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Evaluation of the ECOSSE model for simulating soil organic carbon under *Miscanthus* and short rotation coppice-willow crops in Britain

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Abstract

In this paper, we focus on the impact on soil organic carbon (SOC) of two dedicated energy crops: perennial grass *Miscanthus x Giganteus* (*Miscanthus*) and short rotation coppice (SRC)-willow. The amount of SOC sequestered in the soil is a function of site-specific factors including soil texture, management practices, initial SOC levels and climate; for these reasons, both losses and gains in SOC were observed in previous *Miscanthus* and SRC-willow studies. The ECOSSE model was developed to simulate soil C dynamics and greenhouse gas emissions in mineral and organic soils. The performance of ECOSSE has already been tested at site level to simulate the impacts of land-use change to short rotation forestry (SRF) on SOC. However, it has not been extensively evaluated under other bioenergy plantations, such as *Miscanthus* and SRC-willow. Twenty-nine locations in the United Kingdom, comprising 19 paired transitions to SRC-willow and 20 paired transitions to *Miscanthus*, were selected to evaluate the performance of ECOSSE in predicting SOC and SOC change from conventional systems (arable and grassland) to these selected bioenergy crops. The results of the present work revealed a strong correlation between modelled and measured SOC and SOC change after transition to *Miscanthus* and SRC-willow plantations, at two soil depths (0–30 and 0–100 cm), as well as the absence of significant bias in the model. Moreover, model error was within (i.e. not significantly larger than) the measurement error. The high degrees of association and coincidence with measured SOC under *Miscanthus* and SRC-willow plantations in the United Kingdom, provide confidence in using this process-based model for quantitatively predicting the impacts of future land use on SOC, at site level as well as at national level.

Keywords: ECOSSE model, energy crops, land-use change, *Miscanthus*, process-based model, short rotation coppice-willow, soil organic carbon

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Introduction

The European renewable energy directive 2009/28/EC (E.C., 2009) provides a legislative framework for reducing greenhouse gas (GHG) emissions by 20%, while achieving a 20% share of energy from renewable sources by 2020. Energy crops can contribute to both targets by replacing fossil fuel energy sources, as well as increasing soil organic carbon (SOC) sequestration, that is the long-term storage of carbon (C) in soil (Clifton-Brown *et al.*, 2004). In this paper, we focus on the impact on SOC of two dedicated energy crops: short rotation coppice (SRC)-willow and perennial grass *Miscanthus x Giganteus* (*Miscanthus*).

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Short rotation coppicing is a system of semi-intensive cultivation of fast-growing, woody species. The rotations between harvests are short (3–4 years) in comparison with longer rotations in typical forests (Don *et al.*, 2012), and the frequent harvests enhance root turnover (Block *et al.*, 2006). Annual leaf litter in Europe has been estimated to be on average between 1 and 5 t ha^{-1} (Baum *et al.*, 2009); therefore, inputs of organic matter to soils under SRC are assumed to be relatively high compared to conventional crops. Moreover, no tillage is required during the lifetime of SRC which may enhance SOC sequestration (West & Post, 2002; Walter *et al.*, 2015).

Short rotation coppicing of willow has a high potential to increase SOC due to the abundant above- and belowground biomass input. For example, a study by Tufekcioglu *et al.* (2003) reported that willow trees in

Iowa, USA, can have greater productivity of fine root biomass than corn (5.8 t ha^{-1} vs. 0.9 t ha^{-1} for corn, 7 years after establishment). Zan *et al.* (2001) established a factorial experiment with 4-year-old energy plantations in south-western Quebec, Canada. They reported an average SOC sequestration at 0–60 cm soil depth across sites, not including belowground biomass, of 130 t C ha^{-1} following planting of willow, compared to 110 t C ha^{-1} measured in soil on abandoned agricultural fields used as a baseline for comparison and therefore an estimated SOC sequestration rate under willow of approximately 4 t C ha^{-1} yr^{-1}. In a study of three mixed poplar, aspen and willow plantation sites across Germany, a small increase in SOC (45 and 44 t C ha^{-1}, under current vegetation and former arable soils, respectively) of 0.1–0.6 t C ha^{-1} yr^{-1} in the upper 30 cm soil was observed after 7 years of transition from former arable soil (Jug *et al.*, 1999; Meki *et al.*, 2014).

In the United Kingdom, SRC-willow has been identified as the bioenergy crop with the greatest potential for C mitigation across the United Kingdom (Smith *et al.*, 2000a,b). Willow is an ideal species for SRC in the United Kingdom because of its vigorous shoot regeneration after coppicing, and its suitability to regional climate and soil conditions (Britt *et al.*, 1995; Grogan & Matthews, 2002). Grogan & Matthews (2002) estimated a SOC sequestration rate to 50 cm soil depth of 0.5 t C ha^{-1} yr^{-1} under SRC-willow plantations in the United Kingdom. They developed a model to characterize the essential processes underlying SOC dynamics relating to SOC sequestration but stressed the need for further model development to account for the dynamics of the system within each season, as well as for regional variations in yield and soil C inputs and outputs.

Miscanthus is one of the most promising dedicated energy crops with around 16 000 ha being established in the United Kingdom (Don *et al.*, 2012). Several features of *Miscanthus*' physiology and the agricultural practices associated with its cultivation suggest a large potential for SOC sequestration (Dondini *et al.*, 2009a). *Miscanthus* is usually harvested in spring to allow winter senescence to reduce plant moisture content. Leaving the crop standing over winter increases litter fall, leading to the accumulation of biomass on the soil surface (Zimmermann *et al.*, 2013). In addition, as a rhizomatous crop it allocates a large proportion of the aboveground C to the roots and rhizomes during winter senescence, further increasing SOC stocks (Kuzyakov & Domanski, 2000). When *Miscanthus* is planted on former arable land, the absence of soil tillage results in less soil disturbance which, in turn, enhances SOC stabilization processes (Clifton-Brown *et al.*, 2007).

The amount of SOC sequestered by *Miscanthus* is a function of site-specific factors including soil texture, management practices, initial SOC levels and climate (Lemus & Lal, 2005); for these reasons, both losses and gains in SOC were observed in *Miscanthus* studies (Hansen *et al.*, 2004; Clifton-Brown *et al.*, 2007). Several studies quantifying the changes in SOC on converting arable land to *Miscanthus* energy crop reported an increase in SOC; the reported SOC change rate, however, varied largely across and within experiments, ranging from 0.8 to 2.8 t C ha^{-1} yr^{-1} (Kahle *et al.*, 1999; Hansen *et al.*, 2004; Dondini *et al.*, 2009a,b; Zimmermann *et al.*, 2011; Felten & Emmerling, 2012). Changes from pasture to a *Miscanthus* energy crop have a small effect on SOC. In a review of the effect of land-use change to bioenergy production in Europe, Don *et al.* (2012) estimated a SOC change of −0.09 t C ha^{-1} yr^{-1} if grassland was converted to *Miscanthus*. On the other hand, Zatta *et al.* (2014) reported that planting on semipermanent grasslands with a range of *Miscanthus* genotypes did not deplete SOC significantly after 6 years from establishment. Moreover, the authors suggested that it is highly unlikely that a reduction in SOC levels relative to initial values with increasing stand age will occur.

