# Simulating Field-Scale Soil Organic Carbon Dynamics Using EPIC

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The balance between primary production, decomposition, and lateral transfers of soil organic matter (SOM) determines the amount of organic C sequestered in soils. The evaluation of complex mechanisms and interactions, by which soil use and management affect the nature and concentration of SOC, is best approached by field experimentation coupled with simulation models. Recent developments in SOC simulation models have led

Simulation models integrate our knowledge of soil organic C (SOC) dynamics and are useful tools for evaluating impacts of crop management on soil C sequestration; yet, they require local calibration. Our objectives were to calibrate the Environmental Policy Integrated Climate (EPIC) model, and evaluate its performance for simulating SOC fractions as affected by soil landscape and management. An automated parameter optimization procedure was used to calibrate the model for a site-specific experiment in the Coastal Plain of central Alabama. The ability of EPIC to predict corn (Zea mays L.) and cotton (Gossypium hirsutum L.) yields and SOC dynamics on different soil landscape positions (summit, sideslope, and drainageway) during the initial period of conservation tillage adoption (5 yr) was evaluated using regression and mean squared deviations. Simulated yield explained 88% of measured yield variation, with the greatest disagreement on the sideslope position and the greatest agreement in the drainageway. Simulations explained approximately 1, 34, and 40% of the total variation in microbial biomass C (MBC), particulate organic C (POC), and total organic C (TOC), respectively. The lowest errors in TOC simulations (0-20 cm) were found on the sideslope and summit. We conclude that the automated parameterization was generally successful, although further work is needed to refine the MBC and POC fractions, and to improve EPIC predictions of SOC dynamics with depth. Overall, EPIC was sensitive to spatial differences in C fractions that resulted from differing soil landscape positions. The model needs additional refinement for accurate simulations of field-scale SOC dynamics affected by short-term management decisions.

Abbreviations: CT, conventional tillage; CTm, conventional tillage plus manure; EPIC, Environmental Policy Integrated Climate; FHP, fraction of humus in the passive pool; HI, harvest index; MBC, microbial biomass carbon; MSD, mean squared deviation; NT, no-till; NTm, no-till plus manure; PARM 20, microbial decay rate; PARM 51, microbial activity in the top layer; POC, particulate organic carbon; SOC, soil organic carbon; SOM, soil organic matter; TOC, total organic carbon; WA, biomass/energy ratio.

to an integrated understanding of SOC dynamics in the context of SOC sequestration and climate change (Rosenberg et al., 1999).

Soil organic matter, containing 50 to 58% C, is a complex mixture of organic compounds with different turnover times (Nelson and Sommers, 1982). There is no simple analytical technique for qualifying and quantifying SOM fractions. In fact, the distinction between some fractions is largely conceptual, and convenient for modeling SOC dynamics. Soil organic C is subdivided into several pools with unique characteristics and decomposition rates. Carbon decay in a compartment is assumed to follow first-order kinetics:

$$\frac{\partial C}{\partial t} = -kC + A \tag{[1]}$$

where C is the quantity of C in the compartment, t is time, k is a first-order decomposition coefficient, and A is the annual input of C. Carbon additions from crop residues or animal manures are transferred into different pools varying in stability. The multicompartmental structure of these models provides flexibility as well as the ability to accommodate environmental variables (e.g., water content, temperature, erosion).

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Smith et al. (1997) reported the performance of nine SOM models across 12 long-term data sets. The Century model (Parton et al., 1987, 1994) successfully simulated SOM across a variety of land uses and climates, and was among the models that consistently produced low errors (Kelly et al., 1997; Smith et al., 1997). Century classifies SOC into three pools based on the rate of mineralization and turnover. The labile pool represents easily mineralizable compounds and the microbial and fungal biomass that generally comprises about 5 to 15% of the total SOC, and has a turnover rate of month to years. The slow pool consists of resistant plant material and soil-stabilized microbial products, comprising 20 to 40% of the total SOC with a turnover rate of several decades. The stable or recalcitrant pool comprises the remaining 60 to 70% of the total SOC, and has a turnover time of hundreds to thousands of years.

The EPIC model, developed in the early 1980s, is a process-based model capable of describing interactions among climate, soil, and management at a subwatershed scale (1-100 ha). The acronym initially stood for the Erosion Productivity Impact Calculator, as it was originally designed to estimate erosion impacts on crop productivity (Williams, 1990). Evolution of the model, with incorporation of functions to simulate environmental processes related to water quality and SOC sequestration, merited its name change to the Environmental Policy Integrated Climate model. The EPIC model handles a broad array of crop rotations, soil management systems, and environments, and has been tested in numerous environments. A comprehensive description of development and application of EPIC was presented by Gassman et al. (2004). The original C cycling routine in EPIC was relatively simple and a function of soil N levels, but EPIC v3060 received modification to its C routine with concepts derived from the Century model. A detailed description of the C and N algorithms can be found in Izaurralde et al. (2006).

Model parameters are best determined by experimentation, but spatial variability, measurement errors, and budget constraints often make it necessary to estimate some parameters through calibration. A common calibration approach consists of adjusting model parameters to minimize deviations between simulated and observed values. Manual calibration is subjective and time consuming, but automated iterative procedures have been developed (Eckhardt and Arnold, 2001; Zhai et al., 2004; Wang et al., 2005). Sensitivity analysis, which provides information on the relative importance of each parameter on model output, can be used to identify key parameters. Wang et al. (2005) recently performed a sensitivity analysis on EPIC v3060. They adjusted corn yield and SOC related parameters using an automated optimization procedure, and found parameters of major importance included available water holding capacity, biomass/ energy ratio, potential heat units, harvest index, fraction of organic C in microbial biomass, fraction of humus in the passive pool, and the microbial decay rate coefficient.

