Predicting long-term organic carbon dynamics in organically-amended soils using the CQESTR model

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Abstract

Purpose The CQESTR model is a process-based carbon model recently developed to simulate soil organic matter (SOM) dynamics, and uses readily available or easily measurable input parameters. The current version of CQESTR (v. 2.0) has been validated successfully with a number of datasets from agricultural sites in North America, but still needs to be tested in other geographic areas and soil types under diverse organic management systems.

Materials and methods We evaluated the predictive performance of CQESTR to simulate long-term (34 years) soil organic C (SOC) changes in a SOM-depleted European soil either unamended or amended with solid manure, liquid manure, or crop residue.

Results and discussion Measured SOC levels declined over the study period in the unamended soil, remained constant in the soil amended with crop residues, and tended to increase in the soils amended with manure, especially with solid manure. Linear regression analysis of measured SOC contents and CQESTR predictions resulted in a correlation coefficient of 0.626 ($P < 0.001$) and a slope and an intercept not significantly different from 1 and 0, respectively (95% confidence level). The mean squared deviation and root mean square error were relatively small. Simulated values fell within the 95% confidence interval of the measured SOC, and predicted errors were mainly associated with data scattering.

Conclusions The CQESTR model was shown to predict, with a reasonable degree of accuracy, the organic C dynamics in the soils examined. The CQESTR performance, however, could be improved by adding an additional parameter to differentiate between pre-decomposed organic amendments with varying degrees of stability.

Keywords C sequestration • Crop residue • Manure • Modeling • Organic amendment • Soil organic matter

1 Introduction

Soil organic matter (SOM) plays a paramount role in soil fertility and quality by providing a number of benefits such as increasing soil biodiversity, improving soil structure, water and plant nutrient retention, and protection from soil erosion and degradation (Stevenson 1994; Magdoff and Weil 2004). Consequently, SOM plays a very important role in agronomic production and food security. It has been estimated (Lal 2006) that increasing the SOM pool by 1 Mg ha⁻¹ y⁻¹ might increase food production up to 40 million Mg y⁻¹ in developing countries, which represents an important contribution to meet the increasing demand of the growing population (Lal 2009). Furthermore, SOM has an important role in climate change, since small changes in this large terrestrial C stock, about twice as large as that in the atmosphere, can have significant impacts on atmospheric CO₂ concentrations (Smith et al. 2008; Schmidt et al. 2011).

Strategies to enhance, or at least to preserve the SOM stocks and its related environmental functions include applying organic amendments, growing biomass in situ, minimizing decomposition, decreasing leaching, and reducing erosion (Lal 2009). In particular, crop residue and animal manure have long been used as soil organic amendments (Senesi and Plaza 2007; Senesi et al. 2007). These strategies are especially important in southern Europe, where the decline of SOM represents one of the most serious threats facing many arable lands (CEC 2002; Jones et al. 2004; Fernández et al. 2007).

Carbon models designed to simulate long-term SOM dynamics have become important tools to assess the sustainability of agricultural systems, as well as changes in soil fertility, quality, and C sequestration following soil management change scenarios. The most sophisticated and successful models developed and evaluated during the past three decades (e.g., NCSOIL, RothC, and CENTURY) feature several SOM pools with different turnover rates, which need to be quantified to initiate the simulations (Molina et al. 1983; Jenkinson et al. 1987; Parton et al. 1987; Smith et al. 1997). However, the initial levels of these various SOM pools are difficult, if not impossible, to measure directly (Parton et al. 1996). Unlike other SOM models, the recently developed CQESTR model (Rickman et al. 2001) requires unambiguous input parameters which are readily available or easily measurable. The information needed includes basic weather and tillage data, the aboveground and belowground crop biomass additions, the amount of organic amendments applied, N content of crop residues and organic amendments, and some basic soil data such as the initial SOM content, bulk density, texture, and drainage class (Rickman et al. 2001; Liang et al. 2009).

The current version of CQESTR (2.0) has been validated successfully with long-term datasets from a large number of agricultural sites across North America under diverse climate, soil types, and crop and residue management (Liang et al. 2009). To date, however, the performance of the CQESTR model has never been

tested in the typical SOM-depleted soils of southern Europe. Further, there is no available data in the literature on the ability of CQESTR to predict SOM changes as affected by different organic amendments.

The objective of this work was to evaluate and discuss the predictive performance of the CQESTR model to simulate long-term organic matter dynamics in a SOM-depleted European soil either unamended or amended with solid manure, liquid manure, or crop residues under humid subtropical conditions.

