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Simulating soil organic matter with CQESTR (v. 2.0): Model description and validation against long-term experiments across North America

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ABSTRACT

Soil carbon (C) models are important tools for examining complex interactions between climate, crop and soil management practices, and to evaluate the long-term effects of management practices on C-storage potential in soils. CQESTR is a process-based carbon balance model that relates crop residue additions and crop and soil management to soil organic matter (SOM) accretion or loss. This model was developed for national use in U.S and calibrated initially in the Pacific Northwest. Our objectives were: (i) to revise the model, making it more applicable for wider geographic areas including potential international application, by modifying the thermal effect and incorporating soil texture and drainage effects, and (ii) to recalibrate and validate it for an extended range of soil properties and climate conditions. The current version of CQESTR (v. 2.0) is presented with the algorithms necessary to simulate SOM at field scale. Input data for SOM calculation include crop rotation, aboveground and belowground biomass additions, tillage, weather, and the nitrogen content of crop residues and any organic amendments. The model was validated with long-term data from across North America. Regression analysis of 306 pairs of predicted and measured SOM data under diverse climate, soil texture and drainage classes, and agronomic practices at 13 agricultural sites having a range of SOM (7.3–57.9 g SOM kg^{-1}), resulted in a linear relationship with an r^2 of 0.95 ($P < 0.0001$) and a 95% confidence interval of 4.3 g SOM kg^{-1}. Using the same data the version 1.0 of CQESTR had an r^2 of 0.71 with a 95% confidence interval of 5.5 g SOM kg^{-1}. The model can be used as a tool to predict and evaluate SOM changes from various management practices and offers the potential to estimate C accretion required for C credits.

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Abbreviations: CDD, cumulative degree-days; CT, conventional tillage; NT, no-tillage; SOC, soil organic C; SOM, soil organic matter; ST, sweep tillage.

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1. Introduction

Management of soil organic matter (SOM) is critical for sustaining soil productivity and environmental quality. Soil organic matter influences soil physical, chemical, and biological properties and contributes to crop productivity and soil quality (Jenkinson, 1991; Lal, 1997). Soil is also a major pool (1720 Gt) in the cycling of carbon (C) from the atmosphere to the biosphere (Oades, 1988). There is a growing interest in utilizing soil to store C to reduce carbon dioxide (CO_2) levels in the atmosphere, with implications for the greenhouse effect and global warming (Lal et al., 1998; Paustian et al., 1995).

The amount of soil C in an agro-ecosystem is the net result of C input through primary production and deposition by wind or water erosion, C loss via respiration, loss by wind and water erosion, and translocation of dissolved organic C through soil (Campbell et al., 1996; Mertens et al., 2007). The turnover rate of different SOM compounds varies due to complex interactions between chemical, physical, and biological processes in soil. Soil C in its stable form as SOM responds gradually to agricultural management changes. Although changes in SOM have been detected over a short period of time (e.g. 5 years), when significant management change occurs and soil C pools are far from equilibrium (Conant and Paustian, 2002; West and Post, 2002), most SOM changes require a longer time period (e.g. at least 20 years) to be detectable by present analytical methods (Rasmussen et al., 1998). Simulation models can be useful for projecting short- and long-term effects of many factors that control SOM turnover.

Soil carbon models are needed to predict long-term effects of management practices on C accretion in soils and estimate the benefits of alternative management practices in reducing the greenhouse gas emissions and the impact on global warming. One of the first widely used SOM models (Jenkinson and Rayner, 1977; Jenkinson et al., 1991) divided soil C into active, slow and passive pools with different turnover times ($1/k$) (2, 50 and 1980 years). The model developed by Paul and van Veen (1978) and van Veen and Paul (1981) divided plant material into recalcitrant and decomposable fractions and included the concept of physical protection of SOM. They assumed that physically protected SOM has much lower decomposition rate than non-physically protected SOM. The CENTURY model (Parton et al., 1987; Paustian et al., 1992) established a general approach for splitting plant residue into structural and metabolic material as a function of the initial lignin to nitrogen ratio of the material. Parton et al. (1987) suggested that the soil silt plus clay content influences the turnover rate of the active SOM (higher for sandy soils) and the stabilization of active SOM into slow SOM. The NCSOIL model is a subroutine of NCSWAP (Nitrogen and Carbon Cycling in Soil, Water, Air and Plants) model to simulate N and C transformations in the soil (Molina et al., 1983, 1997) with residues defined into various pools ranging from labile to recalcitrant. It is a complex mechanistic model that integrates water flow dynamics, temperature, solute transport, tillage, crop growth, residue effects, and total and tracer N and C transformations (Gollany et al., 2004). The Environment Policy Integrated Climate (EPIC) model is a widely tested and adapted model originally built to quantify the effects of erosion on soil productivity (Williams et al., 1984). Since its inception, EPIC has evolved into a comprehensive agro-ecosystem model capable of simulating the growth of plant species, including crops, native grass and trees, grown in complex rotations and management operations, such as tillage, irrigation, fertilization and liming. Recently, C and N modules were added to EPIC (Izaurralde et al., 2006). The included C and N routines interact directly with soil moisture, temperature, erosion, tillage, soil bulk density, leaching, and translocation functions in EPIC (Izaurralde et al., 2006).

The detailed nutrient cycling models have typically been used to simulate the dynamics of C and N for a growing season, while the SOM models are used to simulate dynamics for longer time periods (i.e. decades). The major shortcoming of the above mentioned models "is that there is no generally acceptable way to determine the different SOM fractions, either chemically or physically, and thus it is impossible to directly measure SOM pools included in the models" (Parton et al., 1996).

The intergovernmental Panel on Climate Change (IPCC) has developed an inventory method that accounts for changes in soil carbon stocks related to changes in land use and/or agricultural management practices (IPCC, 1997). It is a first-order approach using simple assumptions about the effects of land use on carbon stocks, in the form of a series of coefficients based on climate, soil type, disturbance history, tillage intensity, and residue management. The method estimates SOC stocks over the first 20 years following a shift in management, during which the presumably greatest influence occurs (IPCC, 1997).

With the goal of using readily available input data at the field scale, the CQESTR model was developed to simulate the effect of management practices on short and long-term trends of SOM (Liang et al., 2008; Rickman et al., 2001, 2002). CQESTR also can be used to evaluate the environmental impacts of large-scale crop residue removal from agricultural land (Liang et al., 2008). Extensive evaluation of version 1.0 indicated that the model is easy to use and acceptable in predicting C trends in temperate regions with well drained soils (Rickman et al., 2002, 2005). Our objectives were (i) to revise the model, and make the model more applicable for wider geographic areas, including potential international application, by modifying thermal effect and incorporating soil texture and drainage effects, and (ii) to recalibrate the model with six long-term experiments with a range of climate, and drainage and soil texture classes, and validate it for an extended range of soil properties and climate conditions. The current version of CQESTR (v. 2.0) is presented with the necessary algorithms to simulate SOM at field scale.

