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Title: Simulation of greenhouse gases following land-use change to bioenergy crops using the ECOSSE model. A comparison between site measurements and model predictions.

Running title: Modelling greenhouse gases under bioenergy crops

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Abstract

This paper evaluates the suitability of the ECOSSE model to estimate soil greenhouse gas fluxes from short rotation coppice willow (SRC-Willow), short rotation forestry (SRF-Scots Pine) and *Miscanthus* after land-use change from conventional systems (grassland and arable). We simulate heterotrophic respiration (R_h), nitrous oxide (N_2O) and methane (CH_4) fluxes at four paired sites in the UK, and compare them to estimates of R_h derived from the ecosystem respiration estimated from eddy covariance (EC) and R_h estimated from chamber (IRGA) measurements, as well as direct measurements of N_2O and CH_4 fluxes.

Significant association between modelled and EC-derived R_h was found under *Miscanthus*, with correlation coefficient (r) ranging between 0.54 and 0.70. Association between IRGA-derived R_h and modelled outputs was statistically significant at the Aberystwyth site (r = 0.64) but not significant at the Lincolnshire site (r = 0.29). At all SRC-Willow sites, significant association was found between modelled and measurement-derived R_h ($0.44 \leq r \leq 0.77$); significant error was found only for the EC-derived R_h at the Lincolnshire site. Significant association and no significant error were also found for SRF-Scots Pine and perennial grass. For the arable fields, the modelled CO_2 correlated well just with the IRGA-derived R_h at one site (r = 0.75). No bias in the model was found at any site, regardless of the measurement type used for the model evaluation.

Across all land-uses, fluxes of CH_4 and N_2O were shown to represent a small proportion of the total greenhouse gas balance; these fluxes have been modelled adequately on a monthly time-step. This study provides confidence in using ECOSSE for predicting the impacts of future land-use on greenhouse gas balance, at site level as well as at national level.

Introduction

The interest in using bioenergy crops as an alternative energy source to fossil fuels, and to reduce greenhouse gas (GHG) emissions, has increased in recent decades (Hastings *et al*., 2014). The commitment of the European Union is to increase the percentage of energy from renewable sources to 20% of total energy consumption by 2020 (EU, 2009). Under the Climate Change Act 2008 (Great Britain, 2008), the UK government committed to reduce GHG emissions by 80% in 2050 compared to 1990 levels; the use of bioenergy could contribute to this target using dedicated 'second generation' (2G) lignocellulosic crops/plantations, including short rotation coppice (SRC), *Miscanthus* and short rotation forestry (SRF) (Somerville *et al*., 2010; McKay, 2011; DECC, 2012; Valentine *et al*., 2012). Consequently, a substantial land-use change (LUC) may occur, and it might have considerable environmental and economic impact (Fargione *et al*., 2008, Searchinger *et al*., 2008; Gelfand *et al*., 2011).

Carbon dioxide (CO_2) emissions of bioenergy had previously been assumed to be zero (Gustavsson *et al*., 1995; UK, 2008) on the assumption that emissions during combustion are balanced by the carbon (C) uptake during the growth of these bioenergy plantations, but this fails to take account of GHG emissions following land use change and subsequent crop growth. To this end, it is important to assess the GHG balance of bioenergy crops, particularly during the first years after conversion.

Two approaches have been widely used to monitor CO_2 fluxes: eddy covariance (EC) and the enclosure (or chamber) method. Eddy covariance (McMillen, 1988; Aubinet *et al*., 2012) is a technique developed to estimate land-atmosphere exchange of gas and energy at ecosystem scale. The measured CO_2 flux, known as net ecosystem exchange (NEE), includes ecosystem respiration (R_{eco}) which consists of heterotrophic (R_h) and autotrophic (R_a) respiration, and gross primary production (GPP) at ecosystem scale. As photosynthesis only occurs during daylight hours, the night time flux is typically used to partition the NEE signal between GPP and R_{eco}. A flux-partitioning algorithm that defines a short-term temperature sensitivity of R_{eco} is applied to extrapolate CO_2 fluxes from night to day (Reichstein *et al*., 2005). In a plant removal experiment (Hardie *et al*., 2009), the total R_h from the whole soil profile was found to be approximately between 46 and 59% of the total R_{eco}. Abdalla *et al*. (2014) used these values to simulate R_h from selected European peatland sites using a soil process-based model, ECOSSE.

Enclosure methods have been developed to measure CO_2 efflux from soil; these methods involve covering an area of soil surface with a chamber and the soil CO_2 efflux can be determined using two main modes: dynamic (closed or open) and closed static. In the former mode, a steady stream of air is pumped directly in to the chamber (Christensen, 1983; Skiba *et al*., 1992). The latter mode simply involves closing the chamber for approximately 20-60 min, and taking gas samples at intervals for analysis (Hutchinson and Mosier, 1981), or circulating the chamber air through a non-destructive infrared gas analyser for approximately 2 minutes (IRGA) (Norman *et al*., 1992; Smith and Mullins, 2000). Several studies have used the closed chamber method combined with root exclusion methods, tree grilling or stable isotopes to understand the relative contribution of R_h and R_a to total soil respiration (R_{tot}) under different land uses.