Methods for the determination of SOC involve direct and indirect approaches. Direct methods employ field and laboratory measurements of SOC stocks, but field documentation of SOC changes faces many challenges because of the heterogeneity of soils, environmental conditions, land-use history, sampling methods and analytical errors. Therefore, indirect methods, which require the use of process-based models, are used to predict SOC changes temporally and spatially (Saby *et al.*, 2008). Computer models can also complement and extend the applicability of information collected in field trials (Meki *et al.*, 2013). Combining measurement of SOC with models also provides a useful tool to test the model performance to simulate soil processes with a higher degree of confidence. In fact, model evaluation involves running a model using input values that have not been used during the calibration process, demonstrating that it is capable of making accurate simulations on a wide range of conditions (Moriasi *et al.*, 2007).

Although several soil C models have been developed for conventional agricultural and forest systems, most of them have not been fully parameterized and effectively tested for application on *Miscanthus* and SRC-willow (Dimitriou *et al.*, 2012; Borzęcka-Walker *et al.*, 2013; Robertson *et al.*, 2015). Here we focus on the applicability of the process-based model ECOSSE to predict SOC sequestration and SOC changes after transition to *Miscanthus* and SRC-willow.

The development of the ECOSSE model was mainly due to the need to simulate the C and nitrogen (N)

cycles using minimal input data on both mineral and organic soils (Smith *et al.*, 2010a,b). The ECOSSE model has already been validated and applied spatially to simulate land-use change impacts on SOC and GHG emissions over different soil types, to simulate SOC change under energy crops and to simulate soil N and nitrous oxide (N_2O) emissions in cropland sites in Europe (Smith *et al.*, 2010b; Bell *et al.*, 2012). It has also been previously evaluated against a range of soils under short rotation forestry (SRF) plantations across the United Kingdom (Dondini *et al.*, 2015).

This paper evaluates the suitability of ECOSSE for estimating SOC sequestration from SRC-willow and *Miscanthus* soils in the United Kingdom after land-use change from conventional systems (grassland and arable). Based on the previous published recommendations, a combination of graphical techniques and error index statistics have been used for model evaluation (Moriasi *et al.*, 2007). Model testing is often limited by the lack of field data to which the simulations can be compared (Desjardins *et al.*, 2010) and by inconsistent sampling approaches and soil depths. In this study, the model is evaluated against observations at 29 locations in the United Kingdom, comprising 19 paired transitions to SRC-willow and 20 paired transitions to *Miscanthus*, and two soil depths (0–30 and 0–100 cm), meaning that the mechanistic processes of ECOSSE can be thoroughly evaluated.

Materials and methods

ECOSSE model

The ECOSSE model includes five pools of soil organic matter (SOM), each decomposing with a specific rate constant. Decomposition is sensitive to temperature, soil moisture and vegetation cover, and so soil texture, pH, bulk density and clay content of the soil along with land-use and monthly climate data are the inputs to the model (Coleman & Jenkinson, 1996; Smith *et al.*, 1997). The ECOSSE model simulates the C and N cycles for six categories of vegetation: arable, grassland, forestry, and seminatural, SRC-Willow and *Miscanthus*.

The soil input of the vegetation (SI) is estimated by a modification of the Miami model (Lieth, 1972), which is a simple conceptual model that links the climatic net primary production of biomass (NPP) to annual mean temperature (T) and total precipitation (P) (Grieser *et al.*, 2006). Separate estimates are obtained for NPP as a function of temperature and precipitation according to empirical relationships, and the Miami estimate of NPP is found as the minimum of these two estimates. The NPP estimated by the Miami model is then rescaled for each land-cover type. The scaling factor for *Miscanthus* (1.6) was calculated as the ratio of mean UK yield estimated using Miscanfor (Hastings *et al.*, 2014), converted to NPP, to mean UK NPP estimated by Miami. The scaling factor for SRC-willow (0.875) was calculated by adjusting the *Miscanthus* scaling factor by the ratio of SRC-willow yield values (Styles *et al.*, 2008) to *Miscanthus* yield values. SI is then estimated as a fixed proportion of the rescaled NPP according to the land cover, as described by Schulze *et al.* (2010). The linear rescaling of the nonlinear Miami functions is reasonable given the near-linear behaviour of the Miami functions in the temperature and precipitation range of the United Kingdom. The NPP estimated by the Miami model is a function of climatic variables only; therefore, it does not capture the effects of other local environmental factors such as N inputs. However, the rescaling factors derived for each land-use type implicitly account for standard management practices. For a full description of the ECOSSE model, refer to Smith *et al.* (2010a).

The minimum ECOSSE input requirements for site-specific simulations are as follows:

Climate/atmospheric data:

- Thirty years of average monthly rainfall, potential evapotranspiration (PET) and temperature and
- Monthly rainfall and temperature.

Soil data:

- Initial SOC content,
- Soil sand, silt and clay content,
- Soil bulk density,
- Soil pH and
- Soil depth.

Land-use data:

- Land use for each simulation year.

The initialization of the model is based on the assumption that the SOC is at steady state under the initial land use at the start of the simulation. Previous work has used SOC measured at steady state to determine the plant inputs that would be required to achieve an equivalent simulated value (e.g. Smith *et al.*, 2010a). This approach iteratively adjusts plant inputs until measured and simulated values of SOC converge. Running the simulations to steady state with this adjusted rate of plant input therefore provides an estimate of the activity of the SOM as expressed by the relative C pool sizes of the decomposable plant material, resistant plant material, microbial biomass (BIO) and humified organic matter. However, where input data are missing, most notably the description of the drainage of the soil, the OM in soil with restricted drainage is actually decomposing more slowly than would be calculated from the available soil descriptors. This results in an unrealistically high estimate of plant inputs to compensate for the elevated simulated decomposition rate. In the absence of additional measurements, estimates of plant inputs from the NPP model Miami (Lieth, 1972, 1973) can be used to account for rate modifiers that are missing due to the lack of input data. This approach instead fixes the plant inputs at the rate estimated by the Miami model and then iteratively adjusts an additional decomposition rate modifier until the SOC simulated using long-term climate data converges with the measured value. The same rate modifier is used for all pools, so this approach is adjusting the overall activity of the SOM to account for the missing input data, not the rate constants of the pools, which

Table 1 Details of vegetation type, duration between establishment and sampling, and location of the study sites

Site no.	Transitions (previous land use in bold)	Latitude, Longitude	Duration between establishment and sampling (years)
1	SRC-willow	53.7, −0.8	5
2	SRC-willow		12
1 + 2C	**Arable**		20+
3	SRC-willow	53.2, −0.8	11
4	SRC-willow		7
4C	**Arable**		20+
5	SRC-willow	53.2, −0.7	4
5C	**Grassland**		20+
6	SRC-willow	54.6, −2.7	13
6C	**Arable**		20+
7	SRC-willow		4
7C	**Grassland**		7
8	SRC-willow	50.9, −0.4	4
8C	**Grassland**		12
9	SRC-willow	51.7, −0.9	5
10	*Miscanthus*		5
9 + 10C	**Arable**		32
11	*Miscanthus*	54.0, −1.2	5
11C	**Arable**		20+
12	*Miscanthus*	54.1, −1.1	6
12C	**Grassland**		4
13	*Miscanthus*	53.4, −0.5	2
13C	**Arable**		20+
14	*Miscanthus*	53.2, 0.1	7
14C	**Grassland**		6
15	SRC-willow	51.5, −0.8	6
15C	**Arable**		20+
16	*Miscanthus*	51.5, −1.3	5
16C	**Arable**		20+
17	SRC-willow	51.5, −1.6	22
17C	**Grassland**		Unknown
18	SRC-willow		7
18C	**Arable**		Unknown
19	*Miscanthus*	51.8, −1.6	5
19C	**Arable**		20+
20	SRC-willow	52.2, −1.9	9
22	SRC-willow		22
20, 22C	**Grassland**		32+
23	*Miscanthus*	53.2, −3.7	5
23C	**Grassland**		8
24	*Miscanthus*	52.4, −4.0	1
24C	**Grassland**		22
25	*Miscanthus*	51.2, −2.8	9
25C	**Grassland**		20+
26	SRC-willow	50.7, −2.4	5
26C	**Arable**		20+
27	*Miscanthus*	51.0, −3.1	10
27C	**Arable**		20+
28	*Miscanthus*		10
28C	**Grassland**		29
29	*Miscanthus*	50.5, −4.8	9
29C	**Grassland**		10
30	*Miscanthus*	50.4, −4.6	5
30C	**Arable**		Unknown
31	*Miscanthus*		7
31C	**Pasture**		20+
33	SRC-willow	56.0, −3.6	14
33C	**Arable**		20+
34	SRC-willow	56.2, −3.2	6
34C	**Grassland**		Unknown
35	SRC-willow	51.7, −4.7	9
35C	**Grassland**		20+
36	*Miscanthus*		8
36C	**Arable**		20+
37	SRC-willow	54.8, −2.9	6
37C	**Arable**		Unknown
38	*Miscanthus*	52.6, 2.0	6
38C	**Grassland**		14
39	*Miscanthus*		6
39C	**Arable**		39
40	*Miscanthus*	52.5, −0.5	5
40C	**Arable**		20+
41	SRC-willow		5
42	*Miscanthus*	53.1, −0.4	5
41/42C	**Arable**		20+