2. Materials and methods

2.1. *General description of the CQESTR model*

CQESTR, pronounced sequester, a contraction of 'C sequestration' (meaning C storage), has been in continuous development since 2000. It is a process-based model that uses information stored in crop management files associated with the c-factor of the Revised Universal Soil Loss Equation

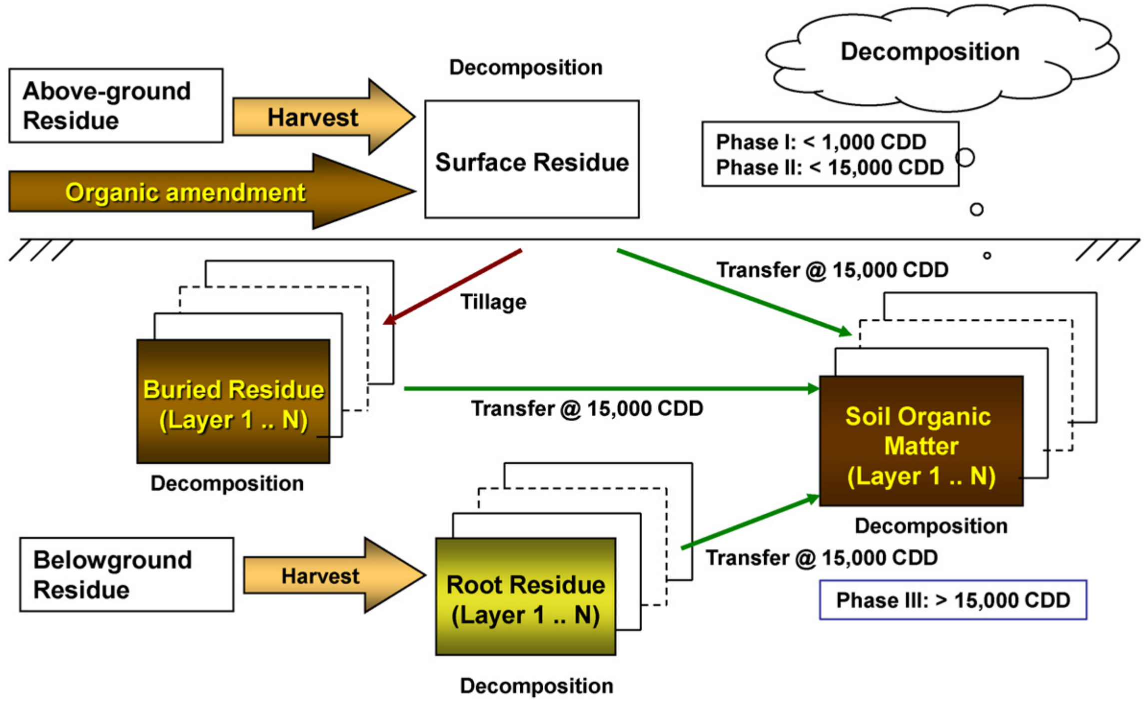

Fig. 1 – Flow diagram for the CQESTR model. The solid arrows depict biomass additions to the residue pools or transfers from the residue pools to the stable SOM pool. CDD is the cumulative degree-days or thermal time.

(RUSLE, version 1, Renard et al., 1996). These inputs include crop rotation, yields (including aboveground and belowground biomass), tillage information, and weather data (i.e. mean monthly air temperature and monthly precipitation). Additional required input data include N content of crop residues and organic amendments, root distribution characteristics of crops, the number and thickness (depth) of soil layers (horizons), and the initial SOM content and bulk density of each layer. Soil layers used in CQESTR are user defined, and are not necessarily delineated by soil characteristics or morphology as is done in most soil process models. Soil layers are defined by the depth increments of available SOC observations. A main consideration in the development of CQESTR was that the model would utilize readily available or easily obtainable inputs instead of detailed physical or chemical fractionations of C sources.

2.1.1. *Description of modified CQESTR model*

The basic model structure and decomposition module of the original version of CQESTR were retained (Rickman et al., 2002) and are illustrated in Fig. 1. Each organic residue addition is tracked separately, without partitioning, according to its placement relative to soil, either on the surface or buried in the soil. Modifications of the CQESTR model are highlighted here and will be explained in detail. A major modification was to quantify soil texture and drainage effects using calibration datasets with a wide range of soil properties. Secondly, the terminating point for organic residue decomposition and residue-to-SOM transfer was changed from calendar-based time to thermal time (explained below). A third modification of CQESTR was to separate the surface residue into two compartments, each with a different water coefficient. This was based on the non-uniform degradation of accumulated surface residue in a no-tillage (NT) cropping system as a result of annual residue layering. A fourth modification involved the inclusion of partially decomposed residue with stable simulated SOM when comparing with SOM observations, since SOM determination unavoidably includes some partially decomposed residue.

2.1.2. *Organic residue decomposition phases*

The model subdivides the organic material decomposition process into three phases (Fig. 1). After each residue addition, decomposition occurs in two phases: Phase I, a rapid phase of the first 1000 cumulative degree-days (CDD or thermal time, a measure of time the organic material decomposes, computed as the summation of mean daily air temperature greater than a base value of 0 °C), approximating the oxidation of readily metabolizable substrate; and Phase II, a slow decomposition phase representing oxidization of more recalcitrant materials. Crop residues and organic amendments are categorized by their placement in the soil and their identities are maintained throughout Phase I and II decomposition. After Phase II is complete (15,000 CDD), the transformed residue is transferred to the stable SOM pool (Phase III) in one step, even though in nature each organic material addition is incorporated in the SOM in a slow and continuous manner. The earlier version of CQESTR used calendar-based four years' worth of CDD for a specific site as the transition point from the residue pools to the common stable SOM pool. However, in general, residue decomposes faster in a warm region (e.g. the middle-Coastal Plain region of South Carolina (34°18′N, 79°44′W) with annual CDD of about 6300) than in a colder region (e.g. Saskatchewan, Canada (50°17′N, 107°48′ W) with annual CDD of about 2600). Since simple calendar-based time calculations allowed more residue decomposition in warm regions, before being transferred into Phase III (slow-degrading SOM pool), we have eliminated one cause of either underestimating SOM content in warmer regions or overestimating in colder regions.

$$R_{SOM,r} = \begin{cases} R_{SOM,p} \times \exp(k \times fN_0 \times fB_{OM} \times fX \times fD \times CDD); & CDD_j < 15{,}000 \\ R_{SOM,p} \times \exp(k \times fN_0 \times fB_{OM} \times fX \times fD \times CDD) + R_{15{,}000,j}; & CDD_j = 15{,}000 \end{cases} \quad (3)$$

2.1.3. *Soil organic C budget and algorithms*

The total soil organic C budget can be represented by Eq. (1), using units of dry weight per unit area within each soil layer.

$$C = (C_{SOM} - C_{DOM}) + \sum_{l=1}^{u}(C_{S,l} - C_{DS,l}) + \sum_{m=1}^{v}(C_{R,m} - C_{DR,m}) + \sum_{n=1}^{w}(C_{A,n} - C_{DA,n}) \quad (1)$$

where C is total SOC, C_{SOM} C in the stable SOM, C_{DOM} decomposed organic matter lost as C dioxide (CO_2), $C_{S,l}$ C in shoot residue l, $C_{DS,l}$ C lost as CO_2 from decomposed shoot residue l, $C_{R,m}$ C in root residue m, $C_{DR,m}$ C lost as CO_2 from decomposed root residue m, $C_{A,n}$ C in organic amendment n, $C_{DA,n}$ C lost as CO_2 from decomposed amendment n, and u, v, w are all applications of organic materials from the initial time to the current day.