Byrne *et al*. (2006) demonstrated that R_a under grassland soil in Ireland accounted for approximately 50% of R_{tot} during the summer months and 38% during the rest of the year. Pacaldo *et al*. (2013) reported a contribution of R_a of about 18-33% of R_{tot} under SRC-Willow at three different development stages in the USA. In a study on commercial farms located across the UK, Koerber *et al*. (2010) reported a contribution of R_h on R_{tot} for wheat of approximately 32% from January to May, 79% from June to September and 67% from

October to December. A meta-analysis of soil respiration partitioning studies reported values for the ratio R_h/R_{tot} for forest soils as ranging from 0.03 to 1.0 (Subke *et al*., 2006). Overall, the ratio was higher for boreal coniferous forests than temperate sites. In temperate, mixed deciduous forests ranges for R_h/R_{tot} of 0.3-0.6 were reported (Gaudinski *et al*., 2000; Borken *et al*., 2006; Millard *et al*., 2010; Heinemeyer *et al*., 2012). Several studies have also shown that bioenergy plantations have low nitrous oxide (N_2O) emissions compared to agricultural crops because of their lower nutrient requirements, thus reducing the fertiliser requirements, and more efficient nutrient uptake , thus increasing competition with microbial organisms of N_2O production (Flessa *et al*., 1998; Hellebrand *et al*., 2010; Drewer *et al*., 2012).

Methane (CH_4) is another important GHG that may be a substantial component of the GHG balance from several terrestrial ecosystems (van den Pol-van Dasselaar *et al*., 1999). In agricultural systems, soil is typically a small net source or sink for CH_4 (Boeckx *et al*., 1998). Bioenergy crops usually present either a small CH_4 sink (Hellebrand *et al*., 2003; Kern *et al*., 2012), or a small CH_4 source (Gelfand *et al*., 2011). The magnitude of the CH_4 flux is typically much smaller than CO_2 and N_2O, in both agricultural soils (Boeckx and Van Cleemput, 2001) and bioenergy crops (Hellebrand *et al*., 2003). However, very few studies (Hellebrand *et al*., 2003; Gelfand *et al*., 2011; Kern *et al*., 2012) have reported on the contribution of CH_4 emission from bioenergy systems, increasing uncertainty in the direction of this small flux (Zona *et al*., 2014).

Several factors control the GHG emissions of both bioenergy and conventional crops, such as site management; e.g. fertilisation (Crutzen *et al*., 2008; Hellebrand *et al*., 2008; Hellebrand *et al*., 2010), previous land use (Smith and Conen, 2004) and climatic conditions (Flessa *et al*., 1995; Hellebrand *et al*., 2003). Despite the high variability of the GHG fluxes, to our knowledge only one study in the UK (Drewer *et al*., 2012) has reported on all three GHG fluxes (CO_2, N_2O and CH_4) from soils under bioenergy crops (*Miscanthus* and SRC-Willow) and, in particular, after transition from former conventional systems. To fill this gap, soil models are a useful tool to predict GHG fluxes when site measurements are not available, especially when studying the effects of the change in land use over time and under different climatic conditions over large areas.

However, soil models need to be extensively tested under a range of climates and soils before being applied under conditions different from those used to parameterise and calibrate the model itself. 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 under a wide range of conditions (Moriasi *et al.*, 2007). A model can only be properly evaluated against independent data and a useful model should be able to simulate those data with some degree of accuracy (Smith and Smith, 2007).

Although several soil models have been developed for conventional agricultural and forest systems, most of them have not been fully parameterised and effectively tested for application on 2G bioenergy crops, such as *Miscanthus*, SRF and SRC (Dimitriou *et al.*, 2012; Borzęcka-Walker *et al.*, 2013; Robertson *et al.*, 2014). Here we focus on the applicability of the process-based model ECOSSE to predict soil CO_2 (heterotrophic respiration), N_2O and CH_4 after transition from conventional to bioenergy crops.

The ECOSSE model was developed mainly 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 been previously evaluated across the UK to simulate the effect on soil C of land-use change to SRF (Dondini *et al.*, 2015a), *Miscanthus* and SRC-Willow (Dondini *et al.*, 2015b), to simulate soil N_2O emissions in cropland sites in Europe (Bell *et al.*, 2012; Smith *et al.*, 2010b) and CO_2 emissions from peatlands (Abdalla *et al.*, 2014).