SRC, short rotation coppice.

remain a fixed characteristic of the model. The rate modifier calculated in this way is then used unchanged for any subsequent calculations to determine the impact of changes in land use. Here we are testing a modelling approach that can also be applied at large scales, so rather than measuring additional values at the specific sites, we used the above approach to evaluate the model using only the input data that would be available in large-scale simulations.

Data

In 2012/2013, 29 sites, including a total of 40 transitions, were sampled in Britain using a paired site comparison approach (Keith *et al*., 2015). The sites and the relative measurements contribute to the ELUM (Ecosystem Land Use Modelling & Soil Carbon GHG Flux Trial) project, which was commissioned and funded by the Energy Technologies Institute (ETI). Each transition consisted of one reference field (arable or grassland, depending on the previous land use of the site) and one adjacent bioenergy field (*Miscanthus* or SRC-willow); some sites contained multiple transitions. At each site, soil samples were collected at two soil depths, for a total of 40 transitions sampled at 0–30 cm soil depth and 38 transitions sampled at 0–100 cm soil depth. In total, 12 arable to SRC-willow transitions, eight grassland to SRC-willow transitions, 11 arable to *Miscanthus* transitions and nine grassland to *Miscanthus* transitions were sampled (Table 1).

The soil of each bioenergy plantation or control field was sampled using a hierarchical design (Keith *et al*., 2015), developed to capture variability across different spatial scales (Conant & Paustian, 2002; Conant *et al*., 2003). Five sampling plots per field were randomly selected, and three soil cores

Table 2 Long-term (30 years) monthly rainfall and temperature at the location of the study sites. Monthly rainfall and temperature were extracted from the E-OBS data set (Haylock *et al.*, 2008; http://eca.knmi.nl/). Monthly PET was estimated using the Thornthwaite method (Thornthwaite, 1948)

Site code	1, 2	3, 4, 5	6, 7	8	9, 10	11	12	13	14	15	16	17, 18	19	20, 22	23	24	25	26	27, 28	29	30, 31	33	34	35	37	38	39	40	41
Rainfall (mm month^{-1})																												
January	52	49	139	80	56	57	57	48	51	63	58	64	63	65	128	152	78	84	85	116	111	107	86	90	104	63	63	50	48
February	40	38	99	53	42	41	41	37	37	45	42	45	46	48	95	112	57	63	63	89	85	74	60	65	77	47	47	38	37
March	43	41	101	55	45	45	45	41	41	48	46	50	51	51	94	124	56	62	62	79	75	77	63	65	79	50	50	41	41
April	45	46	68	47	47	48	48	45	40	49	45	46	48	53	77	86	50	51	53	64	60	51	45	53	56	53	53	44	43
May	44	45	69	45	50	45	45	45	43	52	52	53	55	53	69	82	51	51	54	61	57	58	53	52	61	53	53	47	45
June	57	57	73	49	52	59	59	54	49	52	51	51	53	58	72	93	55	56	58	64	60	63	60	56	67	58	58	53	56
July	50	47	84	43	44	52	52	49	47	44	43	47	50	53	74	105	53	50	57	67	61	67	63	56	74	53	53	48	49
August	57	53	95	51	54	60	60	55	54	56	55	55	58	62	88	114	62	56	67	75	69	74	67	70	80	62	62	54	55
September	50	48	101	61	52	52	52	47	47	54	52	54	57	59	103	121	62	62	68	80	75	82	71	69	83	59	59	50	49
October	54	52	135	86	62	57	57	52	54	66	62	65	65	66	133	174	80	82	89	110	103	102	87	103	105	67	67	53	55
November	54	51	136	86	62	58	58	52	55	68	64	66	64	65	144	171	78	86	87	121	114	96	78	108	103	65	65	54	53
December	57	53	138	82	59	60	60	53	52	64	63	67	67	67	141	168	83	92	89	118	112	95	77	95	104	67	67	52	51
Temperature (°C)																												
January	3.9	4.0	2.3	5.0	4.2	3.5	3.5	4.0	4.1	4.0	4.4	4.2	4.1	4.0	3.4	3.9	5.0	4.7	5.0	5.6	6.3	3.0	3.3	5.9	3.2	3.9	3.9	3.9	4.1
February	4.2	4.2	2.6	4.9	4.3	3.9	3.9	4.2	4.2	4.2	4.5	4.3	4.2	4.1	3.2	3.9	5.0	4.7	5.0	5.4	6.1	3.4	3.7	5.7	3.6	4.0	4.0	4.1	4.4
March	6.1	6.3	4.1	6.7	6.4	5.7	5.7	6.3	6.2	6.2	6.5	6.3	6.2	6.0	4.7	5.4	6.7	6.3	6.6	6.6	7.3	5.1	5.3	6.9	5.3	6.0	6.0	6.2	6.5
April	8.2	8.3	6.3	8.8	8.5	7.7	7.7	8.3	8.1	8.3	8.6	8.4	8.3	8.1	6.5	7.3	8.6	8.1	8.5	8.0	8.8	7.2	7.4	8.5	7.4	8.1	8.1	8.3	8.6
May	11.2	11.4	9.4	12.1	11.8	10.7	10.7	11.4	11.3	11.6	11.8	11.7	11.6	11.3	9.5	10.3	11.8	11.4	11.6	10.8	11.6	10.0	10.2	11.2	10.4	11.3	11.3	11.5	11.6
June	14.1	14.4	12.0	14.9	14.8	13.5	13.5	14.4	14.2	14.6	14.8	14.6	14.5	14.1	12.0	12.6	14.6	14.2	14.4	13.4	14.1	12.8	12.9	13.6	13.0	14.1	14.1	14.4	14.5
July	16.3	16.5	14.0	17.0	17.0	15.7	15.7	16.6	16.4	16.8	17.1	16.8	16.8	16.4	13.9	14.6	16.7	16.3	16.5	15.4	16.0	14.6	14.7	15.5	15.0	16.2	16.2	16.6	16.8
August	16.2	16.4	13.6	17.0	16.9	15.6	15.6	16.5	16.5	16.7	16.9	16.6	16.6	16.1	13.8	14.4	16.6	16.2	16.4	15.5	16.2	14.4	14.6	15.7	14.6	16.0	16.0	16.6	16.6
September	13.8	14.0	11.3	14.8	14.3	13.3	13.3	14.1	14.3	14.1	14.3	14.1	14.0	13.7	11.9	12.6	14.3	13.9	14.2	13.7	14.4	12.0	12.3	14.1	12.3	13.6	13.6	14.1	14.2
October	10.4	10.5	8.3	11.7	10.7	10.0	10.0	10.6	10.8	10.6	10.8	10.7	10.5	10.3	9.1	9.7	11.2	10.9	11.1	11.1	11.8	8.9	9.2	11.6	9.3	10.2	10.2	10.5	10.7
November	6.7	6.7	5.0	8.0	6.9	6.3	6.3	6.8	7.0	6.8	7.1	7.0	6.9	6.7	6.1	6.6	7.7	7.4	7.7	8.2	8.9	5.5	5.8	8.7	5.8	6.6	6.6	6.7	7.0
December	4.4	4.5	2.8	5.7	4.7	4.1	4.1	4.5	4.7	4.5	4.9	4.7	4.6	4.5	4.0	4.4	5.5	5.3	5.6	6.3	7.0	3.4	3.6	6.7	3.6	4.3	4.3	4.4	4.4