Further calibration and validation studies with EPIC v3060 under a range of environmental and management conditions are needed to fully evaluate model performance. With increasing site-specific management, models will need to be effective at the field scale, where soil landscape variability often dictates management and productivity. A challenging aspect of site-specific modeling is to account for the transfer of relevant components within and between landscapes. Most process models consider soil losses, but do not account for gains or deposition (Pennock and Frick, 2001; Polyakov and Lal, 2004). The inability of most models to account for deposition may impair them from detecting management impacts on SOC at cumulative landscape positions.

Since its establishment in 2000, a site-specific experiment at E.V. Smith Research Center (Shorter, AL) has provided information on the interactive effects of soil landscape variation and soil management on soil properties and crop productivity (Terra et al., 2004, 2006). This experiment provides a valuable arena for calibrating SOC simulation models in the Southern Coastal Plain Major Land Resource Area, which makes up a major portion of agricultural lands in the southeastern USA. The experiment also provides a unique opportunity to evaluate short-term changes in SOC during the transition from conventional to conservation management on degraded Ultisols. To date, no studies have evaluated the ability of EPIC v3060 to simulate field-scale variability of SOC, and no calibrationvalidation study of EPIC v3060 has been performed in the southeastern Coastal Plain. Thus, our objective was to evaluate a fully calibrated EPIC v3060 for its ability to simulate shortterm (5-yr) field-scale SOC dynamics as a function of soil landscapes and management.

# MATERIALS AND METHODS EPIC Model Description

The EPIC model is designed to simulate field-scale crop yield and SOC dynamics (Izaurralde et al., 2006). It operates on a daily time step, and can execute long-term simulations (hundreds of years) on watersheds up to 100 ha. Twelve plant species can be modeled simultaneously, allowing intercrop, cover-crop mixtures, and similar scenarios to be simulated. Simulated processes include tillage effects on surface residue, soil bulk density, and mixing of residue and nutrients in the surface layer; along with wind and water erosion, hydrology, soil temperature, C, N, and P cycling, fertilizer and irrigation effects on crops, pesticide fate, and economics (Williams, 1990). Simulations are driven by daily weather (input or simulated) including temperature, radiation, precipitation, relative humidity, and wind speed. Daily crop growth is simulated using solar radiation, and modified by stress factors (e.g., water, temperature, nutrients, and pests).

In EPIC v3060, SOC and N are split into three pools (labile, slow, and recalcitrant), and also can be leached or lost in gaseous forms. Crop residues (including roots) and manure added to the soil are split into two compartments (metabolic and structural) based on lignin and N content. Leaching of organics is estimated by equations that use a linear partition coefficient and soil water content to calculate movement as modified by sorption. Carbon transformation rates are based on temperature and water content calculated with equations originally built in EPIC. Deposition may be estimated by the difference in soil erosion obtained from two equations, the Universal Soil Loss Equation (USLE) and the modified USLE (Izaurralde et al., 2007). The latter accounts for depositional processes that occur in the watershed.

# **Research Location**

We used data from a site-specific experiment located at the Alabama Agricultural Experiment Station E.V. Smith Research and Extension Center in central Alabama (32.4° N, 85.9° W, ~68 m above mean sea level). Background on the experimental site is provided by Terra et al. (2004, 2006). Briefly, the experiment was started in 2000



Fig. 1. Experimental layout at the E.V. Smith Research unit (Shorter, AL). Black area at the north was not included in the simulations. East–west rectangles represent strips with different treatments; gray shading in the background represents the three landscape positions; triangles indicate 2005 soil sampling locations and circles indicate locations where soil pedons were described, sampled, and characterized.

on a 9-ha field that had approximately 30 yr of previous conventional row cropping, mostly cotton, and conventional soil tillage (plowing and disking). Soils are predominantly fine and fine-loamy, kaolin-



Fig. 2. Monthly total precipitation, mean air temperature, and solar radiation for 2001 through 2005. Total rainfall during crop growth is shown with white numbers on black bars.

itic, thermic Typic, Oxyaquic, and Aquic Paleudults. Treatments were conventional and conservation tillage systems with and without dairy manure applied annually in a corn–cotton rotation. The conservation system consisted of no-till (NT) with in-row subsoiling and winter cover crops. Conventional tillage (CT) did not include cover crops, but winter weeds were not controlled. Treatments (CT, NT, CT + manure, and NT + manure) were established in 6.1- by 240-m strips crossing the landscape in a randomized complete block design with six replications (Fig. 1).

# Model Inputs

Weather, soil, and management input files were prepared to conduct 5-yr simulations (January 2001– December 2005).

#### Weather

A daily weather file of maximum and minimum temperature, precipitation, radiation, relative humidity, and wind speed was established from weather data collected at the experiment station (AWIS Weather Services, 2005). We used the Hargreaves method (Hargreaves and Samani, 1985) for estimating evapotranspiration. Monthly mean air temperature, solar radiation, and total precipitation during the study period are shown in Fig. 2. During the 5 yr of simulation, the site averaged 1215 mm of annual precipitation and the mean annual air temperature was 17.7°C.

## Soil

Three major soil landscapes were identified based on previous work (Terra et al., 2004, 2006). The summit was an elevated area of flat topography (0–2% slopes) with well-drained soils (Typic Paleudults), sandy surfaces, and a deep (>150 cm) seasonal high water table

(SHWT). The sideslope (2–6% slopes) was more highly eroded and had an exposed argillic horizon (Typic Paleudults). A concave drainageway occupied the lowest elevation in the field, with more poorly

> drained soils (SHWT = 0.5-1 m; Oxyaquic and Aquic Paleudults). Soil organic C was greater in the drainageway as eroded sediments accumulated and soils were more poorly drained. Model simulations were conducted in these three soil landscapes as they typify the landscape variability of the site and region.