This paper evaluates the suitability of ECOSSE for estimating soil GHG fluxes from SRC-Willow, SRF-Scots Pine and *Miscanthus* soils in the UK after land-use change from conventional systems (grassland and arable). Based on previously published recommendations, a combination of graphical techniques and error 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). In the present study, the model is evaluated against two years of observations at 4 locations in the UK, comprising 1 transition to SRF-Scots Pine, 3 transitions to SRC-Willow and 2 transitions to *Miscanthus*. Modelled GHG fluxes from conventional systems have also been evaluated against field measurements (3 grassland and 2 arable fields).

Materials and Methods

ECOSSE model

The ECOSSE model includes five pools of soil organic matter (SOM), each decomposing with a specific rate constant except for the inert organic matter (IOM) which is not affected by decomposition. Decomposition is sensitive to temperature, soil moisture and vegetation cover; soil texture (sand, silt and clay), pH and bulk density of the soil along with monthly climate and land-use data are the inputs to the model (Coleman and Jenkinson, 1996, Smith *et al*., 1997). The ECOSSE model is able to simulate C and N cycle for six land use categories of vegetation: arable, grassland, forestry, semi-natural, *Miscanthus* and short rotation coppice willow (SRC-Willow).

The vegetation input to the soil (SI) is estimated by a subroutine in the ECOSSE model which uses a modification of the Miami model (Lieth, 1972), a simple model that links the climatic net primary production of biomass (NPP) to annual mean temperature and total precipitation (Grieser *et al*., 2006). For a full description of the ECOSSE model and the plant input estimates refer to Smith *et al*. (2010a) and Dondini *et al*., 2015b.

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

Climate/atmospheric data:

- 30 year average monthly rainfall, potential evapotranspiration (PET) and temperature,
- Monthly rainfall, temperature and PET.

Soil data:

- Initial soil C content (kg ha^{-1}),
- Soil sand, silt and clay content (%),
- Soil bulk density (g cm^{-3}),
- Soil pH,
- Soil depth (cm)

Land-use data:

- Land use for each simulation year.

The initialisation of the model is based on the assumption that the soil column 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. In the absence of additional measurements, estimated plant inputs were calculated from a feature built in the ECOSSE model which combine the NPP model Miami (Lieth, 1972; Lieth, 1973), land-management practices of the initial land use and measured aboveground biomass (details are given in Dondini *et al.*, 2015b).

Data

In 2011-2013, four sites were sampled in Britain using a paired site comparison approach (Keith *et al.*, 2014; Rowe *et al.*, 2015). The sites and the relative measurements contribute to the ELUM (Ecosystem Land Use Modelling & Soil Carbon GHG Flux Trial) project (Harris *et al.*, 2014). Each site consisted of one reference field (arable or grassland, depending on the previous land use of the bioenergy fields) and one or more adjacent bioenergy fields (*Miscanthus*, SRC-Willow, SRF-Scots Pine), for a total of 6 transitions to bioenergy at four site across UK (Table 1). A full description of the sites can be found in (Drewer *et al.*, 2012; Drewer *et al.*, 2015; McCalmont *et al.*, 2015; Harris *et al.*, 2015).

At each bioenergy and reference field, the NEE data were obtained from continuous EC measurements (McMillen, 1988; Aubinet *et al.*, 2012) using open path IRGAs (LI-7500) and sonic anemometers. All details regarding the EC data corrections, quality control, footprint and gap filling procedures can be found in Aubinet *et al.* (2003). The night time fluxes were used to partition the NEE flux measurements into GPP and R_{eco} (Reichstein *et al.*, 2005).

Soil GHG fluxes were measured on a monthly basis at eight points randomly distributed within each field. Soil CO_2 fluxes were measured using an IRGA connected to an SRC-1 soil respiration chamber (PP Systems, Amesbury, MA). Measurements of soil CH_4 and N_2O fluxes were made using a static chamber method (approx. 30 litres) with the addition of a vent to compensate for pressure changes within the chamber during times of sampling. Gas samples were analysed by gas chromatograph (GC). All details regarding the chamber data can be found in Case *et al*. (2014), Drewer *et al*. (2012) and Yamulki *et al*. (2013).

Measurements of soil C, soil bulk density and soil pH to 1 m soil depth, as well as information on the land-use history, were collected for each field (Keith *et al*., 2014; Rowe *et al*., 2015). Soil texture was measured for each site up to a depth of 30 cm; values to 1 m soil depth were extracted from the soil database (1 km resolution) described in Bradley *et al*. (2005), which is a collated soils dataset for England and Wales, Scotland and Northern Ireland. Air temperature and precipitation data at each location were extracted from the E-OBS gridded dataset from the EU-FP6 project ENSEMBLES, provided by the ECA&D project (Haylock *et al*., 2008). This dataset is known as E-OBS and is publicly available (http://eca.knmi.nl/). For each location, monthly air temperature and precipitation for the 30 years before measurements started were used to calculate a long-term average (Table 2). At each site, air temperature and precipitation were collected during the entire study period and monthly values were used as input to the model. Monthly PET was estimated using the Thornthwaite method (Thornthwaite, 1948), which has been used in other modelling studies when direct observational data have not been available (e.g. Smith *et al*., 2005; Dondini *et al*., 2015a).