The rate of biological decomposition of crop residue or organic amendments is a function of environmental conditions, including temperature effect captured by CDD (thermal time) starting at residue addition, water availability, N content of residue, and soil properties (texture and drainage). Organic residues and stable SOM share a similar decomposition equation, but are assigned different values for environmental parameters, according to the biomass type and physical location of the residue addition. Eq. (2) describes the computation of residue remaining at each time-step for each residue or organic amendment (j) in each soil layer. The factors fN, fW, fB, fX, and fD are environmental parameters used to correct decomposition rates for sub-optimal conditions.

$$R_{r,j} = \begin{cases} R_{p,j} \times \exp(k \times fN_j \times fW_j \times fB_j \times fX \times fD \times CDD_j); & CDD_j < 15{,}000 \\ 0; & CDD_j \geq 15{,}000 \end{cases} \quad (2)$$

where:

$R_{r,j}$: residue or organic amendment j remaining at the end of each decomposition time step (weight/area)
$R_{p,j}$: residue or organic amendment j at previous time step (weight/area)
k: universal decomposition rate constant ($^\circ C^{-1}\,d^{-1}$)
fN_j: nitrogen content factor for residue j, with different values assigned either within 1000 CDD or beyond 1000 CDD, and described in the next paragraph
fW_j: water availability factor for residue j
fB_j: biomass or residue type factor for residue j
fX: soil texture factor
fD: soil drainage factor
CDD_j: cumulative degree-days of residue j for this time-step $^\circ$Cd (with a base temperature of 0 °C).

Eq. (3) describes the computation of stable SOM at each time-step in each soil layer.

where:

$R_{SOM,r}$: SOM remaining at the end of each decomposition time step (weight/area)
$R_{SOM,p}$: SOM at previous time step (weight/area)
k: universal decomposition rate constant ($^\circ C^{-1}\,d^{-1}$)
fN_0: nitrogen content factor for the Phase III decomposition
fB_{OM}: biomass type factor for SOM
CDD: cumulative degree-days of SOM for this time step (°C d)
$R_{15{,}000,j}$: residue j remaining after 15,000 CDD of decomposition (weight/area).

The N factor (fN) is assigned based on the initial N content of the residue entering Phase I decomposition of "fresh" organic materials. After Phase I decomposition, a single low value is used for fN (fN_0) for all residues as well as for the stable SOM pool. The water availability factor (fW) is determined by the location of residue as either buried or lying on the soil surface, and the presence or absence of a growing crop. The biomass type factor (fB) distinguishes among shoot residue, root residue, pre-decomposed organic material (e.g. animal manure) and stable SOM. The above parameter values (Table 1), including the universal decomposition constant (k) were originally determined using the exponential equation to best match decomposition of field-scale residue experiment data sets for a variety of crops from more than 10 locations, with a wide range of climate variation from Alaska to Texas, US (Douglas and Rickman, 1992; Rickman et al., 2002). By adjusting decomposition rate coefficients, one acknowledges the various types of components that make up the rapidly decomposed material.

2.1.4. *Soil texture and drainage algorithms*

Although impact of soil texture on the distribution of SOM has been reported (Gregorich et al., 1991; Schimel et al., 1994; Plante et al., 2006), quantitative data for the effect of soil texture on whole-soil organic matter decomposition are lacking. Dijkstra and Cheng (2007) reported higher soil C decomposition from sandy soil than clayey soil due to possible differences of soil C accessibility by microorganisms and oxygen supply. Huggins et al. (1998) speculated that stabilization of labile C with clay could be the primary mechanism for decreased decomposition of SOC at equilibrium under intensive tillage. The silt and clay content decreases the decomposition rate of active SOM (Parton et al., 1987). Numeric texture codes were assigned to the USDA soil texture classes (Gee and Or, 2002) and used to calculate soil texture coefficients based on a linear relationship (Eq. (4)) and calibrated against long-term datasets with a wide range of soil texture. The resulting numeric values for texture codes were −2, −1, −1, −1, −0.5, 0, 0, 0, 0, 0.5, 0.5,

Table 1 – Values of environmental parameters used in the CQESTR decomposition equation.

Environmental parameter		Value	Applicable materials
k		−0.0004	Universal
fN	fN_0	0.8354	N content < 0.55% or soil organic matter
	fN_1	1.2635	0.55% ≤ N content < 1.0%
	fN_2	1.977	1.0% ≤ N content < 1.5%
	fN_3	3.404	N content > 1.5%
fW	$fW_{a,s}$	0.21	Surface "dry" compartment organic matter under arid climate
	$fW_{a,b}$	0.80	Surface "moist" compartment and buried organic matter under arid climate
	$fW_{h,s}$	0.32	Surface "dry" compartment organic matter under humid climate
	$fW_{h,b}$	1.00	Surface "moist" compartment and buried organic matter under humid climate
fB	fB_{rs}	1.00	Crop residue
	fB_{rt}	0.35	Root biomass
	fB_c	0.60	Pre-decomposed organic matter
	fB_{OM}	0.0061	Soil organic matter

and 1 for clay, silty clay, sandy clay, clay loam, silty clay loam, sandy clay loam, silt, silt loam, loam, sandy loam, loamy sand, and sand, respectively. Soil texture coefficients were obtained from the equation

$$fX = 1.0 + 0.01 \times X_k \tag{4}$$

where X_k is the texture code associated with different soil texture classes, ranging from −2 to 1.

The drainage coefficient (fD) was defined as a function of the average number of days per year of soil saturation (Sd) (Eq. (5), Fig. 2). The numbers of saturation days were assigned to the various soil drainage classes (Table 2). Drainage coefficients were obtained from the equation

$$fD = \sqrt{\frac{10}{(Sd \times 100)/(365 \times 2) + 9.3}} \tag{5}$$

where Sd is the number of saturation days associated with drainage classes (Soil Survey Staff, 1975).

Crop rotation and tillage information are required explicitly for the layer-by-layer computation performed by the model. RUSLE c-factor files, used as input files for CQESTR, consist of crop grain yields, shoot-to-grain ratios, dates of all operations (e.g. tillage, seeding, harvest, biomass addition, etc.), effects of tillage on residue (e.g. fraction of pre-tillage residue mass remaining on the soil surface after each tillage, depth of tillage and the fraction of the surface disturbed by each tillage operation). Amount of aboveground biomass was calculated by multiplying grain yield and the shoot-to-grain ratio, and biomass removal (e.g. manual harvest before 1950s and wide use of combines, straw baling, fall or spring residue burning) was explicitly included as model inputs. This makes it possible to simulate the effect of long-term biomass removal on SOM for cellulosic bioenergy production, or other uses (e.g., animal fodder and bedding, mushroom production, etc.).