> Soil property data used for model calibration and validation were from samples collected in 2001, 2003, and 2005. In 2001 and 2003, an average of 10 soil surface (0–30-cm) samples was collected per landscape position and treatment. In addition, composited surface (0–20-cm) samples for the 36 sites (four treatments × three soil landscapes × three repetitions) were collected in 2005 (Fig. 1). The model was initialized with soil surface inputs based on data collected in 2001 for the CT treatment. Other soil properties by horizon were obtained from soil profiles described and sampled in 2005 (Fig. 1). Selected soil properties used for model initialization are shown in Table 1. Carbon fractions were determined for model evaluation on the 2005 soil

samples; i.e., MBC, POC, and TOC. We assumed that the POC fraction corresponded to the slow humus pool in EPIC.

Brief descriptions of the analytical procedures follow. Six soil cores were taken at each sampling location in 2005. Soil cores were cut at 0 to 5 and 5 to 20 cm and air dried. Bulk density was determined for each depth by calculating oven-dry mass per unit volume. Airdry samples were then gently crushed and passed through a 4.75-mm screen. Particulate organic C and MBC were determined with a procedure similar to Franzluebbers et al. (2000). Subsamples (40–60 g) were wet to 50% water-filled pore space and incubated at 25 ± 1°C in 1-L glass jars containing vials with 10 mL of 1.0 *M* NaOH to absorb CO<sub>2</sub>, and small vials containing water to maintain air humidity. At 10 d, a subsample was removed, fumigated with chloroform for 1 d, and then incubated for an additional 10 d under the same conditions to determine the flush of CO<sub>2</sub> representing MBC according to the equation (Voroney and Paul, 1984):

$$SMBC = (mg CO_2 - C kg^{-1} soil)_{fumigated} / k_c$$
[2]

where  $k_{c}$  is an efficiency factor of 0.41.

Evolved CO<sub>2</sub> was determined by titrating the alkali with 1.0 *M* HCl. The particulate organic fraction was determined on the same subsample at the end of 21 d of incubation. Soil was shaken in 100 mL of 0.1 *M* Na<sub>4</sub>P<sub>2</sub>O<sub>7</sub> during 16 h; the suspension was then diluted to 1 L with distilled water and allowed to settle for 5 h, and clay content was determined with a hydrometer. The soil suspension was then passed through a 0.053-mm screen and the retained sand-sized material transferred to a drying bottle and weighed after oven drying; soil C was determined on this fraction. Total organic C was determined

on 0.2 g of finely ground subsamples following the dry combustion method of Nelson and Sommers (1982) using a LECO CN-2000 analyzer (LECO Corp., St. Joseph, MI). The precision of the experiment was calculated by duplicate analysis on 10% of the samples.

On soil pedon samples, particle size distribution was determined by the pipette method following SOM removal with  $H_2O_2$  and dispersion with sodium hexametaphosphate (Kilmer and Alexander, 1949). In situ saturated hydraulic conductivity was measured with a compact constant-head permeameter (Ksat Inc., Raleigh, NC). Water content at field capacity (-33 kPa) and permanent wilting point (-1500 kPa) were determined on soil cores taken from the 0- to -5 and 5- to 20-cm depth, with values for deeper depths estimated by EPIC.

Terrain attributes (e.g., watershed area, slope length and gradient) were obtained with ArcGIS (Version 9.0, ESRI, Redlands, CA).

## **Crop Management**

Tillage, planting, fertilization, harvesting, and associated operation dates and quantities were based on experimental records. Corn in 2001, 2003, and 2005 was fertilized at planting with 56, 45, and 30 kg ha<sup>-1</sup> of N, P<sub>2</sub>O<sub>5</sub>, and K<sub>2</sub>O, respectively. At the V6 to V8 stage, a split application of 112 kg ha<sup>-1</sup> of N was made.

# Model Calibration

The calibration process on the SOC and crop growth modules used data from the CT treatment on the summit landscape position (Fig. 1). Since the summit position is a relatively stable and level area, it was assumed that a steady-state condition was reached in this area under long-term CT. Even though evaluation of the C module was of primary interest, accurate modeling of crop yield and productivity is required for accurate quantification of C additions and their subsequent transformations (Izaurralde et al., 2006).

### **Sensitivity Analysis**

A sensitivity analysis was performed to assess the relative importance of crop growth and soil parameters to model output. Based on data from Wang et al. (2005), the following crop growth parameters were included: (i) biomass/energy ratio (WA), defined as the potential growth rate per unit of intercepted photosynthetically active radiation; (ii) harvest index (HI) or ratio of economic yield to aboveground biomass; (iii) water stress/ harvest index (PARM 3), representing the fraction of the growing season when water stress affects the harvest index; and (iv) Soil Conservation

Table 1. Selected soil properties as affected by landscape position and soil depth used in the 5-yr (2001–2005) EPIC simulation of crop yield and soil organic C fractions.