Model evaluation and statistical analysis

Monthly simulations of soil CO_2, N_2O and CH_4 fluxes were evaluated against monthly chamber measurements. In addition, the soil CO_2 predicted by the ECOSSE model was compared to estimates of R_h derived from the NEE measured by the EC.

At each site, the ECOSSE model has been run for the reference field (i.e. no land-use transition) and the bioenergy crop field (i.e. following transition from the reference land cover). The reference fields have been run for the conventional crop (arable, grassland) with no land-use change and the length of the simulations has been defined by the age of the plantation. At the bioenergy sites, the model has been run for the reference fields (conventional crop) with land-use change to bioenergy crop; the length of the simulations was based on the time after transition to bioenergy crop. Measured soil characteristics and meteorological data have been used as inputs to drive the model (see above for input details), and the results of the simulations were compared to the GHG fluxes measured at the sites.

We expected a monthly underestimate of the soil CO_2 flux simulations because the ECOSSE model simulates R_h (from living micro-organisms + decomposition of old C sources i.e. saprotrophic), while the CO_2 fluxes measured at the sites represent the total CO_2 efflux from the soil profile (R_a + R_h, chamber measurements) or NEE (EC measurements). In order to compare the modelled and measured R_h, we estimated the R_h as a proportion of the measured CO_2 flux, depending on the measurement type (except EC data), vegetation type and growing season.

The eddy covariance measurements of NEE were used to derive R_{eco}; to our knowledge, only the study by Abdalla *et al.* (2014) has reported estimates of R_h from R_{eco}. Abdalla *et al.* (2014) applied the approach proposed by Hardie *et al.* (2009) for peaty soils and reported a contribution of R_h to R_{eco} of 46-59%.

To represent the variations in R_h throughout the year, Abdalla *et al*. (2014) assumed that R_h was at the lowest value of the range (46% R_{eco}) during the summer (June-August), the highest value (59% R_{eco}) during the winter (December-February) and at the mean value (52.5% R_{eco}) during the rest of the year (March-May and September-November). In the present study we used the same approach of Abdalla *et al*. (2014) to derive R_h from EC measurements from all land-use systems.

Chamber measurements represent the total CO_2 flux from the soil as the sum of R_a and R_h, with the exception of grassland where exclusion of full leaves from the chamber is difficult and therefore above ground plant respiration is also included in the measurements. We conducted a literature review to determine the partitioning of R_{tot} measured by the chambers under different vegetation types. Additional experiments within the ELUM project were also undertaken to directly quantify R_h and R_a at selected network sites (data not shown); where available, we used the R_h site data to estimate R_h from R_{tot} measured by the chambers (Lincolnshire – *Miscanthus*, West Sussex – SRC-Willow, Aberystwyth – *Miscanthus*). An overview of the data source and the monthly proportion of R_h for each vegetation type and at each site are shown in table 3.

A quantitative statistical analysis was undertaken to determine the coincidence and association between measured and modelled values, following methods described in Smith *et al*. (1997) and Smith and 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 and Smith (2007).

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. The EC measurements were not replicated, so the coincidence between measured and modelled values was determined using the mean difference (*M*), calculated as the sum of the differences between measured and modelled values and divided by the total number of measurements (Smith *et al*., 1997). The variation across the different measurements was then used to calculate the value of Student's *t* and compared to the *t*-distributions (two-tailed test) to obtain the probability that the mean difference is statistically significant. All statistical results were considered to be statistically significant at $p<0.05$.

Results

The ECOSSE model was evaluated by comparing the outputs to the EC-derived and IRGA-derived R_h fluxes from eleven fields over four sites, representing the following land-use systems: grassland (permanent), arable (barley), *Miscanthus*, SRC-Willow and SRF-Scots Pine.

Soil CO_2 fluxes under *Miscanthus* were measured at two sites, Lincolnshire and Aberystwyth. At both sites, the modelled R_h followed the same seasonal pattern of measured data (Fig. 1). At the Lincolnshire site, a statistically significant association between modelled and EC-derived R_h (r = 0.54) was found, but a small significant bias in the model simulations when tested against the EC-derived R_h was also found (Table 4). On the other hand, the IRGA-derived R_h did not correlate well with the modelled outputs (r = 0.29) but no bias was found in the model simulations (Table 4).

At the Aberystwyth site, significant association between modelled and measurement-derived R_h was found, regardless the type of measurement used. A slightly higher correlation coefficient was calculated correlating the modelled R_h with the EC-derived R_h (r = 0.70) compared to the one arising from the correlation with the IRGA-derived R_h (r = 0.64). No significant error between simulated and IRGA-derived R_h was found for this site, but a bias in the model was found when it was tested against the EC-derived R_h (Table 4).