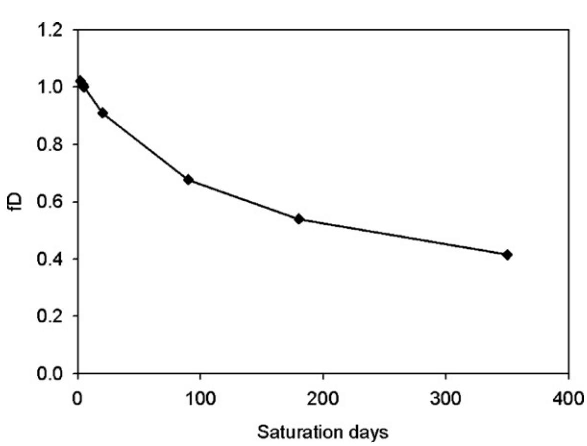

Fig. 2 – Relationship of drainage factor and the saturation days for various soils defined by $fD = \sqrt{\frac{10}{(Sd\times100)/(365\times2)+9.3}}$.

2.1.5. *Belowground biomass algorithms*

Belowground biomass in the upper 10 cm (0.1 m or 4 in.) soil layer is obtained from croplist.dat of the RUSLE c-factor files. This input data is used to calculate the total belowground biomass based on a mathematical equation reported by Gerwitz and Page (1974). They determined the relationship between total root biomass and soil depth by taking the reciprocal of the slope of a logarithmic plot of percentage of total roots within a soil horizon plotted against horizon depth [Eq. (6)].

$$\frac{dP}{dx} = e^{-fx+C} \tag{6}$$

Table 2 – Drainage classes and their assigned saturation days which are used in drainage factor (fD, Fig. 2) calculation.

Drainage class	Saturation days
Excessively drained	2
Somewhat excessively drained	4
Well drained	5
Moderately drained	20
Somewhat poorly drained	90
Poorly drained	180
Very poorly drained	350

Table 3 – Root distribution coefficients (*f*) of different crops used in the model simulation.

Crops	Root distribution coefficient
Legume: soybean (*Glycine max* L.); navy bean (*Phaseolus vulgaris* L.)	12
Cereal: wheat (*Triticum aestivum* L.); oat (*Avena sativa* L.); rye (*Secale cereale* L.); etc.	10
Maize (*Zea mays* L.), sorghum (*Sorghum bicolor* L.), clover (*Trifolium*)	8
Alfalfa (*Medicago sativa* L.), cotton (*Gossypium* hirstum L.)	3

where dP is the percentage of root within a horizon of thickness dx at a depth of x cm; f is the slope of the line relating the logarithm of percentage of root to depth, which is crop specific; and C is the intercept. From Eq. (6) an expression was derived to give the total root biomass ($P_{R,m}$) based on the belowground biomass of the upper 4 in. soil layer ($P_{R,m,top4}$) and the characteristics of root distribution (the constant 0.1016 meters is the equivalent of 4 in.).

$$P_{R,m} = \frac{P_{R,m,top4}}{1 - e^{-f \times 0.1016}} \tag{7}$$

Each plant species has its characteristic root systems and distribution, and their growth are greatly dependent on the crop variety, soil, and environmental conditions. However, due to limited root data, root distribution coefficients (*f*) for crops were developed and used in the model. The root distribution coefficients were determined based on root development experiments reported in the literature (Weaver, 1926; Barraclough et al., 1991; Barber and Kovar, 1991; Gao et al., 1998; Sainju et al., 1998, 2005; Scheiner et al., 2000) and summarized in Table 3. Deep rooted crops (e.g., alfalfa; *Medicago sativa* L.) have smaller root distribution coefficients than shallow rooted crops. The derivation of the soybean (*Glycine max* L.) root distribution coefficient resulted in a root mass comprising of 70% of total root mass in the top 10 cm (0.1016 m, 4 in.), while the top 10 cm of root mass in alfalfa comprised of 26% of total root. This general approximation does not reflect any specific crop variety, soil or environmental interactions.

2.1.6. *Surface residue algorithms*

No-tillage management can result in a large amount of crop residue accumulating on the soil surface after a number of years. Decomposition rates of surface residues can vary depending on their position relative to the soil surface and moisture condition. Newly added residues are exposed to direct sunlight and can dry quickly. On the other hand, residue that lies beneath the recently applied residue layer is under a less arid condition and subject to a higher degree of microbial (e.g. fungal) degradation. In the model, surface residues are separated into two compartments, with a different water coefficient (fW) assigned for each compartment. A concept of target cover was developed as a criterion to separate the residues into an upper "dry" compartment and a "moist" compartment underneath. The target cover is the dry weight of residue sufficient to cover 95% of the soil surface, and calculated by Eq. (8) (Renard et al., 1996).

$$RC = 1 - \exp\left[-\sum_{i=1}^{n}(\alpha_i R_{DW,i})\right] \tag{8}$$

where:

RC: residue cover in percentage (%)
α_i: the ratio of area covered by residue to the weight of that residue (area/weight) for each residue layer encountered
$R_{DW,i}$: the dry weight of crop residue on the soil surface per unit area for each layer (weight/area)
n: the number of residue layers.

Two assumptions are made when calculating target cover. First, residue is added to the soil surface in layers of uniform thickness. Second, each tillage operation only reduces the amount of the surface residue, and does not alter the sequence of added residue layers. At any time step, the mass of the surface residue is summed from the top layer downward (i.e. the most recent residue being added first) consecutively until the target cover is reached. Those layers of residue that were used in the summation to reach target cover are assigned to the "dry" compartment, while the layers of surface residue that were not used in the summation are assigned to the "moist" compartment. Layers in the dry compartment, which undergo a slower decomposition than the moist compartment, were assigned a low fW value ($fW_{a,s}$ or $fW_{h,s}$, Table 1), while layer(s) in the moist compartment, which undergo a relatively faster decomposition, were assigned higher fW values ($fW_{a,b}$ or $fW_{h,b}$, Table 1). In conventional tillage (CT), where the majority of residue is incorporated into soil by moldboard plow, the amount of target cover is rarely met. Consequently, all surface residues in a CT system decompose in a slow manner, corresponding to a dry condition.

Agricultural soil contains successive accumulations of organic matter derived from plants, other organisms and organic amendments in different stages of decomposition, ranging from fresh litter to well-humified SOM (Oades, 1988; Stevenson, 1994). The commonly used soil preparation method (air-drying, grinding, sieving) for SOC analysis (e.g. Leco C analyzer, Carlo Erba automated analyzer)[2] unavoidably includes some fine undecomposed organic residues (plant debris) in the results. Therefore, model-simulated SOM contents are assumed to be contributed from different stages of decomposition, which includes both the stable SOM and active SOM. The active SOM defined by CQESTR is the balance of various residue pools after undergoing certain CDD of decomposition. A threshold of 3700 CDD was selected to exclude relatively fresh residue and partially decomposed organic materials. These combined simulated stable and active SOM contents were compared with SOM observations.