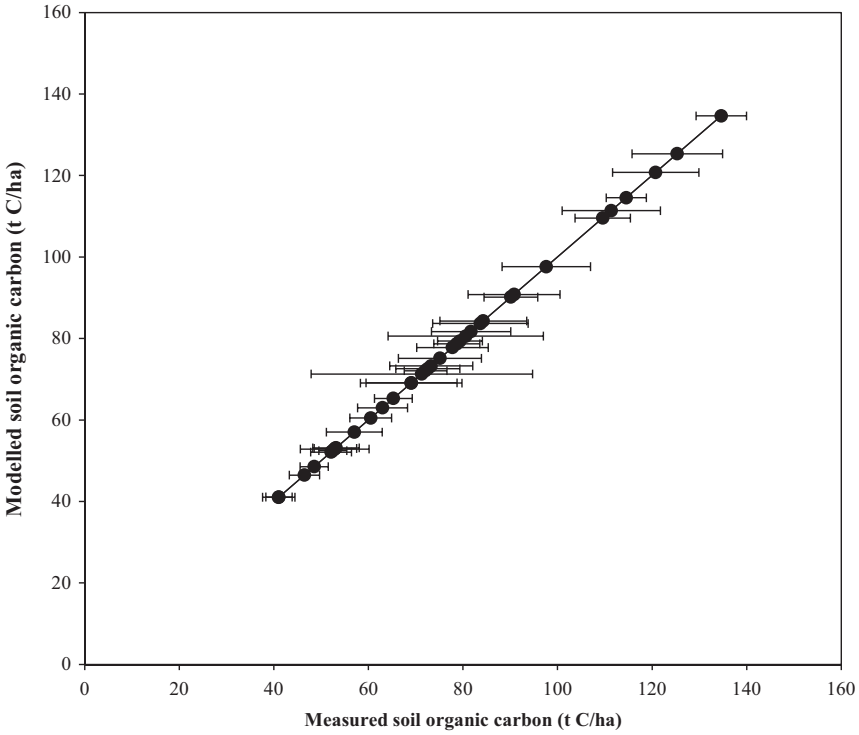

Fig. 1 Correlation between measured and modelled SOC at the reference sites at 0–30 cm soil depth. Error bars represent 95% confidence interval of measured values. SOC, soil organic carbon.

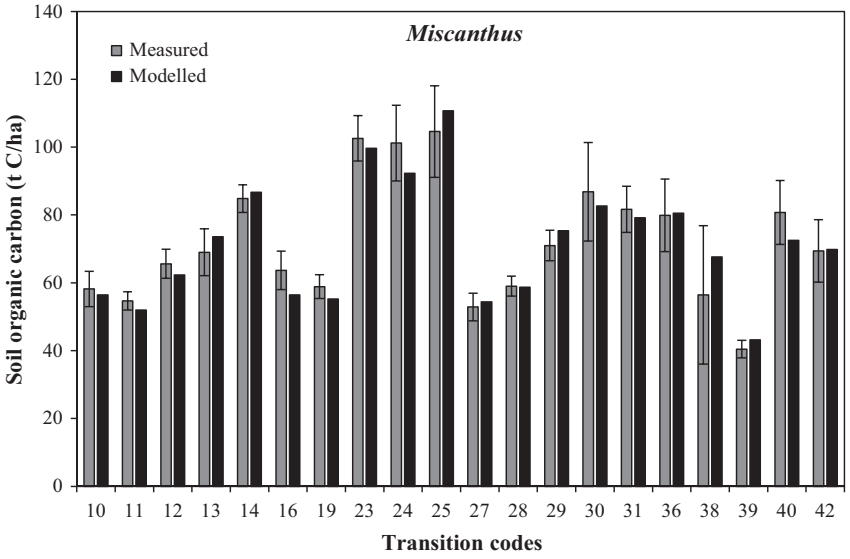

Fig. 2 Comparison between modelled and measured SOC at the *Miscanthus* sites at 0–30 cm soil depth. Error bars represent 95% confidence interval of measured values. SOC, soil organic carbon.

were taken to a depth of 30 cm within each sampling plot. Soil cores were divided in the field into 0–15 and 15–30 cm (measuring from the base of the core). One of the five sampling plots was randomly selected and three 1-m cores were taken, except for site 38. Due to the high stones content at site 38, it was possible to sample just two 1-m cores. On return to the laboratory, the 1-m cores were divided into four sections: 0–15, 0–30, 30–50 and 50–100 cm. The rationale behind the sampling approach for the 1-m soil cores was largely based on feasibility and practicality.

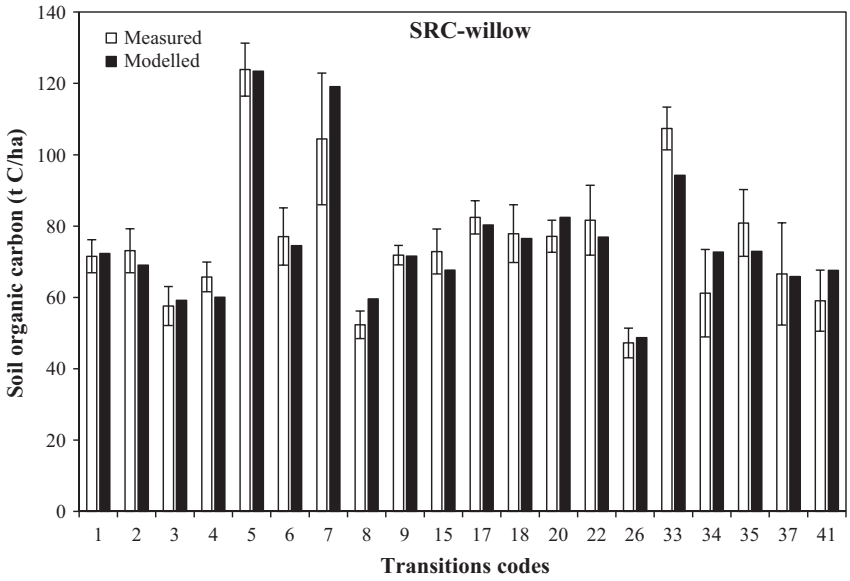

Fig. 3 Comparison between modelled and measured SOC at the SRC-willow sites at 0–30 cm soil depth. Error bars represent 95% confidence interval of measured values. SOC, soil organic carbon; SRC, short rotation coppice.