The model performance to simulate soil CO_2 fluxes under SRC-Willow was tested against measurements taken at three sites: Lincolnshire, West Sussex and East Grange (Fig. 2). At all sites a good agreement was found between simulations and measurement-derived R_h with r values ranging from 0.44 to 0.77. Also, no significant error between simulated and measurement-derived R_h was found, with the exception of the EC-derived R_h at the Lincolnshire site (Table 4).

Model performance to simulate soil CO_2 fluxes under SRF-Scots Pine has been evaluated against data collected at the East Grange site (Fig. 3). The modelled outputs followed the same pattern of the measured values and the statistical analysis showed good correlation with both IRGA- and EC-derived R_h. Moreover, we found no statistically significant error between modelled and measured values as well as no bias in the model (Table 4).

Model simulations of soil R_h have also been evaluated for conventional crops (arable and grassland). Overall, the simulated CO_2 follows the same pattern as the measured values at all sites (Fig. 4 and 5). The statistics highlighted a significant correlation (ranging between 0.48 and 0.87 across all sites and measurements types) and no significant error between modelled and measured values as well as no model bias under perennial grass (Table 4). For the arable fields, the modelled CO_2 was significantly correlated to the measured value just for the IRGA-derived R_h at the Lincolnshire site ($r = 0.75$); however no bias in the model was found at any site, regardless of the measurement types used for the model evaluation (Table 4).

Monthly fluxes of CH_4 and N_2O were shown to be highly variable, both spatially and temporally, across all land uses, so we present an example of the correlation between modelled and measured soil N_2O and CH_4 fluxes for each land use. Both N_2O and CH_4 are very small fluxes and the model outputs were within the errors of the measurements, for both GHGs and at all sites (data not shown). However, low correlation between measured and modelled values has been found for the majority of the sites, ranging from -0.02 to 0.61 for N_2O and from -0.29 to 0.53 for CH_4. The high variability of the measured N_2O and CH_4 fluxes led to a statistically significant error between simulated and measured values at most of the study sites (Table 5 and 6).

Discussion

Soil CO_2 emissions under *Miscanthus* have been quantified at two sites (Lincolnshire and Aberystwyth) using two different sampling methods (EC and IRGA methods). At both sites, we found a high correlation between measured and modelled R_h, ranging from 0.54 to 0.60, except for the IRGA values at Lincolnshire site ($r = 0.29$, Table 4). The lack of association at this site was mainly due to differences between modelled and IRGA-derived R_h in the year

2013 (Fig. 1b). In April 2013, the soil was harrowed and disked to break up the rhizomes for improved yield, so the system was out of balance; the farmer also applied waste wood products, which led to high CO_2 emissions, undetected by the model (May-August 2013 in Fig. 1b) since this was not included in the management file. In the ECOSSE model, the patterns of C and N debris return during the growing season follow a standard exponential relationship, as originally derived by Bradbury *et al*. (1993). Any alteration, such as harrowing or waste application, cannot be easily entered by the user. The scope of the present study is to evaluate the model using independent data which has not been used to develop the model. Therefore, we deliberately chose not to apply any modifications to the model to fit the measured data. However, the model was able to simulate independent data derived from two different sources with a good degree of accuracy.

Soil CO_2 emissions under SRC-Willow and SRF-Scots Pine plantations have been quantified using the same sampling methods. At all sites, the modelled R_h significantly correlated with all types of measurements, showing no significant error between measured and modelled values (Fig. 2).

The model has also been tested against CO_2 fluxes measured under conventional crops. At all three grassland sites (West Sussex, Aberystwyth and East Grange), the measured CO_2 fluxes correlate significantly with the modelled values and the statistical analysis showed no error between measured and modelled values, and no bias in the model (Fig. 5). This is a striking result which underlines the good quality of the data provided for the model evaluation, as well as the good model performance to simulate soil CO_2 fluxes.

Under grassland, R_h derived from the IRGA measurements does not always show a high correlation with the modelled values, particularly during the summer months (Fig. 5). This lack of correlation is mainly due to the difficulties in the separation of soil respiration from grassland, due to the possible inclusion of vegetation within the chamber. When deriving R_h from grassland, we estimated that 60% of the measured CO_2 can be attributed to plant (leaf) respiration, as reported by Byrne and Kiely (2006), but this crude estimate doesn't always reflect the field conditions. For an accurate quantification of the proportion of the CO_2 derived from the plant occluded in the chambers, field experiments would be needed to explicitly quantify plant respiration and biomass.