[2] Mention of trade names or commercial products in this manuscript is solely for the purpose of providing specific information, and does not imply recommendation or endorsement by USDA.

3. Statistical evaluation of model performance

Regression analysis and mean square deviation (MSD) statistics were used to evaluate the predictive performance of the model against measured data for 13 long-term agricultural sites. The MSD is partitioned into three components: squared bias (SB), nonunity slope (NU) and lack of correlation (LC) or scatter (Gauch et al., 2003). All three components relate to terms of the linear regression equation ($Y = a + bX$) and the regression coefficient (r^2).

Given a set of observed (X) and simulated values (Y), the MSD is defined as $\text{MSD} = \sum (X_n - Y_n)^2/N$ for $n = 1, 2, \ldots, N$. The first component of MSD, $\text{SB} = (\bar{X} - \bar{Y})^2$, gives a measure of the inequality between the two means $\bar{X}$ and $\bar{Y}$. According to Gauch et al. (2003), the second component, non-unity (NU), measures the degree of rotation of the regression line and is defined as $\text{NU} = (1 - b)^2 \times \sum x_n^2/N$, where b is the slope of the least-square regression of Y on X, $b = \sum x_n y_n / \sum x_n^2$, $x_n = X_n - \bar{X}$, and $y_n = Y_n - \bar{Y}$. The third component, lack of correlation or scatter (LC), is calculated as $\text{LC} = (1 - r^2) \times \sum y_n^2/N$ where r^2 is the coefficient of determination $(\sum x_n y_n)^2/(\sum x_n^2 \sum y_n^2)$.

Simulated SOC results from three long-term sites (Lancaster, WI, 24 years; Sidney, NE, 20 years; Swift Current, SK, 24 years) were compared with IPCC method. Vegetation in two of the three locations was either native prairie (Sidney, NE) or alfalfa-bromegrass meadow (Lancaster, WI) prior to the experiments. The area of Swift Current, SK was used for various cereal experiments before onset of the experiment resulting in different initial SOC values in 1976. The final SOC (Mg C ha^{-1}) is estimated as described by Ogle et al. (2003) using the following equation

$$\text{SOC} = R_{\text{SOC}} \times \text{TF} \times \text{IF} \tag{9}$$

where R_{SOC} is the SOC stock at the initiation of experiments, TF is the tillage factor (i.e. no-tillage vs. conventional tillage practices), and IF is the input factor (cropping intensity and productivity of various cropping rotations). High input refers to cropping systems that included a year of hay, legumes, or pasture in rotation, while low input refers to rotations with bare summer-fallow, or crops producing low amounts of residue, such as vegetables and cotton.

4. Results

4.1. Model calibration

4.1.1. *Site descriptions*

Descriptions of the six long-term experiments (Florence, SC, 19 yrs; Lincoln, NE, 26 yrs; Hoytville, OH, 31 yrs; Breton, AB, 60 yrs; Pendleton, OR, 76 yrs; and Columbia, MO > 100 yrs) having a range of soil properties and climate used in calibrating CQESTR are presented in Table 4. These studies represent a variety of crop rotations, tillage practices, fertility management, and crop residue removal and their effects on grain yields and soil C dynamics (Hunt et al., 1996; Buyanovsky et al., 1997; Darmody and Peck, 1997; Lyon et al., 1997; Paul et al., 1997; Rasmussen and Albrecht, 1997; Rasmussen and Smiley, 1997; Rickman et al., 2002; Wilhelm and Wortmann, 2004; Novak et al., 2007). Three wheat (*Triticum aestivum* L.)–fallow treatments from long-term experiments at Pendleton were originally used to calibrate the k, fN, fW and fB parameters of CQESTR model (Rickman et al., 2002). The three treatments were (1) fall burn—no fertilizer added, with stubble burned in the fall and the soil plowed in the spring before the fallow summer for minimum residue return; (2) fertilizer—90 kg N ha^{-1} applied to each wheat crop, with stubble plowed in the spring and summer fallow; and (3) manure—22 Mg ha^{-1} wet manure (mixed with straw bedding) added before plowing in the spring of the fallow year (Rasmussen and Albrecht, 1997; Rasmussen and Smiley, 1997; Rickman et al., 2002). All three treatments used the same fallow methods. The three treatments represent various amounts of C inputs under well-drained silt loam soil and similar cropping rotation. Five long-term experiments (Florence, SC; Lincoln, NE; Hoytville, OH; Breton, AB; and Columbia, MO) with different crop rotations and a wider range of soil texture and drainage classes across North America (Table 4) were used to calibrate the fX and fD factors of the modified model. No changes were made to the original calibration parameters k, fN, or fW. The calibration values for the environmental parameters are reported in Tables 1 and 2, and Fig. 2.

Several calibration and validation sites originally had poorly drained soil but were tile-drained during the course of the experiments. It was assumed that the installation of drainage tile changed the soil drainage class to the moderately drained category.

4.1.2. *Simulation results for Pendleton long-term experiments*

The observed and simulated SOM contents for the three treatments in 0–30 cm and 30–60 cm depth at Pendleton are illustrated in Fig. 3. The bars represent 95% confidence intervals for the observed SOM content for each treatment at each sample date, and for each depth. The simulations demonstrate that crop management practices that are beneficial to grain and residue production, such as the application of fertilizers, organic amendment, also improve SOM content (Fig. 3). Addition of source C such as farmyard manure resulted in decreased soil C losses in the winter wheat–fallow system. Simulation trends show that management practices that increase biomass contributions to the soil (fertilization, manure application, etc.), and return root and shoot biomass to the soil annually promote SOM accretion. Manure addition is the only management practice that can maintain SOM content in wheat–fallow rotation for these soils under conventional tillage and semiarid condition.

4.1.3. *Model validation*

Data from 13 long-term cropping experiments in the United States and Canada (Paul et al., 1997) were used for the validation of the model (Table 5). The data included agricultural cropping experiments ranging from 8 to 100 years in duration, with a range of mean annual temperature (4–16 °C), precipitation (350–1250 mm), soil texture (i.e. silty clay, silty clay loam, loam, silt loam, sandy clay loam, sandy loam, loamy sand)

Table 4 – Management practices, experiment duration, soil sampling, soil texture and drainage classes for calibration sites.

Site	Crop rotation[a]	Management[b]	Duration[c] (years)	Sampling depth (cm)	Earliest sample[d]	Latest sample	Soil texture[e]	Soil drainage class
Breton, AB	W–F	CR Residue removal 3 fertility levels	60	0–15	1971	1995	L	Well drained
Florence, SC	C–W, CO C–W, SB	CT CS	19	0–5 5–10 10–15 15–20	1979	2004	SL	Well drained
Hoytville, OH	C	CT NT	31	0–7.5 7.5–15	1962	1980	SiL	Moderately drained
Pendleton, OR	W–F	CT One residue burning One fertility One manure	76	0–12 12–24	1931	1995	SiL	Well drained
Lincoln, NE	C SB C–SB SB–C	CT CH CT	26	0–12	1985	1999	SiCL	Moderately drained
Columbia, MO (Sanborn Field)	C W	CT Fertilizer Manure	>100	0–20	1915	1986	SiL or L	Moderately drained

[a] Crop abbreviations: C, corn; CO, cotton; F, fallow; SB, soybean; W, wheat. "–", separates years, and ",", separates crops within a year.
[b] Tillage abbreviations: CR, cultivation and rod-weeding; CS, conservation tillage; CT, conventional tillage; CH, chisel tillage; NT, no-tillage.
[c] Refers to the duration time period for reported data used in calibration.
[d] Earliest soil sample does not necessarily occur at the initiation of an experiment.
[e] Texture abbreviations: C, clay; L, loam; S, sand; Si, silt.