Soil properties	Layer 1	Layer 2	Layer 3	Layer 4	Layer 5	Layer 6
	Summit					
Lower depth limit, m	0.05	0.20	0.30	0.46	1.04	1.42
Bulk density, Mg m <sup>-3</sup>	1.59	1.65	1.55	1.36	1.36	1.37
Wilting point, m <sup>3</sup> m <sup>-3</sup>	0.11	0.11	0.11	0.14	0.15	0.15
Field capacity, m <sup>3</sup> m <sup>-3</sup>	0.18	0.18	0.18	0.31	0.32	0.30
Sand, %	58.37	54.50	53.72	44.90	41.85	45.16
Silt, %	19.97	26.83	24.63	21.60	20.02	16.24
Clay, %	21.66	18.67	21.65	33.50	38.13	38.60
Soil organic C, %	0.70	0.53	0.53	0.33	0.28	0.26
Saturated conductivity, mm h <sup>-1</sup>	1.20	1.20	1.20	1.48	0.15	0.15
			<u>Side</u>	<u>eslope</u>		
Lower depth limit, m	0.05	0.20	0.28	0.46	0.80	1.00
Bulk density, Mg m <sup>-3</sup>	1.64	1.60	1.37	1.40	1.37	1.35
Wilting point, m <sup>3</sup> m <sup>-3</sup>	0.09	0.09	0.13	0.17	0.19	0.19
Field capacity, m <sup>3</sup> m <sup>-3</sup>	0.20	0.20	0.32	0.33	0.34	0.35
Sand, %	59.53	50.00	41.21	37.96	35.18	32.45
Silt, %	18.20	28.00	25.87	23.45	21.55	22.38
Clay, %	22.27	22.00	32.92	38.59	43.27	45.17
Soil organic C, %	0.58	0.47	0.32	0.28	0.27	0.27
Saturated conductivity, mm h <sup>-1</sup>	6.25	6.25	1.68	0.20	0.08	0.08
	<u>Drainageway</u>					
Lower depth limit, m	0.05	0.20	0.40	0.62	0.98	1.20
Bulk density, Mg m <sup>-3</sup>	1.58	1.69	1.44	1.46	1.34	1.30
Wilting point, m <sup>3</sup> m <sup>-3</sup>	0.05	0.05	0.08	0.14	0.18	0.20
Field capacity, m <sup>3</sup> m <sup>-3</sup>	0.18	0.18	0.27	0.32	0.35	0.36
Sand, %	62.90	57.07	52.66	40.92	31.46	28.27
Silt, %	21.23	30.13	34.31	28.08	22.44	19.31
Clay, %	15.87	12.80	13.03	31.00	46.10	52.42
Soil organic C, %	0.76	0.55	0.38	0.29	0.31	0.31
Saturated conductivity, mm h <sup>-1</sup>	1.96	1.96	3.19	3.33	0.17	0.07

Service curve number index (PARM 42), which regulates the effect of potential evapotranspiration on runoff volume. Different from Wang et al. (2005), we did not include the potential heat unit parameter, because it was estimated as the accumulation of daily mean air temperature above the plant's base temperature (10°C for cotton and 8°C for corn) from planting to maturity.

Soil parameters included for sensitivity analysis as well as ranges and sources are listed in Table 2. Wang et al. (2005) included FHP (the fraction of humus in the passive pool), PARM 20 (microbial decay rate), and FBM (the fraction of organic C in the microbial biomass pool) in their sensitivity analysis, and found that FBM was not influential. For that reason, and because we had analytical data to estimate FBM, we did not include this parameter.

The sensitivity analysis identified relevant parameters for subsequent optimization. We used the extended FAST method (Saltelli et al., 1999; Ratto et al., 2001) to ascertain how variation in EPIC output was apportioned to variation in parameters. This method is model independent, and allows the determination of not only the individual effects of parameters, but also the cumulative interaction effect among parameters.

The extended FAST is based on the estimation of fractional contribution from each input parameter to the variance of the model output. The main effect or first-order sensitivity index  $(S_i)$  represents the average output variance reduction that could be achieved if the parameter  $(X_i)$  were fully known and fixed (Saltelli et al., 1999):

$$S_i = \frac{V[E(Y | X_i)]}{V_Y}$$
[3]

where  $S_i$  is the first-order sensitivity index,  $V[E(Y|X_i)]$  is the expected reduction of total output variance, if the true value of  $X_i$  were known, and  $V_V$  is the output variance.

The total sensitivity index  $(S_{Ti})$  for  $X_i$  was defined as the average output variance that would remain as long as  $X_i$  stayed unknown, and collected in one single term all the interactions involving  $X_i$ :

Table 2. The EPIC parameters included in the sensitivity analyses of the 5-yr (2001–2005) EPIC simulations of crop yield and soil organic C fractions.

Parameter	Description	Range
Yield related		
WA	Riomass operation ka ha-1 MI-1	30-45 (corn)†
	Diomass-energy ratio, kg na mj	11-20 (cotton)‡
HI	Harvest index	0.45-0.60 (corn)†
	That vest muex	0.30-0.60 (cotton)§
PARM 3	Water stress-harvest index	0.3-0.7†
PARM 42	SCS curve number index	0.5-2.0†
Soil organic C	related	
FHP	Fraction of humus in passive pool	0.3-0.9†
PARM 20	Microbial decay coefficient	0.05-1.50+
PARM 45	Humus transformation ratio	0.001-0.05§
PARM 47	Slow humus transformation rate, d <sup>-1</sup>	0.00041-0.00068§
PARM 48	Passive humus transformation rate, d <sup>-1</sup>	0.0000082-0.000015§
PARM 51	Microbial activity in top layer	0.1–1.0§
PARM 52	Residue decay tillage coefficient	5–15§
PARM 53	Microbial activity at depth	0.8–0.95§
PARM 54	Root growth water use coefficient	2.5-7.5§
PARM 55	Root growth water use/depth ratio	0–1§
PARM 56	Root growth depth coefficient	5–10§
+Wang et al. (2)	005)	

†Wang et al. (2005).

‡Rosenthal and Gerik (1991).