The analysis of the soil R_h fluxes from the arable fields reveals reasonable model performance at the Lincolnshire site, while at the East Grange site, correlation between modelled and measured IRGA values was poor (Table 4). This discrepancy between modelled and measurement-derived R_h appears to be due to the nature of the source data; in fact, the IRGA-derived R_h is estimated from a single data point which is taken to represent monthly CO_2 fluxes. Therefore, the monthly CO_2 flux might not be properly represented if high flux variation occurred within the month. Another explanation could also be the discontinuity of the IRGA measurements taken at the East Grange site (Fig. 4b). The latter hypothesis is supported by the R_h results of the arable field at the Lincolnshire site. In fact, the IRGA measurements at the Lincolnshire site have been taken over a 2-year period, and the statistical analysis shows a good correlation against the model output (r = 0.75; Table 4). Therefore, we conclude that the low correlation at the East Grange arable field is mainly due to the variability and quantity of the measurements, and that the model accurately describes the CO_2 emissions from arable crop.

Generally, the model was able to predict seasonal trends in R_h at most of the sites; however, the model occasionally over/underestimated the flux values during the warm weather in spring and summer. This is particularly evident at the Lincolnshire site, resulting in a high mean difference between modelled and EC-derived R_h (Table 4). Despite using a generic method to estimate R_h from R_{eco}, therefore providing a challenging test for the model, we found no significant mean difference between modelled and EC-derived R_h at 3 sites (for a total of 4 land uses), proving that the model adequately simulates soil processes under different land-use systems and climate/soil conditions.

Low correlation between measurements and model simulations arose predominantly when comparing model outputs against the IRGA-derived dataset; this is mainly due to the nature of the measurements (single data point representing total monthly CO_2 flux), an aspect not related to the soil processes described in the model. However, it is to notice that the IRGA-derived R_h has been estimated from direct measurements of total soil respiration and the degree of correlation between measured and modelled R_h is also related to the R_h:R_{tot} ratio adopted. On the other hand, the EC-derived R_h was estimated from the R_{eco} during daytime, which is a modelled flux driven by air temperature and other environmental factors. Further model evaluation should be based on comparison of the model output with direct measurements of soil R_h fluxes, possibly using automatic chambers on soil plots where roots have been excluded. This measurement technique would provide continuous R_h measurements which would be directly comparable to the model outputs and therefore would provide a more accurate evaluation of the performance of the model. However, given the very limited input data used to run the model and the number of sites/locations used for the model evaluation, we conclude that the simulations are robust and the model adequately simulate soil CO_2 fluxes under five land-use systems.

Model simulations of N_2O and CH_4 fluxes resulted in low correlation and association at most of the study sites (Table 5 and 6), which is expected with such low fluxes, and does not represent a failure of the model. In fact, the measured N_2O and CH_4 fluxes are pooled from sample data points containing outliers and extreme variation between sample points in each site, which results in a high standard error of the measured values. But the N_2O and CH_4 flux simulations are within the 95% confidence interval of the measured values, showing that the model cannot be improved to better fit these data, and suggesting that the lack of correlation between modelled and measured values is due to the high variation in the measured fluxes, which is a common phenomenon verified in many N_2O (e.g. Oenema *et al*., 1997; Skiba *et al*., 2013; Cowan, 2015) and CH_4 flux measurement experiments (Parkin *et al*., 2012; Savage *et al*., 2014). Moreover, if the measured values do not show any seasonal trend, a significant correlation with the model outputs cannot be obtained (Smith and Smith, 2007) and low correlation is expected.

Measured fluxes of CH_4 were shown to be negligible across all land-uses and their contribution to the total GHG balance, when converted to CO_2 equivalent, was on average less than 0.2%, except for the *Miscanthus* field at the Aberystwyth site (3% of the total GHG balance). The high mean value recorded for *Miscanthus* in 2012 is driven by one replicate with very high CH_4 production and there was large standard error associated with the measurements. In general, CH_4 production or consumption was negligible also for this field.

Across all land uses, measured fluxes of N_2O represent a small proportion (< 1.5%) of the total GHG balance, with the exception of the arable field at the Lincolnshire site and the *Miscanthus* field at the Aberystwyth site (6% of the total GHG balance over the two years measurement period at both fields). Due to technical issues and issues regarding access to sites for sampling, the dataset for the arable and SRC-Willow fields at East Grange is missing a substantial number of months and therefore it was not possible to determine the annual GHG balance.

Despite the very low values of the CH_4 and N_2O fluxes, and their small contribution to the total GHG balance at all experimental sites, both fluxes have been modelled adequately on a monthly time-step and no improvements can be made to the model with the available flux data.

In this study, all major GHG fluxes from five land-use systems were reasonably well-estimated using the ECOSSE model. The results from this evaluation exercise show that ECOSSE is robust for simulating GHG fluxes from cropland, grassland, SRC-Willow, SRF-Scots Pine and *Miscanthus* (and transitions from the former two land uses to the latter three energy crops). This validation builds confidence that the model can be used to investigate the impacts of land-use transitions spatially in the UK, and to investigate the effects of converting large areas to grow bioenergy crops.