Table 5 – Management practices, experiment duration, soil sampling, soil texture and drainage classes for validation sites across North America.

Site	Crop rotation[a]	Management[b]	Duration[c] (yr)	Sampling depth (cm)	Earliest sample[d]	Latest sample	Soil texture[e]	Soil drainage class
Akron, CO	W–F	ST NT	11	0–10 10–20	1982	1989	SiL	Well drained
Arlington, WI	C	CT 3 fertility levels	33	0–15	1958	1990	SiL	Well drained
Lancaster, WI	C C–C–O–A–A C–SB–C–O–A	CT 3 fertility levels	24	0–15	1966	1990	SiL	Well drained
Athens, GA	GS, RY	CT NT	11	0–5 5–15 15–22.5	1982	1990	SCL	Well drained
Watkinsville, GA	GS, CL GS	DK NT	8	0–8	1986	1991	SL	Well drained
Champaign, IL	C C-O C-O-Hay	CT 3 fertility levels Residue removal before 1950s	106	0–15	1904	1993	SiL	Moderately drained
East Lansing, MI	C grain C silage	CT 3 fertility levels	19	0–20	1972	1982	LS	Well drained
Saginaw Valley, MI	C–C–C–BT C–C–NB–BT O–NB–BT NB–BT C–BT	CT 3 fertility levels	18	0–25	1972	1991	SiC	Moderately drained
Lethbridge, AB	W W–F	CT 2 fertility levels	81	0–15	1910	1990	SCL	Well drained
Lexington, KY	C, RY	CT NT 3 fertility levels	21	0–15 15–30	1975	1989	SiL	Well drained
Mead, NE	C C–SB–C, CL	CT 2 fertility levels	16	0–15	1971	1990	SiCL	Well drained
Sidney, NE	W–F	CT ST NT	20	0–10 10–20	1982	1991	L	Well drained
Swift Current, SK	W W–F W–F–F	CR	24	0–15	1976	1990	L	Well drained

[a] Crop rotation abbreviations: A, alfalfa; BT: sugar beet; CL, clover; C, corn; F, fallow; NB, navy bean; GS, grain sorghum; O, oat; RY: rye; SB: soybean; W: wheat. "–", separates years, and ",", separates crops within a year.
[b] Tillage abbreviations: CR, cultivator and rod-weeder; CT, conventional tillage; CH, chisel tillage; DK, disking; NT, no-tillage; ST, sweep tillage.
[c] Refers to the duration time period for reported data used in validation.
[d] Earliest soil sample does not necessarily occur at the initiation of experiments.
[e] Soil Texture abbreviations: C, clay; L, loam; S, sand; Si, silt.

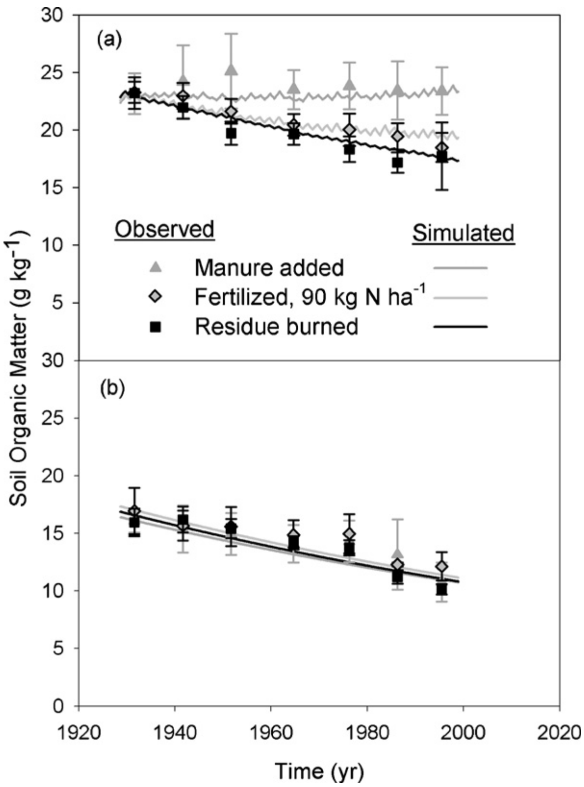

Fig. 3 – Comparison of observed and simulated soil organic matter (SOM) contents for the manure, fertilizer and fall burn treatments for (a) 0–30 cm (b) 30–60 cm depth at Pendleton, OR. The treatments were: manure, 22 Mg ha^{-1} wet manure added in the spring and plowed with the stubble before the fallow summer; fertilizer, 90 kg N ha^{-1} applied to each wheat crop and stubble plowed in the spring during the fallow summer; and fall burn, no fertilizer added and stubble burned in the fall, soil plowed in the spring of the fallow summer, for minimum residue return. The bars represent 95% confidence intervals for the observed data.

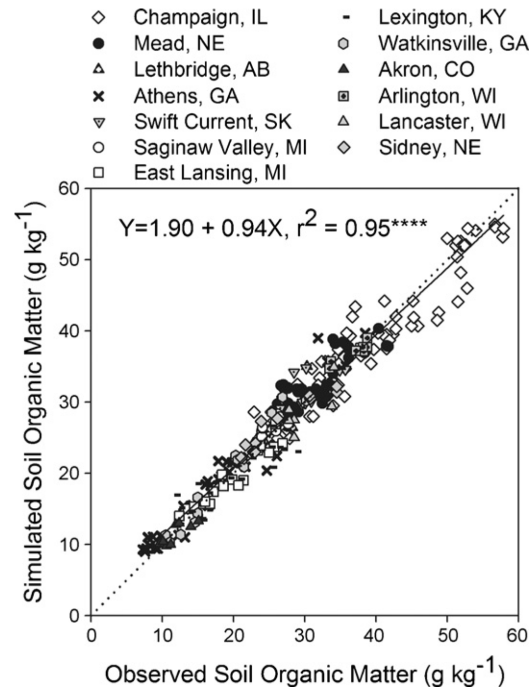

Fig. 4 – Comparison of simulated and observed soil organic matter (SOM) contents at 13 agricultural sites under diverse climate, soil types and crop and residue management. The linear fit of simulated vs. observed SOM explained 95% of the variation ($P<0.0001$), had a slope of 0.94, and a 95% confidence interval of 4.35 g SOM kg^{-1}. ****Significant at the 0.0001 probability level.

and soil drainage (i.e. moderately drained and well-drained). In some cases, crop residue was removed with grain at harvest for certain periods during the long-term experiments (e.g. Champaign, IL). Five locations included NT treatments, with a maximum duration of 21 years. The initial SOM content for each treatment was chosen to ensure CQESTR simulation matched the first available observed SOM content from each field experiment.