Table 3 ECOSSE model performance at simulating soil C at the reference sites at 0–30cm soil depth, *Miscanthus* and SRC-willow fields for two soil depths (0–30 and 0–100 cm). Association is significant for $t > t$ (at $P = 0.05$). Model bias is not significant for $E < E_{95}$. Error between measured and modelled values is not significant for $F < F$ (critical at 5%)

	0–30 cm depth			0–100 cm depth	
	Reference	*Miscanthus*	SRC-willow	*Miscanthus*	SRC-willow
r = Correlation coefficient	1.0	0.95	0.72	0.93	0.9
t-value	79.38	12.27	4.37	10.24	8.15
t-value at ($P = 0.05$)	2.03	2.11	2.1	2.11	2.13
E = Relative error	0	2	2	3	−3
E_{95} (95% Confidence limit)	9	13	10	92	87
F	0	0.01	0.08	0	0
F (Critical at 5%)	1.48	1.69	1.69	1.71	1.77
Number of values	40	20	20	20	18

SRC, short rotation coppice.

Air-dried soil samples were sieved to 2 mm, and the mass and volume of stones and roots remaining on the sieve were recorded. A subsample of the sieved soil was oven-dried (105 °C for 12 h) and subsequently ball-milled (Fritsch Planetary Mill); samples were analysed for %C using a LECO TruSpec CN analyser (Leco, TruSpec CN, St. Joseph, MI, USA), and a 100 mg subsample was used for the assessment of OC concentration using an elemental analyser (Leco, TruSpec CN). Prior to OC analysis, soil subsamples that were either from sites located on soil types known to contain inorganic C or which had pH values >6.5 were tested for the presence of inorganic C. Samples that tested positive were treated to remove inorganic C by acid fumigation following the procedure detailed by Harris *et al.* (2001).

The change in SOC was assumed to be the difference between the bioenergy and non-bioenergy pair. Measurements of SOC, soil bulk density, soil texture and soil pH, as well as information on the land-use history, were collated for each field. Soil texture was determined for the top 30 cm soil depth; therefore, soil texture data for the 30–100 cm soil depth were extracted from soil data at 1 km resolution for England and Wales, Scotland and Northern Ireland as described in Bradley *et al.* (2005), first used to run RothC in support of the Land use, land-use change and forestry (LULUCF) inventory (Falloon *et al.*, 2006).

Air temperature and precipitation data at each location were extracted from the E-OBS gridded data set from the EU-FP6 project ENSEMBLES, provided by the ECA&D project (Haylock *et al.*, 2008), publicly available at http://eca.knmi.nl/. For each location, monthly air temperature and precipitation for each simulated year was collated and a long-term (30 years before transition) average was also calculated (Table 2). Monthly PET was estimated using the Thornthwaite method (Thornthwaite,

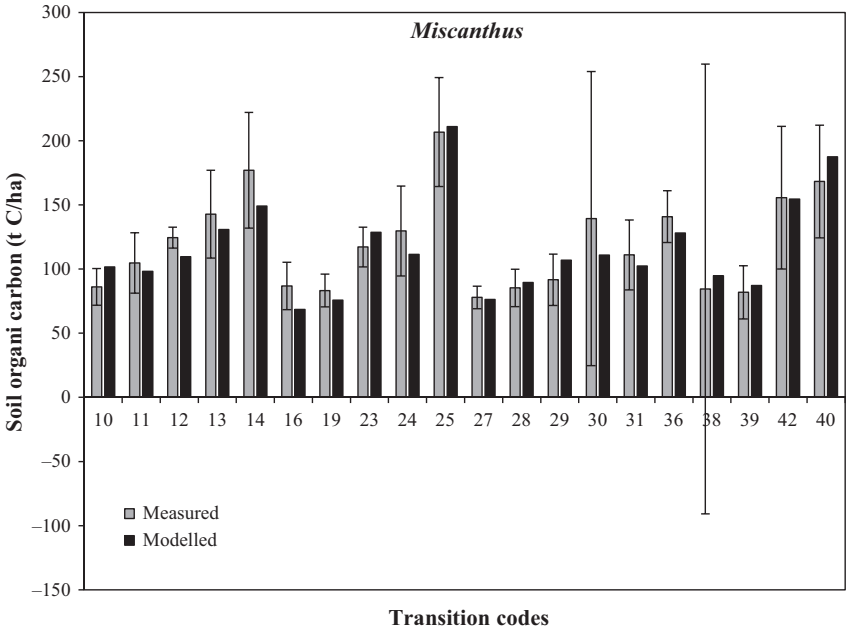

Fig. 4 Comparison between modelled and measured SOC at the *Miscanthus* sites at 0–100 cm soil depth. Error bars represent 95% confidence interval of measured values. SOC, soil organic carbon

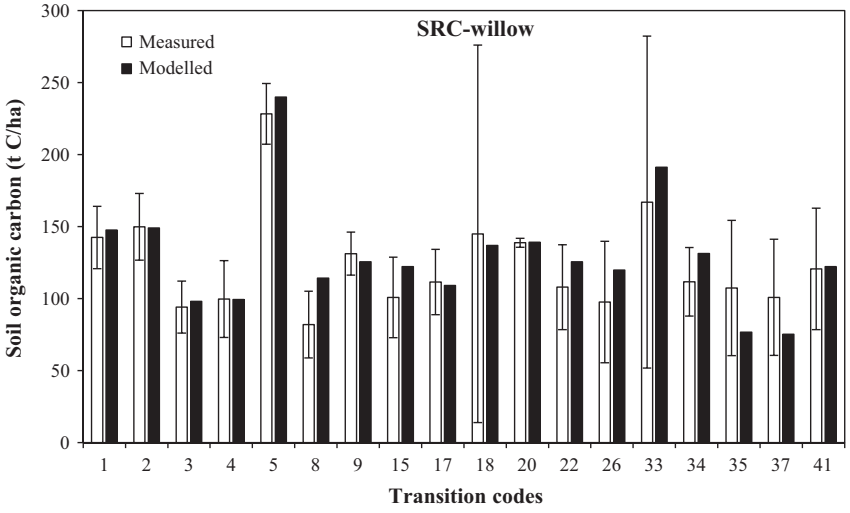

Fig. 5 Comparison between modelled and measured SOC at the SRC-willow sites at 0–100 cm soil depth. Error bars represent 95% confidence interval of measured values. SOC, soil organic carbon; SRC, short rotation coppice.

1948), which has been used in other modelling studies when direct observational data have not been available (e.g. Smith *et al*., 2005; Yokozawa *et al*., 2010; Bell *et al*., 2012).

Model evaluation

At each site, each transition from conventional (arable or grassland) to bioenergy crop (*Miscanthus* or SRC-willow) was modelled and the simulated SOC was compared to the measured SOC. Based on the site information provided, the measured SOC at each reference arable/grassland site was used as the starting C input to the model, assuming that the soil at the reference site had been in equilibrium before the transition. The model has not been recalibrated or reparameterized using the data presented in this study; therefore, the presented results are an independent test of the ability of the model to simulate SOC under *Miscanthus* and SRC-willow as well as change in SOC from grassland/arable.