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Figure legends

Figure 1: Eddy covariance derived (dotted line with diamond markers), IRGA derived (filled triangle) and modelled (solid line with circle markers) monthly

heterotrophic CO_2 (R_h) under *Miscanthus* plantations during the measurement period.

Figure 2: Eddy covariance derived (dotted line with diamond markers), IRGA derived (filled triangle) and modelled (solid line with circle markers) monthly heterotrophic CO_2 (R_h) under SRC-Willow plantations during the measurement period.

Figure 3: Eddy covariance derived (dotted line with diamond markers), IRGA derived (filled triangle) and modelled (solid line with circle markers) monthly heterotrophic CO_2 (R_h) under SRF-Scots Pine plantation during the measurement period.

Figure 4: Eddy covariance derived (dotted line with diamond markers), IRGA derived (filled triangle) and modelled (solid line with circle markers) monthly heterotrophic CO_2 (R_h) under arable plantations during the measurement period.

Figure 5: Eddy covariance derived (dotted line with diamond markers), IRGA derived (filled triangle) and modelled (solid line with circle markers) monthly heterotrophic CO_2 (R_h) under grassland plantation during the measurement period.

Tables

Table 1

Site	Land use	Latitude, longitude	Establishment year	Carbon (%)	Nitrogen (%)	Bulk density (g cm^{-3})

West Sussex	SRC-Willow	50.9,-0.4	2008	0.63	0.17	1.50
	Grassland	50.9,-0.4	2000	0.53	0.17	1.55
East Grange	SRF-Scots Pine	56.0,-3.6	2009	0.95	0.18	1.47
	Grassland	56.0,-3.6	2009	1.30	0.17	1.49
	SRC-Willow	56.0,-3.6	2009	1.57	0.17	1.38
	Arable	56.0,-3.6	pre 1990	1.37	0.18	1.57
Lincolnshire	SRC-Willow	53.1 - 0.3	2006	1.26	0.11	1.41
	Miscanthus	53.1 - 0.4	2006	1.30	0.13	1.53
	Arable	53.1 - 0.5	pre 1990	1.47	0.13	1.37
Aberystwyth	Miscanthus	52.4,-4.0	2012	0.98	0.25	1.21
	Grassland	52.4,-4.0	pre 2007	1.16	0.26	1.45

Table 1: Details of soil C, soil bulk density and soil pH to 1 metre soil depth, as well as information on the land-use history at the study fields. Soil texture to 1 m soil depth was extracted from the soil database (1 km resolution) described in Bradley *et al*. (2005).

Table 2

	Aberystwyth			East Grange			Lincoln			West Sussex		
Month	Rain (mm)	Temperature (C°)	PET (mm)	Rain (mm)	Temperature (C°)	PET (mm)	Rain (mm)	Temperature (C°)	PET (mm)	Rain (mm)	Temperature (C°)	PET (mm)
January	152	4	15	103	3	11	48	4	13	80	5	16
February	112	4	17	72	3	15	37	4	17	54	5	18
March	124	5	29	74	5	27	41	6	30	55	7	30
April	86	7	45	53	7	47	43	9	48	46	9	48
May	82	10	69	61	10	72	45	12	73	47	12	73
June	93	13	89	60	13	96	56	14	97	48	15	95
July	105	15	101	67	14	105	49	17	112	49	17	110
August	114	14	93	77	14	96	55	17	103	52	17	103
September	121	13	71	84	12	70	49	14	76	60	15	79
October	174	10	46	100	9	43	55	11	46	99	12	51
November	171	7	27	94	5	22	53	7	25	88	8	29
December	168	4	17	91	3	12	51	4	14	86	6	18

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

Table 3

		Arable	**SRC-Willow**	***Miscanthus***	**Grassland**	**SRF-Scots Pine**
		(Koerber *et al*., 2010)	(Pacaldo *et al*., 2013)		(Byrne and Kiely, 2006)	(Millard *et al*., 2010)
Lincolnshire	January	32% R_{tot}	75% R_{tot}	41% R_{tot}*		
	February	32% R_{tot}	75% R_{tot}	41% R_{tot}*		
	March	32% R_{tot}	75% R_{tot}	85% R_{tot}*		
	April	32% R_{tot}	75% R_{tot}	85% R_{tot}*		
	May	32% R_{tot}	75% R_{tot}	85% R_{tot}*		
	June	79% R_{tot}	75% R_{tot}	85% R_{tot}*		
	July	79% R_{tot}	75% R_{tot}	44% R_{tot}*		
	August	79% R_{tot}	75% R_{tot}	44% R_{tot}*		
	September	79% R_{tot}	75% R_{tot}	44% R_{tot}*		
	October	67% R_{tot}	75% R_{tot}	44% R_{tot}*		
	November	67% R_{tot}	75% R_{tot}	41% R_{tot}*		
	December	67% R_{tot}	75% R_{tot}	41% R_{tot}*		
West Sussex	January		82% R_{tot}*		60% R_{tot}†	
	February		82% R_{tot}*		60% R_{tot}†	