2 Materials and methods

2.1 Site description and long-term datasets

The datasets used in this model evaluation exercise were collected from a long-term experiment conducted at the research and outreach farm of the University of Bologna near Cadriano (Bologna), northern Italy (44°33' N, 11°24' E; 31 m above sea level). The experiment was started in 1966 on a site that had been under arable rotation for 8 years and meadow for 3 years. The site is characterized by a humid subtropical climate with an average annual rainfall of 714 mm and an average annual temperature of 13.0 °C over the study period (1966-2000). The soil is a well-drained sandy clay loam (560 g kg⁻¹ sand, 160 g kg⁻¹ silt, and 280 g kg⁻¹ clay) Haplic Calcisol (IUSS Working Group WRB 2006). In 1966, the 0-20 cm soil layer had a bulk density of 1.16 Mg m⁻³, pH of 6.9, traces of carbonates, 7.7 g kg⁻¹ of total organic C, 1.1 g kg⁻¹ of total N, and a C/N ratio of 7.0.

The experimental design was a split plot arrangement with four replicates. All plots were in a corn (*Zea mays* L.)-winter wheat (*Triticum aestivum* L.) rotation. The main plot treatments were four types of organic amendment: control without any amendment, cattle manure, cattle slurry, and crop residue (either wheat straw or corn stalk). The subplot treatments were four levels of mineral N fertilizer: 0, 100, 200, and 300 kg N ha⁻¹. The organic amendments were applied every year in early October at rates of either 7.5 Mg ha⁻¹ after corn crops or 6.0 Mg ha⁻¹ after wheat crops, and immediately buried by moldboard plowing to a depth of 40 cm.

From 1972 to 2000, soil samples representative of the plow layer were taken randomly from each plot soon after harvest every year. The samples were air-dried, crushed, and passed through a 2-mm sieve. Total soil organic C (SOC) content was determined on 0.5-mm ground soil samples by oxidation with K₂Cr₂O₇ and H₂SO₄ at 150°C for 30 min followed by titration with FeSO₄ (Lotti and Galoppini 1967).

More detailed descriptions of the site, experimental design, sampling and analysis methods, main chemical properties of organic amendments and soils, and crop yields were reported previously (Triberti et al. 2008). The average organic C contents of the applied cattle manure, cattle slurry, wheat straw, and corn stalk were 331, 390, 328, and 326 g kg⁻¹, with total N contents of 26.8, 28.1, 4.7, and 7.0 g kg⁻¹, and C/N ratios of 12.4, 13.9, 69.8, and 46.6, respectively. Only the treatments with no mineral N fertilization were used in the model evaluation exercise, since mineral N fertilization was beyond the scope of our objectives and did not significantly affect total SOC content.

2.2 Model description

The CQESTR model is a process-based soil organic C balance model that computes the rate of biological decomposition of organic amendments or crop residue as they convert to SOM or SOC during oxidation by microbial metabolism (Liang et al. 2009; Rickman et al. 2001). The structure and underlying assumptions of the CQESTR model (version 2.0) are described in detail elsewhere (Liang et al. 2009). Briefly, total SOM content is calculated on a daily time-step as the sum of stable SOM content plus crop residue and organic amendment

contents. The organic material decomposition is a three phase process. After each residue placement in the soil, decomposition occurs in two phases. Phase I is a rapid phase covering the first 1000 cumulative degree-days (CDD), approximating the oxidation of readily metabolizable substrate. Phase II is a slow decomposition phase representing oxidization of more recalcitrant materials. After 15000 CDD when Phase II is complete, the composted residue is transferred to the stable SOM pool (Phase III). The amount of stable SOM, crop residue, or organic amendment remaining at a given thermal-time, R , is calculated by the exponential formula:

$$R = R_i \exp(k \cdot fN \cdot fW \cdot fB \cdot fX \cdot fD \cdot CDD) \text{ Eq. [1]}$$