We demonstrated the CQESTR model's capability to simulate different residue management and tillage operations for the majority of sites. The observed versus simulated SOM values for the 13 validation sites are presented in Fig. 4. Predicted and observed values from all sites were closely related ($r^2 = 0.95$, $n = 306$, $P < 0.0001$) with a 95% confidence interval of 4.35 g SOM kg^{-1} and aligned along the 1:1 regression line. The model simulated SOM content reasonably well for most of the agricultural sites, and is an improvement over version 1.0. The previous version 1.0 of CQESTR with a 95% confidence interval of 5.5 g SOM kg^{-1} explained 71% of the variation in the SOM data, while the current version explains 95% of the variation in the SOM data.

4.1.4. *Statistical evaluation of CQESTR simulation results*

The least square linear regressions of simulated vs. observed SOM for individual sites were all significant at the $P = 0.05$ level (Table 6). The mean square deviations for each validation site were calculated to evaluate how well the model had captured the spatial–temporal dynamics of SOM with various crop rotations for different climatic regions (Fig. 5). Relatively small MSDs were observed at three sites (Akron, CO; Arlington, WI; and East Lansing, MI), while larger MSDs were observed at four sites (Morrow Plots in Champaign, IL; Mead, NE; Swift Current, SK; and Lexington, KY). The Morrow plots have been greatly altered during the course of their existence (e.g., a building was placed on the site) and only a small fraction of the original plots exist today. This might explain the rather large scatter in these plots. Most of the prediction errors were associated with a lack of correlation (LC) or scatter at all sites, except for three sites (Arlington, WI; Saginaw Valley, MI; and Sidney, NE).

4.1.5. *CQESTR simulation vs. IPCC estimates*

The observed vs. simulated/calculated soil organic C stocks for three relatively long-term experiments were compared at the end of 20+ years of cultivation (Fig. 6). At the Sidney experiment site (Fig. 6a), decreasing tillage intensity increased SOC stocks for the winter wheat–fallow rotation of both observed and estimated or simulated by IPCC and CQESTR models,

Table 6 – Regression parameters (slope, intercept, regression correlation and standard error) for simulated soil organic matter contents as a function of observed soil organic matter contents at the 13 agricultural sites.

Site	Slope		Intercept		r^2	SE of regression	*P* value
	Estimate	SE[a]	Estimate	SE[a]			
Akron, CO	0.67	0.18	3.60	2.21	0.69	0.93	0.011
Arlington, WI	0.57	0.09	15.91	3.29	0.86	0.53	0.0003
Lancaster, WI	0.64	0.26	10.14	7.67	0.43	2.00	0.040
Athens, GA	0.98	0.03	1.26	0.68	0.95	1.92	<0.0001
Watkinsville, GA	1.14	0.07	−1.97	1.41	0.96	1.55	<0.0001
Champaign, IL	0.89	0.03	3.86	1.25	0.91	2.75	<0.0001
East Lansing, MI	0.82	0.05	3.02	0.94	0.93	1.00	<0.0001
Saginaw Valley, MI	0.37	0.16	17.1	4.20	0.34	0.73	0.047
Lethbridge, AB	0.96	0.17	1.70	1.39	0.73	1.63	<0.0001
Lexington, KY	0.81	0.07	3.60	1.49	0.86	2.21	<0.0001
Mead, NE	0.67	0.07	11.19	2.24	0.68	1.96	<0.0001
Sidney, NE	0.73	0.05	7.36	1.45	0.91	0.92	<0.0001
Swift Current, SK	0.48	0.22	16.77	6.64	0.33	1.97	0.051

[a] SE, standard errors of the estimates.

although both methods underestimated SOC stocks under three tillage practices by up to 11%.

At the Swift Current site (Fig. 6b), CQESTR simulation and IPCC estimation of SOC stock were within 5% of each other for three rotations. However, SOC observation for continuous wheat in 1990 was substantially lower than estimations, indicating possible error from soil sampling or analysis.

In the Lancaster experiment (Fig. 6c), two rotations that included alfalfa (categorized as "high input" or IF of 1.1 in IPCC methods) increased estimated SOC stocks to 40.5 Mg C ha^{-1},

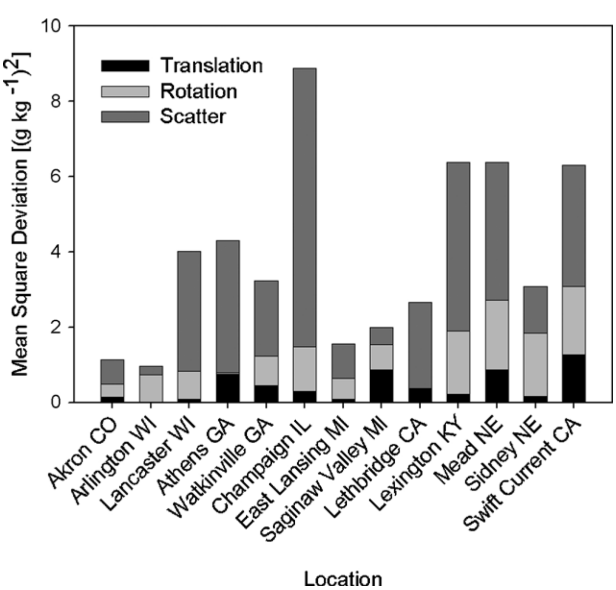

Fig. 5 – Comparison of mean square deviations (MSD) for model simulations of long-term soil organic matter changes at 13 agricultural sites. The translation (Squared Bias, SB) component of MSD is a measure of the inequality of the means. The rotation (Nonunity, NU) component contributes to the MSD when the slope of the regression line between simulated and observed values is $\neq 1$. The scatter (Lack of Correlation, LC) component of MSD gives a measure of the scatter in the data.

while CQESTR simulated SOC stocks of 44.1 and 37.2 Mg C ha^{-1} for the two rotations, respectively. The IPCC estimates of SOC for continuous corn under three fertility levels resulted in the same stock values because of the identical "medium input" factor used in IPCC estimates. However, CQESTR simulated an increase in SOC stocks with increased fertility levels, because the actual grain and corresponding biomass yields were used as inputs in the model. Relatively large difference between observed and CQESTR simulated values for continuous corn under no fertilizer may be caused by a lower harvest index (low grain yields but similar biomass inputs).

4.1.6. *CQESTR simulation vs. CENTURY results*

The CQESTR model-simulated SOC values for three tillage systems (NT, CT, and RT–one heavy disc harrow and one harrow leveling) were compared to the simulation results from the CENTURY model (Parton et al., 1987), using the same data from tropical soils to evaluate the performance of the models (Leite et al., 2009). The estimated SOC stocks for RT were similar for both models, however CQESTR predicted higher SOC stocks for NT and CT compared to the CENTURY model (Leite et al., 2009).