§EPIC default range.

$$S_{\mathrm{T}i} = \frac{E[V(Y \mid X_{-i})]}{V_{\mathrm{Y}}}$$

$$[4]$$

where  $S_{Ti}$  is the total sensitivity index,  $E[V(Y|X_{-i})]$  is the expected output variance that would remain unexplained if  $X_i$  were unknown but all other parameters were known  $(X_{-i}$  indicates all the parameters but  $X_i$ .

In general, the sensitivity analysis involved four steps: (i) selection of a range for each input parameter (Table 2); (ii) generation of 1500 parameter sets from the ranges specified in the first step (using a triangular distribution); (iii) evaluation of the model output for each parameter set; and (iv) calculation of sensitivity indices. The second and fourth steps were performed using the public domain software SIMLAB (Version 2.2, Joint Research Centre, European Commission). The third step was facilitated by i\_EPIC (Version 1.1, Center for Agricultural and Rural Development, Ames, IA), a public domain software that manages input and output of multiple EPIC simulations within a single database. We first conducted the sensitivity analysis for crop growth parameters and then for SOC parameters.

#### **Uncertainty Analysis**

After parameters were identified by the sensitivity analysis, an array of 1500 parameter sets was generated, and their respective simulations were conducted. The uncertainties associated with EPIC outputs were estimated with the GLUE technique of Beven and Binley (1992). On the basis of comparing predicted with observed values, each parameter set was assigned a likelihood of being an accurate simulator of the system. For our purposes, likelihood was defined as

$$L(\theta_i \mid X) = \exp\left(-\frac{\text{MSD}_i}{\min(\text{MSD})}\right), \ (i = 1, 2, 3, ..., N)$$
[5]

where X is the observation vector, N is the total number of simulations,  $MSD_i$  is the mean squared deviation for the *i*th model run, and min(MSD) is the minimum MSD. The MSD was calculated as

$$MSD = \frac{1}{n} \sum_{i=1}^{n} (Y_i - X_i)^2$$
 [6]

where  $Y_i$  and  $X_i$  are predicted and observed values, respectively. The likelihood measures were weighted  $[L_w(\theta)]$  using

$$L_{w}(\theta) = \frac{L(\theta_{i} \mid X)}{\sum_{i}^{N} L(\theta_{i} \mid X)}$$
[7]

Weighted likelihood measures had a sum of 1 and yielded a relative probability of acceptability for the parameter sets (Beven, 1993). The uncertainty estimation was performed by computing the model output cumulative distribution and the prediction quantiles. Weighted likelihood measures were calculated using the public domain software GLUEWIN (Version 1.0, Joint Research Centre, European Commission).

#### **Determination of Parameter Values**

At the conclusion of the uncertainty analyses, multiobjective functions were defined for crop yields and C pools (Wang et al., 2005), respectively, as

$$F_{\text{yields}} = \sqrt{\frac{1}{2}L(\theta_i \mid \overline{Y}_{\text{cotton}})^2 + \frac{1}{2}L(\theta_i \mid \overline{Y}_{\text{corn}})^2} \quad [8]$$

$$F_{\text{carbon}} = \sqrt{\frac{1}{3}L(\theta_i \mid \text{TOC})^2 + \frac{1}{3}L(\theta_i \mid \text{POC})^2 + \frac{1}{3}L(\theta_i \mid \text{MBC})^2} \quad [9]$$

where  $L(\theta_i | \overline{Y}_{\text{cotton}})$  and  $L(\theta_i | \overline{Y}_{\text{corn}})$  are the average cotton (2002 and 2004) and corn (2001, 2003, and 2005) yield likelihood weights, respectively; and  $L(\theta_i | \text{TOC}), L(\theta_i | \text{POC})$ , and  $L(\theta_i | \text{MBC})$  are the TOC, POC, and MBC likelihood weights, respectively (calculated using Eq. [7]).

The largest  $F_{yields}$  and  $F_{carbon}$  among the 1500 measurements were identified and the corresponding set of parameter values were used as the calibrated parameters for the site.

#### **Model Validation**

The validation process focused on the crop growth and C modules using data corresponding to the three landscape positions (summit, sideslope, and drainageway) and four treatments (CT, NT, CTm, and NTm).

#### **Statistical Evaluation of Model Performance**

The agreement between simulated (Y) and observed (X) values after model calibration was assessed with a combination of the following criteria: (i) linear regression relating simulated to observed values with intercept not significantly different from zero and slope not significantly different from unity, and (ii) the MSD and its components.

The MSD is the sum of squared deviations between X and Y, divided by the number of observations (Eq. [6]). On perfect equality with Y = X, MSD = 0. The MSD statistic was partitioned into three components (Gauch et al., 2003): (i) inequality of means,

$$IM = (\overline{X} - \overline{Y})^2$$
[10]

(ii) non-unity mean square, defined as

$$NU = (1-b)^2 \left( \sum x_n^2 / N \right)$$
[11]

where *b* is the slope of the least-squares regression of *Y* on *X*, and  $x_n = X_n - \overline{X}$  measures the degree of rotation of the regression line, and (iii) lack of correlation mean square,

$$\mathrm{LC} = \left(1 - r^2\right) \left(\sum y_n^2 / N\right)$$
 [12]

where  $r^2$  is the square of the correlation and  $y_n = Y_n - \overline{Y}$ .

# RESULTS AND DISCUSSION Model Calibration Sensitivity Analysis

The extended FAST sensitivity indices for crop yield and SOC parameters are shown in Tables 3 and 4, respectively. The first-order index for a particular parameter indicates the amount of variance that would be removed from the total output variance if the true value of that parameter were known. Therefore, it shows the relative importance of an individual

Table 3. First and total sensitivity indices for crop yield related parameters (from Table 2) of the 5-yr (2001–2005) EPIC simulations of crop yield and soil organic C fractions.