where R_i is the amount of stable SOM or residue at the previous time step (same units as R ; e.g., dry weight per unit area), k is a universal decomposition rate constant ($^{\circ}\text{C}^{-1} \text{ d}^{-1}$), fN is a N content factor, fW is a water availability factor, fB is a biomass type factor, fX is a soil texture factor, fD is a soil drainage factor, and CDD or cumulative degree-days is the summation of daily air temperatures greater than a base value of 0°C . The value of k is $-0.0004^{\circ}\text{C}^{-1} \text{ d}^{-1}$ for the stable SOM pool or any organic material independently of its nature and location relative to the soil (either on the surface or buried); fN (unitless) is 0.8354, for stable SOM or organic materials with N content less than 0.55%, and 1.2635, 1.9770, and 3.4040 for organic materials with N contents from 0.55 to 1.0%, from 1.0 to 1.5%, and more than 1.5%, respectively; the value of fW (unitless) is 0.21, 0.32, 0.80, and 1.00 for residue on the soil surface under dry condition, residue on the soil surface under wet condition, buried organic matter under dry condition, and buried organic matter under wet condition, respectively; and fB value (unitless) is 1.0, 0.35, 0.60, and 0.0061 for shoot residue, root biomass, pre-decomposed organic matter (i.e., organic amendment), and stable SOM, respectively; fX (unitless) is calculated using a linear equation in which the independent variable corresponds to a numeric texture code assigned by the United States Department of Agriculture (USDA) soil texture class; and fD (unitless) is calculated using a function of the average number of days per year of soil saturation associated with the USDA drainage class. After 1000 CDD , a single fN value of 0.8354 is assigned to all organic residues and amendments. After 15000 CDD , all residues and amendments are considered stable SOM and the fW and fB values are modified accordingly.

2.3 Input data

Input data required to run the CQESTR model include (a) average monthly mean air temperature, (b) average monthly precipitation, (c) aboveground and belowground crop biomass, (d) root distribution characteristics of crops, (e) rates of organic amendments, (f) percentages of crop residues and organic amendments buried and left on the soil surface after tillage, (g) dates of amendment applications and tillage operations, (h) depth of tillage, (i) initial N contents of crop residues and organic amendments, (j) soil texture class, (k) soil drainage class, (l) number and thickness of soil layers, (m) initial soil bulk density, and (n) initial SOM content of each layer. For the study site, all of this information was available from experimental records (Triberti et al. 2008), apart from the belowground crop biomass, root distribution characteristics, amount of organic residues left on the soil surface after harvest and tillage, and initial soil SOM content for the top 40 cm at the beginning of the experiment in 1966. Belowground crop biomass and root distribution characteristics were obtained from the CQESTR database, which was based on a large number of root development experiments reported in the literature (Liang et al. 2009). Aboveground crop biomass removal after harvest was estimated at 85% and the percentage of crop residue and organic amendment left on the soil surface after incorporation into soil by moldboard plow was estimated at 10%. Finally, the initial SOM content was set to the value that resulted in the

best model fits by iteratively varying this parameter until the sum of the residual differences between the observed and CQESTR-estimated SOM contents for all the treatments was minimized.

2.4 Evaluation of model performance

The predictive accuracy of CQESTR was evaluated by means of linear regression, correlation coefficient, (r) and root mean square error (RMSE) between the model-based estimations and measured values of SOC contents. The significance of RMSE was assessed by comparison with the RMSE obtained assuming a deviation corresponding to the 95% confidence interval of the measurements (Smith et al. 1997). To gain further insight into the CQESTR model performance, the mean squared deviation (MSD) was also calculated and partitioned into three components, namely squared bias (SB), nonunity slope (NU), and lack of correlation (LC), as proposed by Gauch et al. (2003). Specifically, the MSD was calculated as $\sum(X_n - Y_n)^2/N$, where N is the number of observations and X and Y are the predicted and observed values, respectively, for $n = 1, 2, \dots, N$; SB, which measures the inequality between the arithmetic means of the X and Y values ($\bar{X}$ and $\bar{Y}$, respectively), was calculated as $(\bar{X} - \bar{Y})^2$; NU, which measures the degree of rotation of the regression line, was calculated as $(1 - b)^2(\sum x_n^2/N)$, where b is the slope of the least-square regression of Y on X and x_n is $X_n - \bar{X}$; and LC, which measures the scatter, was calculated as $(1 - r^2)(\sum xy_n^2/N)$, where r^2 is the coefficient of determination and y_n is $Y_n - \bar{Y}$.

3 Results and discussion

3.1 Soil organic C dynamics

Soil organic C dynamics as affected by the organic treatments are summarized in Fig. 1 and Table 1. Briefly, organic C levels decline with time in the unamended soil, remain constant in the soil amended with crop residues, and tend to increase in the soils amended with cattle manure, especially with solid manure (Fig. 1). Thus, averaged over the study period and after 34 years, SOC contents increase in the order unamended soil, soil amended with crop residues, soil amended with liquid manure, and soil amended with solid manure (Table 1).