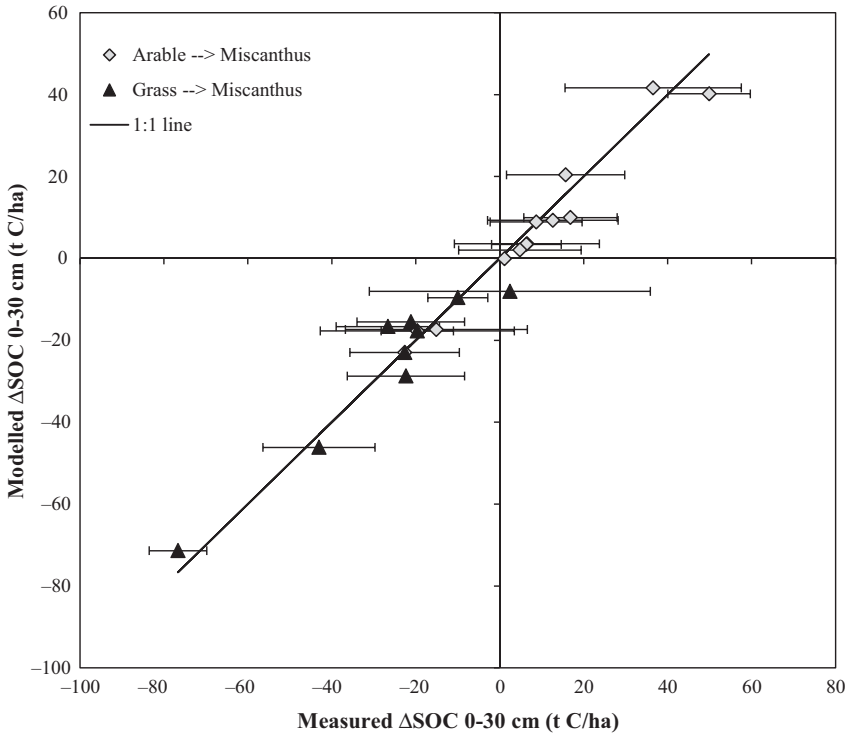

Fig. 6 Measured and modelled change in SOC after transition to *Miscanthus* at 0–30 cm soil depth. Error bars represent 95% confidence interval of measured values. Solid line represents 1 : 1 correlation between measured and modelled values. SOC, soil organic carbon.

The model was evaluated using input data of measured SOC at the start of the simulation, bulk density and soil texture. Simulations were carried out for 0–30 and 0–100 cm soil depths.

A quantitative statistical analysis was undertaken to determine the coincidence and association between measured and modelled values, following the methods described in Smith *et al.* (1997) and in Smith & Smith (2007). The statistical significance of the difference between model outputs and experimental observations can be quantified if the standard error of the measured values is known (Hastings *et al.*, 2010). The standard errors (data not shown) and 95% confidence intervals around the mean measurements were calculated for all field sites.

The degree of association between modelled and measured values was determined using the correlation coefficient (r). Values for r range from −1 to +1. Values close to −1 indicate a negative correlation between simulations and measurements, values of 0 indicate no correlation, and values close to +1 indicate a positive correlation (Smith *et al.*, 1996). The significance of the association between simulations and measurements was assigned using a Student's t-test as outlined in Smith & Smith (2007).

The bias was expressed as a percentage using the relative error, E. The significance of the bias was determined by comparing to the value of E that would be obtained at the 95% confidence interval of the replicated values (E_{95}). If the relative error is less than the 95% error (i.e. $E < E_{95}$), the model bias cannot be reduced using these data.

Analysis of coincidence was undertaken to establish how different the measured and modelled values were. The degree of coincidence between the modelled and measured values was determined using the lack of fit statistic (*LOFIT*) and its significance was assessed using an F-test (Whitmore, 1991) indicating whether the difference in the paired values of the two data sets is significant. All statistical results were considered to be statistically significant at $P < 0.05$.

Results

The model simulations of the SOC show a good fit against the measured SOC, for both reference (Fig. 1) and bioenergy crops (*Miscanthus* and SRC-willow), at 0–30 cm soil depth (Figs 2 and 3, respectively).

All the reference sites have been simulated for a time period of ≥30 years without any land-use change and using the field measurements as inputs to the model. Based on the site histories, we assumed that all the reference sites were in equilibrium at the time of sampling. The r value (1) of the reference sites at 0–30 cm soil depth showed a significant ($P < 0.05$) association between modelled and measured values, as well as no significant model bias ($E < E_{95}$) (Table 3).

The correlations between modelled and measured SOC at the *Miscanthus* and SRC-willow fields, at

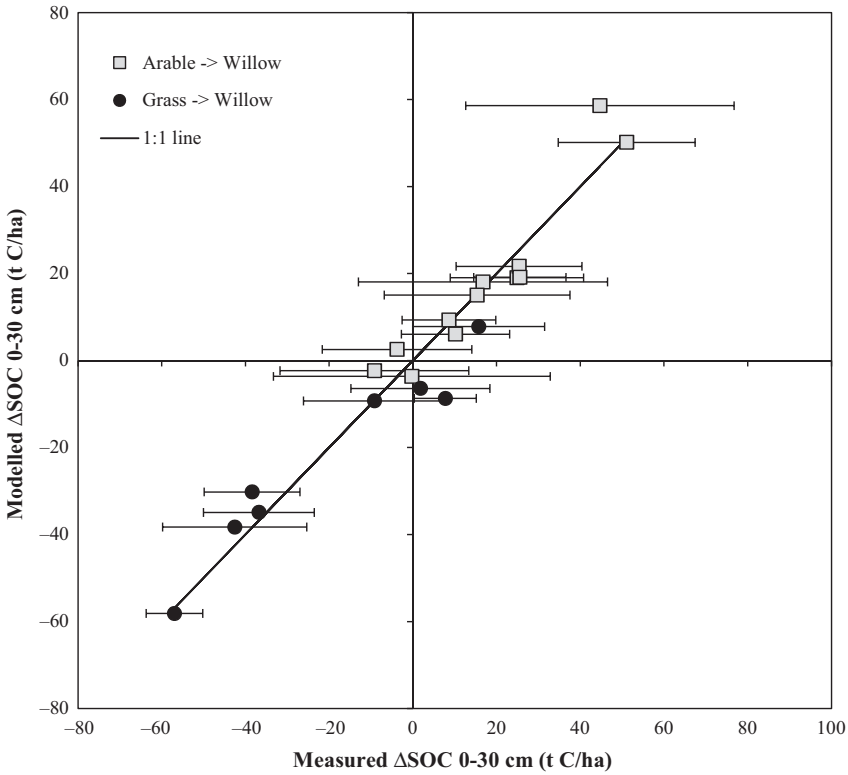

Fig. 7 Measured and modelled change in SOC after transition to SRC-willow at 0–30 cm soil depth. Error bars represent 95% confidence interval of measured values. Solid line represents 1 : 1 correlation between measured and modelled values. SOC, soil organic carbon; SRC, short rotation coppice.

0–30 cm soil depth, are presented in Figs 2 and 3, respectively. Overall, the simulated C correlates well with the measured SOC (Table 3).

The r value of the SOC at both *Miscanthus* ($r = 0.95$) and SRC-willow ($r = 0.72$) sites showed a significant ($P < 0.05$) association between simulated and measured values. The calculated value of E indicated that the simulations at both *Miscanthus* and SRC-willow sites show no significant bias ($E < E_{95}$). Finally, the *LOFIT* value showed that the model error was within (i.e. not significantly larger than) the measurement error.

At most of the *Miscanthus* sites, the simulated SOC was within the 95% confidence interval of the measured SOC (error bars in Fig. 2). At sites 11, 16 and 19, the model estimated a lower SOC compared to the measured values (51.9 vs. 54.6 t C ha^{-1}, 56.4 vs. 63.6 t C ha^{-1}, 55.2 vs. 58.9 t C ha^{-1}, respectively).