5. Discussion and model evaluation

One of the unique features of CQESTR is to use thermal time (CDD) as the primary driver for decomposition. This is based on the findings that the natural logarithm of the remaining residue fraction is linearly dependent on thermal time (cumulative degree-days) regardless of geographic location. This relationship was obtained from the residue decomposition model created from field-scale residue experimental data of various regions (Douglas and Rickman, 1992). The change of residue-to-SOM transition criterion from a calendar based-time to thermal time in the current version of CQESTR is a natural extension of this feature.

A few limitations exist in the current approach that may have contributed to the simulation discrepancy. The amounts of aboveground and belowground biomass are equally impor-

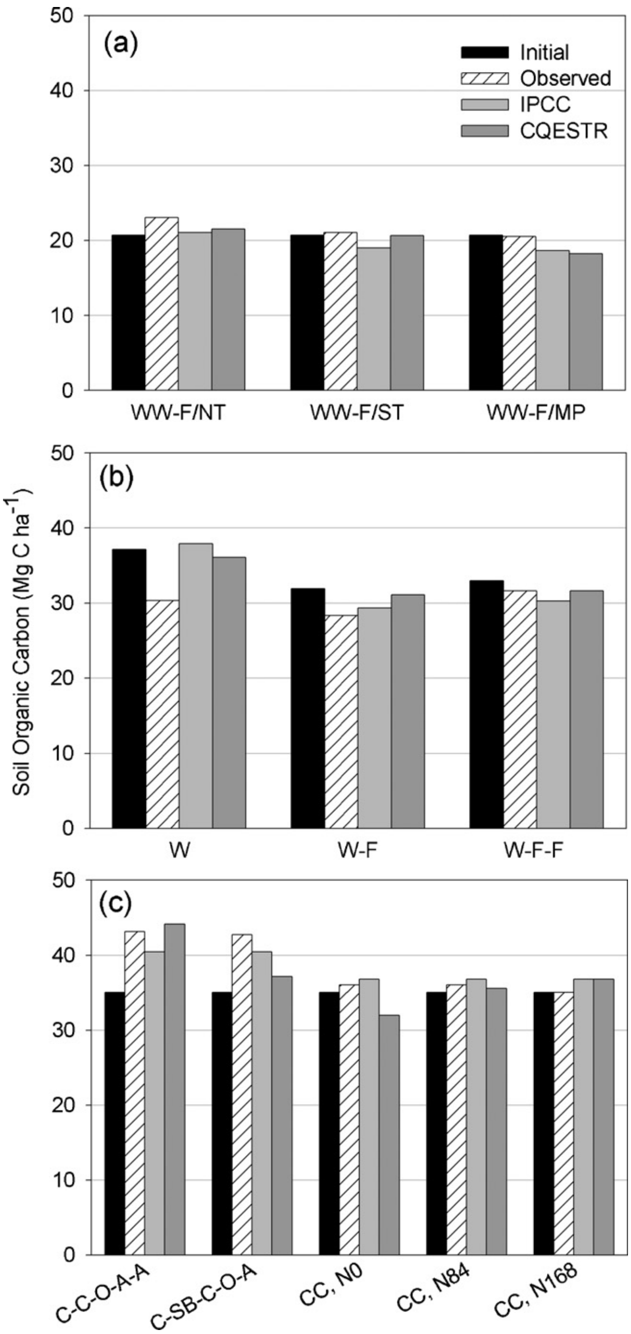

Fig. 6 – Observed and estimated or simulated soil organic carbon stocks (SOC) by IPCC method and CQESTR. (a) Tillage experiment, 0–10 cm soil layer for winter wheat–summer fallow (WW-F) under three tillage treatments (NT—no-tillage, ST—sweep tillage, and MP—moldboard plow) at Sidney, NE; (b) crop–rotation experiment, 0–15 cm soil layer for continuous spring wheat (W), wheat–fallow (W–F), and wheat–fallow–fallow (W–F–F) under reduced tillage at Swift Current, SK; and (c). Crop rotation and nitrogen fertility experiment, 0–15 cm soil layer for corn–corn–oat–alfalfa–alfalfa (C–C–O–A–A), corn–soybean–corn–oat–alfalfa (C–SB–C–O–A) and coutinuous corn (CC) with three fertility levels (N_0, N_{84}, N_{168}, at 0, 84, and 168 kg N ha^{-1}) at Lancaster, WI.

tant as input data for the CQESTR model. However, limited information is available for root biomass and root distribution pattern of certain crops or in certain geographical regions. In most cases, belowground biomass was generally not measured, therefore estimates were derived from published root-to-shoot ratios, and might not reflect the local condition. Root biomass used in the simulation were mostly adopted from the RUSLE vegetation database file without verification under actual growing conditions. Additionally, data on root-to-shoot ratios for non-commodity crops (e.g. root crops) are nearly non-existent, which may have contributed to the low coefficient of determination ($r^2 = 0.34$) of Saginaw Valley, MI, with navy bean (*Phaseolus vulgaris* L) and sugar beet (*Beta vulgaris* L.) in the crop rotation. There is also a relatively poor understanding of the fate of C from root exudates.

A second limitation in CQESTR may be a missing parameter to account for the complex relationship between soil nitrogen level and plant N uptake (e.g. the interaction of crop with indigenous soil N). A poor relationship ($r^2 = 0.43$) for Lancaster WI occurred where observed SOM levels were greater in the unfertilized treatment than in two fertilized treatments in 1990 (data not shown). This is consistent with findings of Khan et al. (2007) that N fertilizer promoted the decomposition of crop residue and SOM. Furthermore, Warembourg and Estelrich (2001) reported that the highest C use efficiency would occur in the low fertility soil when expressed in units of C being translocated belowground per unit of root C. In unfertilized crops, N stress decreased shoot growth more than root growth, and root-to-shoot ratios were higher than those found in the fertilized crop (Hansson et al., 1987; Paustian et al., 1992). A more appropriate root-to-shoot ratio, if known, can be inserted into the RUSLE c-factor files, to improve prediction values.

Thirdly, loss or deposition of C at the soil surface from erosion by wind and water is not considered, nor is the physical transfer between soil layers or consumption of residue by worms, insects nor small mammals, or C loss through the soil profile by dissolved organic C leaching. However, C loss from erosion can be calculated using RUSLE, and the output combined with a CQESTR simulation can provide the C balance for a selected field.

6. Conclusions

CQESTR has been modified to respond to agronomic practices for an extended range of soil properties and climates. The model was modified to account for soil texture and drainage interaction with organic residue decomposition and validated with long-term data from across North America. The revised CQESTR model successfully simulated long-term SOM based on crop management, soil properties, aboveground and belowground biomass yields and climate conditions for the majority of agricultural sites. The result demonstrates that long-term SOM dynamics under an array of widely different cropping systems and soil conditions can be adequately modeled using a relatively simple approach. However, there is a pressing need for root biomass data and long-term SOM data, especially from NT experiments, to test and further refine CQESTR. The revised CQESTR model can be used to examine the effect of planned changes in agricultural management on soil C stocks at the field-scale level. As such, CQESTR can estimate the amount of C that can be sequestered for C credit, and offers the potential to guide crop residue removal (e.g., biofuel production) while maintaining the SOM content.

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