The decline of SOC in the unamended soil is consistent with many other long-term studies (e.g., Odell et al. 1984; Rasmussen et al. 1998; Kapkiyai et al. 1999; Nardi et al. 2004; Lugato et al. 2007) and may be attributed to the termination of centuries long manure application practice, the minimal crop residue returned to the soil, and the physical disturbance associated with the increased depth of tillage at the beginning of the experiment. The latter accelerates the turnover of soil aggregates, increases the exposure of aggregate-associated SOM to decomposition, and inhibits the formation and stabilization of recalcitrant organic compounds within microaggregates (Paustian et al. 2000). Similar findings of higher organic C contents in organically-amended soils with respect to unamended soils are also widely reported in the literature (e.g., Ohno et al. 2005; Sleutel et al. 2006; Bhattacharyya et al. 2007; Lugato et al. 2007; Zhao et al. 2009). The larger accumulation of SOC with the application of solid manure compared to liquid manure and especially to crop residues may be related to the different stability of their organic constituents against biological mineralization. Other studies also suggested that cattle manure is richer in C compounds with resistant molecular structures than crop residues, whereas liquid manure is richer in fresh, readily degradable substances than solid manure (Nardi et al. 2004; Monaco et al. 2008; Bertora et al. 2009).

3.2 CQESTR performance

Organic C dynamics in the soils examined as estimated by CQESTR is shown in Fig. 1. Except for the soil amended with solid manure at the end of the study period, the CQESTR model prediction fits very well the experimental datasets. In fact, the residual differences between the observed and model-predicted values are very small, except for the soil amended with solid manure at the end of the experiment (Table 1).

In general, the CQESTR-estimated SOC contents averaged over the study period and after 34 years are in agreement with the trends of the measured values, and increase in the order unamended soil, soil amended with crop residues, and soils amended with manure (Table 1). However, the actual organic C contents of the soil amended with solid manure are markedly greater than those of the soil amended with liquid manure, whereas the CQESTR estimations are similar (Table 1). These results indicate that the CQESTR model can hardly distinguish between the two manure treatments, even though the organic stability of solid manure is known to be higher than that of liquid manure and different priming effects could be expected (Nardi et al. 2004; Monaco et al. 2008; Bertora et al. 2009). This is because both solid manure and liquid manure contain more than 1.5% of N and both materials are considered by CQESTR as pre-decomposed organic matter, so the N content factor, the biomass type factor, and obviously the rest of the CQESTR factors are the same for both materials. Perhaps insertion of a new parameter such as lignin content of the manure into the model could improve the CQESTR-predicted values. However, there are limited long-term experiments available worldwide with both liquid and solid manure with which to calibrate and validate the model. The slightly higher estimations of organic C contents for the soil amended with solid manure are only due to the slightly higher crop yields obtained with this treatment (Triberti et al. 2008) and, therefore, the slightly higher crop residues left on the soil surface.

Linear regression analysis of actual measured and CQESTR-predicted values results in an r value of 0.626 ($P < 0.001$), an intercept of -0.86 not significantly different from 0, a slope of 1.15 not significantly different from 1 at the 95% confidence level (Fig. 2), and a random distribution of residuals (Fig. 3). In general, these results indicate that CQESTR simulates long-term organic C dynamics reasonably well under the humid subtropical conditions of this study. Previous regression analysis for long-term data from across North America (Liang et al. 2009), however, resulted in a higher r (0.975), possibly due to the larger number (306) of pairs of predicted and measured data analyzed and to the much wider range of SOM examined (7.3 to 57.9 g kg⁻¹). When regression analysis is performed separately for the individual treatments in this study, the r values between simulated and observed SOC are also highly significant ($P < 0.001$), except for the unamended soil, but the intercepts and slopes are far from 0 and 1, respectively (Table 2, Fig. 2). These results may be attributed to the narrow spread of paired observed and estimated data (Smith et al. 1997) and suggest that linear regression analysis is not useful for evaluating the model performance in simulating the individual datasets, especially that of the unamended soil because of the limited changes measured in SOM.