The simulated SOC at the SRC-willow sites was within the 95% confidence interval of the measured SOC (error bars in Fig. 3). The only exceptions were found at sites 4 and 33 where the model estimated a lower SOC compared to the measured values (60.0 vs. 65.7 t C ha^{-1}, 94.3 vs. 107.4 t C ha^{-1}, respectively) while for sites 8 and 20 the model simulated a higher accumulation of SOC compared to the site measurements. However, simulated SOC showed a good fit against soil measurements at all sites (Table 3).

The model simulations of the total C at 0–100 cm soil depth again showed a good correlation with the measured SOC, for both *Miscanthus* (Fig. 4) and SRC-willow fields (Fig. 5). High variation of the measured SOC was found at certain *Miscanthus* (site 30 and site 38) and SRC-willow (site 18 and site 33) sites. The statistics of the SOC at the 0–100 cm soil depth reflected the good model performance found for the top soil layer, with a high correlation between simulated and measured values and no significant bias for both *Miscanthus* and SRC-willow sites (Table 3).

The change in SOC (ΔSOC) has been calculated as the difference between the SOC at the bioenergy sites and the SOC at the reference. These results are important as they directly show the effect of the land-use transition itself, that is the long-term accumulation or loss of SOC due to the transition occurring. At 0–30 cm soil depth, the modelled transitions from conventional crops (arable and grassland) to *Miscanthus* and SRC-willow lead to a ΔSOC that was within the 95% confidence intervals of the measured values (Figs 6 and 7).

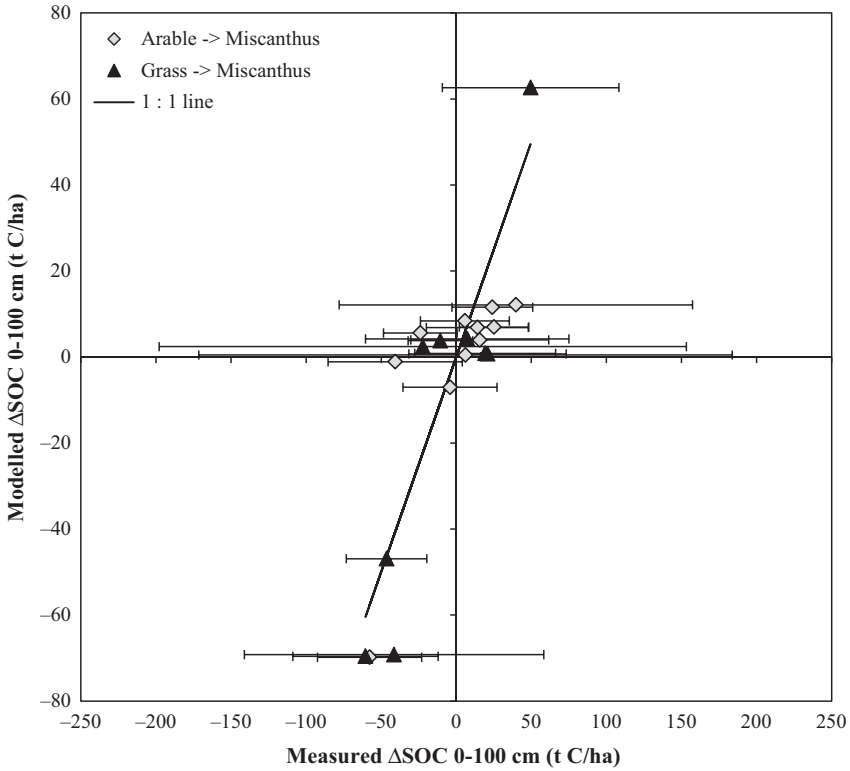

Fig. 8 Measured and modelled change in SOC after transition to *Miscanthus* at 0–100 cm soil depth. Error bars represent 95% confidence interval of measured values. Solid line represents 1 : 1 correlation between measured and modelled values. SOC, soil organic carbon.

Overall, at 0–100 cm, the ΔSOC simulated by the model followed the same direction of the measured SOC changes, for both transitions to *Miscanthus* (Fig. 8) and SRC-willow (Fig. 9). All the ΔSOC simulated by the model is within the 95% confidence intervals of the measured values.

The simulated changes in SOC are well associated with the measured values, with a r value for *Miscanthus* of 0.98 and 0.97 at 0–30 and 0–100 cm soil depth, respectively, and for SRC-willow of 0.98 and 0.84 at 0–30 and 0–100 cm soil depth, respectively. Furthermore, the statistical analysis on the ΔSOC showed no model bias ($E < E_{95}$) and a good coincidence [$F < F$ (critical at 5%)] between modelled and measured changes in SOC after transition to *Miscanthus* and to SRC-willow (Table 4).

Discussions

The present study emphasizes the high accuracy of the ECOSSE model to simulate SOC and SOC changes after transitions to SRC-willow and *Miscanthus* crops in the United Kingdom. The statistical analysis of the SOC and SOC changes at both 0–30 and 0–100 cm soil depths highlights the absence of significant error between simulated and measured values as well as the absence of significant bias in the model. As for the bioenergy plantations, SOC in the reference fields has been accurately simulated by the model. The extremely high correlation for the reference fields shows a good performance of the model spin-up, which is used by the model to reach a state of equilibrium under the specified inputs. However, it is important to stress that it does not confirm that the reference sites are in an equilibrium condition. In fact, at certain bioenergy sites, the model under/overestimated the SOC at 0–30 cm soil depth. A possible explanation of such model underestimates could be that the soil at the reference sites, all arable cultivations established before 1990, were not in equilibrium at the time of the transitions. The initialization of the model is based on the assumption that the soil column is at a stable equilibrium under the initial land use at the start of the simulation (T_0); therefore, the SOC measured at the reference site at the time of sampling (T_1) is assumed to be at the same level as at the time of the transition to the new crop. The equilibrium level depends on several factors: the input of organic material and its rate of decomposition, the rate at which existing SOM is mineralized, soil texture and climate.

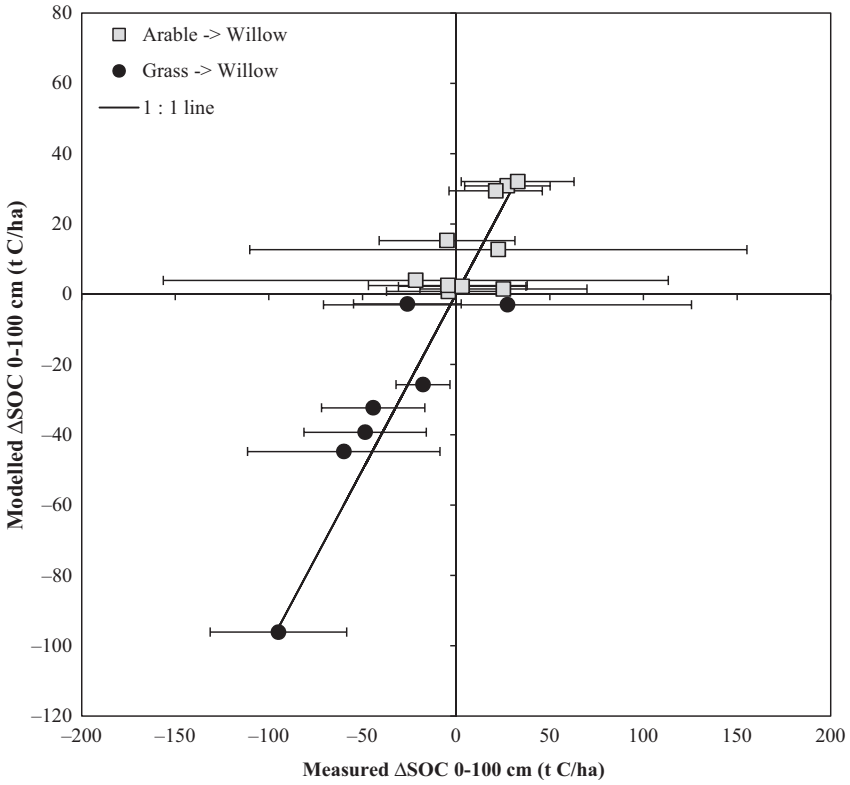

Fig. 9 Measured and modelled change in SOC after transition to SRC-willow at 0–100 cm soil depth. Error bars represent 95% confidence interval of measured values. Solid line represents 1 : 1 correlation between measured and modelled values. SOC, soil organic carbon; SRC, short rotation coppice.