First-orde	er indices	Total-order indices		
Cotton	Cotton Corn		Corn	
0.00	0.51	0.01	0.50	
0.00	0.49	0.01	0.47	
0.37	0.00	0.36	0.01	
0.62	0.00	0.60	0.01	
0.00	0.00	0.01	0.01	
0.00	0.00	0.01	0.01	
	First-orde Cotton 0.00 0.37 0.62 0.00 0.00	First-order indices           Cotton         Corn           0.00         0.51           0.00         0.49           0.37         0.00           0.62         0.00           0.00         0.00           0.00         0.00	First-order indices         Total-order           Cotton         Corn         Cotton           0.00         0.51         0.01           0.00         0.49         0.01           0.37         0.00         0.36           0.62         0.00         0.60           0.00         0.00         0.01           0.00         0.00         0.01	

parameter. For cotton and corn, WA and HI explained >99% of the output variance. For the C module, FHP and PARM 20 explained most of the variance; FHP was the most influential parameter for MBC and POC, while PARM 20 was for TOC. In addition, PARM 51 (microbial activity in the top layer) was relatively important for MBC.

The total-order index for a particular parameter  $(X_i)$  represents the sum of all sensitivity indices, including all interaction effects. This index indicates those parameters that are relatively unimportant, either alone or in combination with others; therefore, all parameters having low total index can be fixed to any value within their range of uncertainty. Total-order indices for parameters of the crop growth module and for the C module were similar to first-order indices, suggesting minimal interaction.

According to the sensitivity analysis, parameters WA and HI for corn, WA and HI for cotton, and three parameters for the C module (FHP, PARM 20, and PARM 51) were chosen as the most influential on model outputs. Except for PARM 51, parameter selection for the crop growth and SOC modules agreed with Wang et al. (2005).

#### **Uncertainty Analysis**

Distribution of predicted average crop yields (corn and cotton) and SOC fractions (MBC, POC, and TOC) are shown in Fig. 3. The height of the bars is the sum of likelihood weights of the simulations. Distributions were approximately normal. Observed crop yields, except corn in 2005, were within the 90% confidence interval of simulated values. Overall, EPIC accurately simulated cotton yields, with differences between observed and average predicted yields of 53 (1325 - 1272) and -29 kg ha<sup>-1</sup> (1526 – 1555) in 2002 and 2004, respectively. Simulation of corn yield was not as accurate as cotton, with differences between observed and predicted yields of -552 (9728 - 10280), 120 (12890 - 12770) and -1941 (6085 – 8026) kg ha<sup>-1</sup> in 2001, 2003, and 2005, respectively. There was a dry period at the time of corn silking and pollination in 2005 that reduced actual corn yield and was largely not simulated well by EPIC. Guerra et al. (2004) pointed out that EPIC tends to overestimate low yields, especially under conditions of pronounced water stress. In spite of the poor agreement between observed and predicted average yield in 2005,

Table 4. First and total sensitivity indices for soil organic C related parameters (from Table 2) of the 5-yr (2001–2005) EPIC simulations of crop yield and soil organic C fractions microbial biomass C (MBC), particulate organic C (POC), and total organic C (TOC).

Parameter	First-order indices			Total-order indices			
	MBC	POC	TOC	MBC	POC	TOC	
FHP	0.396	0.538	0.394	0.575	0.584	0.416	
PARM 20	0.316	0.260	0.415	0.492	0.284	0.451	
PARM 45	0.001	0.000	0.000	0.022	0.024	0.015	
PARM 47	0.016	0.049	0.051	0.056	0.069	0.070	
PARM 48	0.001	0.000	0.001	0.029	0.017	0.016	
PARM 51	0.182	0.021	0.035	0.207	0.042	0.064	
PARM 53	0.002	0.000	0.000	0.024	0.016	0.015	
PARM 52	0.001	0.001	0.002	0.025	0.017	0.018	
PARM 54	0.005	0.005	0.004	0.022	0.027	0.023	
PARM 55	0.065	0.006	0.008	0.089	0.019	0.024	
PARM 56	0.005	0.001	0.002	0.027	0.016	0.020	

all simulated crop yields fell within the range of observed yields (minimum and maximum observed yields are not shown).

In 2005, measured MBC, POC, and TOC were within the 90% confidence interval of the simulated values. The EPIC model accurately simulated SOC fractions at the 0- to 20-cm depth, with differences between measured and predicted values of  $-52 \text{ kg C ha}^{-1}$  (855 – 907) for MBC, 80 kg ha<sup>-1</sup> (6624 – 6544) for POC, and  $-313 \text{ kg ha}^{-1}$  (19277 – 19590) for TOC. The relatively close agreement between measured and simulated SOC fractions indicates that the analytical methods used to characterize these fractions were adequate.

## **Parameter Estimation**

From the uncertainty analysis and the use of aggregated likelihood functions for crop yields and SOC fractions (Eq. [8–9]), the parameter values were set at 32.42 kg ha<sup>-1</sup> MJ<sup>-1</sup> for WA and 0.50 for HI in corn, and 13.00 kg ha<sup>-1</sup> MJ<sup>-1</sup> for WA and 0.54 for HI in cotton. Parameter values for the C module were set at 0.70 for FHP, 0.55 for PARM 20, and 0.80 for PARM 51.