The RMSE for the individual datasets and the complete range of data examined varies between 8.3 and 11.6 (Table 2), and are very close to the smallest values reported by Smith et al. (1997) for a large number of datasets using other successful SOM models. The RMSE values are in any case less than the corresponding RMSE_{95%} values, indicating that the simulated values fall within the 95% confidence interval of the measurements (Smith et al. 1997). Similarly, the MSD values (< 0.5) are very small (Table 2), even smaller than the values commonly found in comparable studies (Leite et al. 2009; Gollany et al. 2010). With the only exception of the soil amended

with crop residues, the highest contributing component of MSD is the LC (Table 2). When all the data are pooled together, the highest contributing component of MSD is also the LC (Fig. 2), which indicates that prediction errors can be mainly associated with data scattering.

3.3 Conclusions

The CQESTR model, with an acceptable degree of accuracy, predicted the long-term organic C dynamics of a SOM-depleted soil as affected by solid manure, liquid manure, and crop residues under humid subtropical conditions. The results obtained also indicated that model performance could be improved by capturing the composition difference and stability degrees for different pre-decomposed organic amendments with variant C/N ratios and contents of N, lignin, and humic-like substances. This could be achieved by including other categories for the biomass type factor, which requires long-term experimental datasets with various types of manures. Further research will be needed for calibration and validation of a modified model with new parameters.

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Table 1 Means over the entire study period (1972-2000) and final values after 34 years (2000) of measured and CQESTR-estimated organic C contents of soils unamended (UN) and amended with solid manure (SM), liquid manure (LM), and crop residues (CR), and the corresponding residual differences

	1972-2000			2000		
	Measured organic C (g kg ⁻¹)	Estimated organic C (g kg ⁻¹)	Residual difference (%)	Measured organic C (g kg ⁻¹)	Estimated organic C (g kg ⁻¹)	Residual difference (%)
UN	5.12	5.36	-4.8	5.21	4.94	+5.2
SM	6.62	6.24	+5.8	8.55	6.49	+24.0
LM	6.07	6.24	-2.8	6.76	6.49	+4.1
CR	5.81	5.65	+2.8	6.12	5.42	+11.5

Table 2 Intercept and slope ($\pm$ margin of error at the 95% confidence level) of the linear regression, correlation coefficient (r), root mean square error (RMSE), RMSE corresponding to the 95% confidence interval of the measurements (RMSE_{95%}), mean squared deviation (MSD), squared bias (SB), nonunity slope (NU), and lack of correlation (LC) between measured and CQESTR-estimated organic C contents of soils unamended (UN) and amended with solid manure (SM), liquid manure (LM), and crop residues (CR)

	Intercept	Slope	r	RMSE	RMSE _{95%}	MSD	SB	NU	LC
UN	5.73($\pm$ 3.92)**	-0.11($\pm$ 0.73)	-0.062	11.6	30.9	0.353	0.061	0.078	0.215
SM	-8.70($\pm$ 7.31)*	2.46($\pm$ 1.17)***	0.638***	10.2	35.8	0.453	0.146	0.060	0.247
LM	-6.51($\pm$ 6.76)	2.02($\pm$ 1.08)***	0.592***	8.5	26.3	0.266	0.029	0.028	0.208
CR	20.52($\pm$ 7.70)***	-2.61($\pm$ 1.36)***	-0.602***	11.2	33.4	0.421	0.027	0.205	0.188

*, **, and ***, significant at the 0.05, 0.01, and 0.001 probability level, respectively.

FIGURE CAPTIONS

Fig. 1 Measured (symbols) and CQESTR-predicted (lines) total organic C contents in the 0-40 cm layer of soils unamended and amended with solid manure, liquid manure, and crop residues from 1966 to 2000. Bars are standard errors of the mean ($n = 4$).

Fig. 2 Scatter plots and linear regressions of measured versus CQESTR-predicted soil organic C contents of soils unamended (UN) and amended with solid manure (SM), liquid manure (LM), and crop residues (CR). Superimposed is the linear regression line of all measured versus CQESTR-predicted soil organic C contents for the four treatments and the associated slope and intercept ($\pm$ margin of error at the 95% confidence level), correlation coefficient (r), root mean square error (RMSE), RMSE corresponding to the 95% confidence interval of the measurements (RMSE95%), mean squared deviation (MSD), squared bias (SB), nonunity slope (NU), and lack of correlation (LC); ***, significant at the 0.001 probability level.

Fig. 3 Residuals versus CQESTR-predicted soil organic C contents of unamended soil (UN) and soils amended with solid manure (SM), liquid manure (LM), and crop residues (CR).