Table 4 ECOSSE model performance at simulating soil C changes (ΔC) at the *Miscanthus* and SRC-willow fields for two soil depths (0–30 cm and 0–100 cm). Association is significant for $t > t$ (at $P = 0.05$). Model bias is not significant for $E < E_{95}$. Error between measured and modelled values is not significant for $F < F$ (critical at 5%)

	0–30 cm depth		0–100 cm depth	
	Miscanthus	SRC-willow	*Miscanthus*	SRC-willow
r = Correlation coefficient	0.98	0.98	0.97	0.84
t-value	21.59	20.92	16.99	6.52
t-value at ($P = 0.05$)	2.10	2.10	2.1	2.1
E = Relative error	−34	47.51	114	−134
E_{95} (95% Confidence limit)	−253	657.24	657	−962
F	0.02	0.03	0.04	0.2
F (Critical at 5%)	1.69	1.69	1.69	1.7
Number of values	20	20	20	18

SRC, short rotation coppice.

The time to reach such equilibrium between vegetation and soil system is extremely unpredictable as all the factors involved in the stabilization process are in constant interaction with each other (Jenkinson, 1990).

Another source of discrepancy between modelled and measured SOC could also be attributed to the divergence between model estimates of the plant inputs to the soil and the actual field value. In the ECOSSE model, the SI is estimated by a modification of the Miami model (Lieth, 1972), which is a simple conceptual model that links the NPP to annual mean temperature and total precipitation (Grieser *et al*., 2006). The NPP is rescaled for each land-cover type, and SI is then estimated as a fixed proportion of the NPP according to the land cover. The rescaling factors for *Miscanthus* and SRC-willow have been derived from comparison of unadjusted Miami results with published yield data for *Miscanthus* in the United Kingdom (Hastings *et al*. 2013) and SRC-willow (Styles *et al*., 2008). The Styles *et al*. (2008) publication reports an expected annual yield of 9 t DM ha^{-1} yr^{-1} for SRC-willow in Ireland; this figure is comparable with UK estimates reported by Tallis *et al*. (2013) (9.0 t DM ha^{-1} yr^{-1}) and Hastings *et al*. (2014) (6.1–12.1 t DM ha^{-1} yr^{-1}). The application of the

rescaling factors has been necessary as the Miami model has been developed to estimate NPP at a global scale and based on environmental variables only, while land-cover type is a key aspect in the ECOSSE model. In the present study, this approach has provided good plant input predictions, and consequently SOC figures, at 17 *Miscanthus* and 16 SRC-willow sites in the United Kingdom; it has also been previously applied with good results on the prediction of SOC in 29 transitions to SRF (Dondini *et al.*, 2015). However, localized weather conditions at some sites may cause divergent yields compared to that predicted by the Miami model. A study by Hastings *et al.* (2014) reported estimated yield potential for current and future climates across Great Britain; *Miscanthus* yield, estimated using the Miscanfor model, ranged from 7.4 to 13.1 t DM ha^{-1} yr^{-1} across regions in Great Britain, whereas estimates of willow yield (from the ForestGrowth-SRC model) ranged from 6.1 to 12.1 t DM ha^{-1} yr^{-1} under current climate.

High variability in the measured SOC at 1 m depth was found at the *Miscanthus* site 38 (error bars in Fig. 4). The high variability in SOC at this site is mainly due to the higher stone content in the soil cores compared to the other *Miscanthus* fields and to a lower number of soil cores collected at this site. In fact, due to the high stone content, two soil cores (instead of three) have been collected at site 38, leading to a bigger 95% confidence interval of the measured values compared to other sites. A high error in the measured SOC has also been found at site 30 and at two SRC-willow sites (sites 18 and 33).

Many factors influence SOC, including temperature, precipitation, NPP and soil physical characteristics (Parton *et al.*, 1987), all of which are spatially variable. The result is substantial variability in SOC, with coefficients of variation as high as 20% even in a visually uniform cultivated field (Robertson *et al.*, 1997). As variability increases, the minimum number of samples needed to detect a given level of change increases. Furthermore, short-term changes in SOC are usually small relative to the amount of C in soil (Conant & Paustian, 2002). Therefore, all transition units reported in the current study were sampled using a hierarchical design, developed to capture variability across different spatial scales (Conant & Paustian, 2002; Conant *et al.*, 2003), especially for the top 30 cm soil.

The results of the present work revealed a strong correlation between modelled and measured SOC and SOC changes to *Miscanthus* and SRC-willow plantations, at two soil depths (Tables 3 and 4). Previous studies on ECOSSE have used large spatial data sets (Smith *et al.*, 2010a,b) to evaluate the model accuracy to simulate SOC. Smith *et al.* (2010a) presented an evaluation of the ECOSSE model to simulate SOC at a national scale, using data from the National Soil Inventory of Scotland. This data set provided measurements of SOC and SOC change for the range of soils, climates and land-use types found across Scotland. The results of the present work are in agreement with the publication of Smith *et al.* (2010a), which reported a high degree of association of the ECOSSE modelled values with the measurements in both total C and change in C content in the soil.

The performance of the ECOSSE model in simulating SOC and SOC changes was recently evaluated for SRF plantations in the United Kingdom (Dondini *et al.*, 2015). The same approach has been used in the present study to test its application for transitions to *Miscanthus* and SRC-willow in the United Kingdom. The statistical analysis of the results presented here is in accordance with the results presented by Dondini *et al.* (2015) for SRF, revealing no significant error between modelled and measured SOC and SOC changes, as well as no significant model bias. The latter is a promising result, given that this work is an independent evaluation of ECOSSE, and therefore, the model had not been further improved or parameterized to produce the outputs under *Miscanthus* and SRC-willow plantations.

This work reinforces previous studies on the ability of ECOSSE to simulate SOC and SOC changes at field level and using limited data to initialize the model. The high degrees of association with measured SOC under *Miscanthus*, SRC-willow and SRF (Dondini *et al.*, 2015) plantations in the United Kingdom allow confidence in using this process-based model for quantitatively predicting the impacts of future land use on SOC, at site level as well as at national level.

Acknowledgements

This work contributes to the ELUM (Ecosystem Land Use Modelling & Soil Carbon GHG Flux Trial) project, which was commissioned and funded by the Energy Technologies Institute (ETI). We acknowledge the E-OBS data set from the EU-FP6 project ENSEMBLES (http://ensembles-eu.metoffice.com) and the data providers in the ECA&D project (http://www.ecad.eu).

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