The value for WA was consistent with reports in the literature. Sinclair and Muchow (1999) summarized 11 studies on radiation use efficiency in corn at different locations and calculated WA values of 32 to 34 kg ha<sup>-1</sup> MJ<sup>-1</sup>. Wang et al. (2005), using a similar EPIC calibration procedure as



Fig. 3. Probability distribution of predicted crop yields and soil organic C fractions. The 5 and 95% quantiles are shown as vertical dotted lines; the mean of predictions across the 1500 simulations is represented by a vertical solid line, and the corresponding measured value is shown as a vertical dashed line.

this in a corn field in south-central Wisconsin, reported WA as  $35.4 \text{ kg ha}^{-1} \text{ MJ}^{-1}$ . Our value for HI of corn was close to values reported in agronomic studies across nine states in the USA (Kiniry et al., 1997), and the value of 0.48 reported by Wang et al. (2005). The value for WA in cotton was similar to the average of three cotton cultivars (14.43 kg ha<sup>-1</sup> MJ<sup>-1</sup>) reported by Rosenthal and Gerik (1991).

Nonhydrolyzable C has been considered the extractable fraction most closely related to the passive SOC pool (Wang et al., 2005). The FHP value we identified was higher than the value (0.51) reported by Paul et al. (1997) for nonhydrolyzable C in a cultivated soil profile of the central USA. Our value for PARM 20, which can be related to the potential transformation of the various C pools, was higher than the value of 0.13 identified by Wang et al. (2005). This could be related to a climate effect, since the warmer and more humid conditions in our study favor an increase in C transformation rates. Overall, the automatic calibration procedure was useful for identifying influential parameters and their values for our experimental site.

## Model Validation Crop Yields

Measured and simulated yields are compared in Fig. 4. In 2001, treatments were in their first year and neither tillage system

nor manure application affected measured crop yields. In addition, it was a dry year with corn receiving only 441 mm of rain during the growing period (Fig. 2). The EPIC model simulated yield variation trends among landscape positions, but mostly overestimated measured yields on summit positions and underestimated measured yields on sideslope and drainageway positions.

Tillage system effects on measured cotton yields were apparent in 2002. This was the driest year for cotton, with rainfall amounts of 354 mm during the growing season. Water use efficiency was maximized under NT, resulting in higher relative yields than the CT systems, especially on summit positions with sandy, well-drained soils, and on the sideslopes with higher runoff. Overall for 2002, EPIC underestimated yield but adequately showed the difference between tillage systems and landscape positions. Manure application did not have a clear effect on either measured or simulated yields.

Corn received 774 mm of rain during the 2003 growing season (wettest year). There were only small differences in measured corn yields among management systems and landscape positions. The greatest difference between tillage systems occurred in the drainageway. The best fit between measured and simulated yields occurred in 2003; overall, EPIC underestimated corn yields, especially on the summit and sideslope positions, but accurately simulated



Fig. 4. Measured and simulated yields affected by landscape position and treatment. CT = conventional tillage; NT = no tillage; CTm = conventional tillage + manure; NTm = no tillage + manure. Standard error bars are shown.

the positive NT effect. There was no clear effect of manure application on measured or simulated corn yields in 2003.

In 2004, EPIC underestimated yields but the effect of landscape position on cotton yield was well simulated. In 2005, EPIC overestimated corn yield on the summit and sideslope positions, but more adequately simulated yield in the drain-ageway. Although the amount of rainfall received by the crop (435 mm) was similar to that in 2001, the driest period happened when corn was silking and pollinating—critical stages for corn grain development. This dry period had greater effects on the crop on summit and sideslope positions, as these soils have less available water than within the drainageway.

Overall, 58% of the simulated yields were within 20% of measured yields (60 simulations were run: 5 yr × four treatments × three soil landscapes). Simulated yield explained 88% of the variation in measured yield (Fig. 5). The regression relating simulated to measured values had a slope of 0.78 and an intercept of 0.81, however, which were significantly different from 1 and 0, respectively. The EPIC model has been shown to accurately simulate long-term mean yields, but may be less accurate for reflecting year-to-year variability (Kiniry et al., 1995). Greater disagreement between simulated and measured yields occurred in dry years, suggesting that the model needs further adjustments on parameters controlling soil hydrology and water use by plants.





#### Mean Squared Deviations of Crop Yields

Gauch et al. (2003) proposed the MSD approach to evaluate the source of error in simulation models. They claimed that MSD and its components were better suited to the X-Y comparison and easier to interpret than regression. The main objective in evaluating model performance is to compare predicted with measured values, rather than fitting the model output to measurements. The three MSD components are additive (their sum equals MSD) and provide further insight into model performance.

Mean squared deviations of crop yield and its components as affected by management and landscape position are shown in Fig. 6. Lowest MSDs were found in the drainageway, followed by the summit and sideslope positions. Within a particular landscape position, the greatest MSD occurred with manure treatments. The highest contributing component of MSD differed among soil landscapes. At the summit position, lack of correlation between measured and pre-



Fig. 6. Mean squared deviations among 12 simulations of crop yields during a 5-yr period on three landscape positions. LC = lack of correlation; NU = non-unity; IM = inequality of means; CT = conventional tillage; NT = no tillage; CTm = conventional tillage + manure; NTm = no tillage + manure.



Fig. 7. Measured and simulated soil microbial biomass C as affected by landscape position and treatment (2005 data) at 0- to 5-, 5- to 20-, and 0- to 20-cm depths. CT = conventional tillage; NT = no tillage; CTm = conventional tillage + manure; NTm = no tillage + manure. Standard error bars are shown.

dicted yield was the major component of MSD. Equality between measured and predicted means was greatest on the summit position. At the sideslope position, the major component of MSD was lack of correlation, although the difference in unity of the regression slope between measured and predicted yield was also important. The lowest MSD was in the drainageway, where the major component of MSD was inequality of means in treatments without manure, and lack of correlation in treatments that received manure.

