

The soil columns were placed in closed jars with 100 ml 0.15 M NaOH at the bottom, absorbing the mineralized CO_2, which was released from the soil columns between two measuring dates. The absorbed CO_2 was precipitated as $BaCO_3$ through the addition of 10 ml 1.5 M $BaCl_2$ solution and measured by titration with 0.3 M HCl and phenolphthalein as indicator. Measurement dates were 1, 3, 7, 14, 21, 35, 56, 77, 98, 120, 162, 217 and 301 days after start of incubation. The apparent decomposition of plant residues was calculated as difference between evolved CO_2 from soil columns with and without plant residue. The course of EOC-induced CO_2 release was calculated by summing up the EOC-induced CO_2 release between two subsequent measurement dates.

APPENDIX 3

TABLE A1 Ratio of coarse roots to fine roots for crops, received from field experiments (Höcker, 2017)

Crop	Coarse roots [%]	Fine roots [%]
Maize	58	42
Sorghum	55	45
Green rye	30	70

APPENDIX 4

TABLE A2 Mean calculated masses [t*ha^{-1}] and standard deviation of stubble (st) and roots (rt) calculated by the CCB model with the method R2, from 2011 (*2012) to 2020

Treatment	Winter rye st	Winter rye rt	Maize st	Maize rt	Sorghum st	Sorghum rt
CRL	0.773 ± 0.71	2.17 ± 1.99	1.462 ± 0.71	2.093 ± 1.02	2.002 ± 1.01	3.802 ± 1.827
CAN	2.423 ± 0.85	6.807 ± 2.38	1.996 ± 1.01	2.857 ± 1.45	3.540 ± 1.87	6.403 ± 3.39
FYM*	1.92 ± 7.7	5.4 ± 2.15	2.000 ± 0.8	2.863 ± 1.15	3.071 ± 1.75	5.554 ± 3.17
SLY	2.332 ± 0.78	6.554 ± 2.2	2.358 ± 0.97	3.375 ± 1.39	3.493 ± 1.86	6.317 ± 3.37
DG A	1.947 ± 0.73	5.470 ± 2.08	2.273 ± 0.88	3.253 ± 1.25	2.945 ± 1.57	5.326 ± 2.84
DG B	1.719 ± 0.72	4.829 ± 2.03	2.235 ± 0.96	3.198 ± 1.37	3.095 ± 1.57	5.597 ± 2.84
DG C	1.964 ± 0.7	5.519 ± 1.98	2.466 ± 0.68	3.529 ± 0.98	3.118 ± 1.74	5.64 ± 3.14
DG D-s	2.247 ± 0.63	6.315 ± 1.78	2.292 ± 0.69	3.280 ± 0.98	3.456 ± 1.96	6.25 ± 3.54
DG D-l*	1.383 ± 0.816	3.887 ± 2.292	2.031 ± 0.49	2.906 ± 0.7	2.450 ± 1.02	4.43 ± 1.84