## **Soil Organic Carbon Fractions**

Measured and simulated fractions of SOC are presented in Fig. 7, 8, and 9. The EPIC model overpredicted MBC (Fig. 7). Tillage and manure effects were not adequately simulated, especially at the 5- to 20-cm depth, where the substrate for microbial activity was lower in NT and NTm than in CT and CTm (residues remained on the surface). Our results suggest there is need for improved simulation of the vertical distribution of MBC. The analytical method used to characterize MBC was similar to the method of Jenkinson and Powlson (1976), which was suggested by Izaurralde et al. (2006) as an appropriate method to initialize the MBC fraction in EPIC. Possibly adjustment of other model parameters would be beneficial, rather than altering MBC methods.

Simulated POC was mostly lower than measured POC (Fig. 8). At the 5- to 20-cm depth, differences between measured and simulated values were small, but EPIC did not adequately estimate variations due to tillage. Higher POC at lower depths



Fig. 8. Measured and simulated particulate organic C as affected by landscape position and treatment (2005 data) at 0- to 5-, 5- to 20-, and 0- to 20-cm depths. CT = conventional tillage; NT = no tillage; CTm = conventional tillage + manure; NTm = no tillage + manure. Standard error bars are shown.

of CT and CTm soils was expected, because tillage operations mix residues to lower depths. Cambardella and Elliott, (1992) suggested that POC closely matches the slow humus pool conceptualized in the Century model. We obtained a relatively close agreement between measured and simulated POC during the calibration process. Therefore, adjustment of other EPIC parameters is suggested, rather than altering POC determination.

The best agreement between measured and simulated SOC fractions was obtained for TOC (Fig. 9). The EPIC model adequately simulated SOC at the 0- to 5-cm depth and satisfactorily simulated other depths. Accuracy in estimation of TOC at the 0- to 20-cm depth has been the strength of Century (Kelly et al., 1997; Pennock and Frick, 2001).

# Mean Squared Deviations of Soil Organic Fractions at the Zero- to Twenty-Centimeter Depth

The MSD for each landscape position was calculated to evaluate how well EPIC had captured the spatial-temporal dynamics of SOC fractions (i.e., MBC, POC, and TOC; Fig. 10). Most of the error associated with the prediction of MBC was related to the inequality of means, while the second significant source of error was lack of correlation.

The largest discrepancy between measured and simulated POC was found on the sideslope and in the drainageway. There was also poor agreement between measured and simulated POC



Fig. 9. Measured and simulated total organic C as affected by landscape position and treatment (2005 data) at 0- to 5-, 5- to 20-, and 0- to 20-cm depths. CT = conventional tillage; NT = no tillage; CTm = conventional tillage + manure; NTm = no tillage + manure. Standard error bars are shown.

means in the drainageway (large inequality of means), while the opposite was true for the sideslope and summit positions.

The largest MSD for TOC was in the drainageway and the smallest was on the sideslope. Most error associated with the prediction of TOC was related to the inequality of means and lack of correlation between measured and simulated values. The slope of the regression between measured and simulated values was closer to unity in the three landscape positions.

Across landscape positions, EPIC explained about 1, 34, and 40% of the total variation (0–20-cm depth) in MBC, POC, and TOC, respectively. Thus, the simulations in this study were relatively less accurate than Izaurralde et al. (2006), where EPIC simulated up to 91% of total variation in soil C for uniform landscapes and management.

# **Temporal Changes in Total Organic Carbon**

Comparison between simulated and measured temporal changes in TOC is shown in Fig. 11. Dairy manure additions and conservation tillage practices increased TOC, but measured C stocks at the 0- to 30-cm depth of these degraded soils were still low. The EPIC model tended to overestimate TOC, but mimicked variations with time. Izaurralde et al. (2006) reported that EPIC overpredicted at low TOC, and suggested that continued development of the model is needed. Sixteen of the 36 simulations were within the standard error of measured



Fig. 10. Mean squared deviations among four simulations of microbial biomass C, particulate organic C, and total organic C (0-20 cm) at the end of 5 yr. LC = lack of correlation; NU = non-unity; IM = inequality of means.

means. Irrespective of landscape position, the best agreement between simulation and measurements was obtained with the CT treatments. Model overestimation on the NT treatments suggests that parameters controlling residue transformation rates warrant further investigation.

## CONCLUSIONS

Automated parameter optimization procedures can be applied to EPIC. Our results generally suggest that the integration of meaningful ranges of parameters with a numerical optimization routine has the potential to estimate valid crop and SOC parameter values.

Simulated crop yields were lower than measured crop yields in most years; however, management effects on crop yields were adequately simulated. Greater disagreement between simulated and measured yields occurred in dry years, suggesting that EPIC



Fig. 11. Measured and simulated total organic C as affected by landscape position and treatment (0–30 cm) in 2001, 2003, and 2005. CT = conventional tillage; NT = no tillage; CTm = conventional tillage + manure; NTm = no tillage + manure. Standard error bars are shown.

needs further refinement on parameters controlling soil hydrology and water use by plants.

The EPIC model adequately explained the variability of total organic C (0–20 cm) as affected by management during a 5-yr simulation. Agreement between measured and simulated active (MBC) and slow pools (POC) was poor, however. We suggest that adjustment of other model parameters is needed. Further studies are needed to improve EPIC predictions of SOC dynamics with depth. Parameters regulating root distribution and residue decomposition with depth should be considered during the calibration process.

Overall, EPIC was sensitive to spatial differences that resulted from differing soil landscapes. The model still needs additional work for accurate simulations of field-scale SOC dynamics affected by short-term management decisions.

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