	March		82% R_{tot}*		60% R_{tot}†	
	April		82% R_{tot}*		60% R_{tot}†	
	May		82% R_{tot}*		60% R_{tot}†	
	June		82% R_{tot}*		40% R_{tot}†	
	July		82% R_{tot}*		40% R_{tot}†	
	August		82% R_{tot}*		40% R_{tot}†	
	September		82% R_{tot}*		60% R_{tot}†	
	October		82% R_{tot}*		60% R_{tot}†	
	November		82% R_{tot}*		60% R_{tot}†	
	December		82% R_{tot}*		60% R_{tot} †	
Aberystwyth	January			62% R_{tot}*	60% R_{tot}†	
	February			62% R_{tot}*	60% R_{tot}†	
	March			36% R_{tot}*	60% R_{tot}†	
	April			36% R_{tot}*	60% R_{tot}†	
	May			36% R_{tot}*	60% R_{tot}†	
	June			36% R_{tot}*	40% R_{tot}†	
	July			36% R_{tot}*	40% R_{tot}†	
	August			36% R_{tot}*	40% R_{tot}†	
	September			36% R_{tot}*	60% R_{tot}†	
	October			36% R_{tot}*	60% R_{tot}†	
	November			62% R_{tot}*	60% R_{tot}†	
	December			62% R_{tot}*	60% R_{tot}†	
East Grange	January	32% R_{tot}	25% R_{tot}		60% R_{tot}†	61% R_{tot}
	February	32% R_{tot}	25% R_{tot}		60% R_{tot}†	61% R_{tot}
	March	32% R_{tot}	25% R_{tot}		60% R_{tot}†	61% R_{tot}
	April	32% R_{tot}	25% R_{tot}		60% R_{tot}†	61% R_{tot}
	May	32% R_{tot}	25% R_{tot}		60% R_{tot}†	61% R_{tot}
	June	79% R_{tot}	25% R_{tot}		40% R_{tot}†	61% R_{tot}
	July	79% R_{tot}	25% R_{tot}		40% R_{tot}†	61% R_{tot}
	August	79% R_{tot}	25% R_{tot}		40% R_{tot}†	61% R_{tot}
	September	79% R_{tot}	25% R_{tot}		60% R_{tot}†	61% R_{tot}
	October	67% R_{tot}	25% R_{tot}		60% R_{tot}†	61% R_{tot}
	November	67% R_{tot}	25% R_{tot}		60% R_{tot}†	61% R_{tot}
	December	67% R_{tot}	25% R_{tot}		60% R_{tot}†	61% R_{tot}

Table 3: Contribution of heterotrophic respiration (R_h) on total respiration (Rtot) at the study sites.

*Values derived from direct measurements on root-exclusion plots

†Where R_{tot} is 60% of measured CO_2 to account for plant respiration

TTable 4

Land-use system	*Miscanthus*				SRC-Willow					SRF-Scots Pine		Grass				Arable		
Site	**Aberystwyth**		**Lincolnshire**		**West Sussex**		**East Grange**	**Lincolnshire**		**East Grange**		**West Sussex**		**Aberystwyth**	**East Grange**	**Lincolnshire**		**East Grange**
Measurement type	EC	IRGA	EC	IRGA	EC	IRGA	IRGA	EC	IRGA	EC	IRGA	EC	IRGA	IRGA	IRGA	EC	IRGA	IRGA
***r* = Correlation Coeff.**	0.70	0.64	0.54	0.29	0.77	0.75	0.73	0.70	0.44	0.66	0.62	0.87	0.48	0.52	0.54	0.50	0.75	0.03
t* = Student's *t* of *r	4.65	3.92	2.88	1.44	3.99	5.41	3.72	4.32	2.32	4.10	3.60	5.33	2.66	2.85	2.98	1.91	5.31	0.12
***t*-value at (*p*=0.05)**	2.07	2.07	2.09	2.07	2.20	2.07	2.18	2.09	2.07	2.07	2.08	2.26	2.07	2.07	2.08	2.20	2.07	2.16
LOFIT = Lack of Fit																		
F	N/A	0.88	N/A	0.42	N/A	0.51	0.60	N/A	0.55	N/A	0.40	N/A	0.50	1.47	1.14	N/A	0.61	0.27
***F* (Critical at 5%)**	N/A	1.60	N/A	1.58	N/A	1.58	1.84	N/A	1.58	N/A	1.61	N/A	1.58	1.60	1.61	N/A	1.60	1.80
M = Mean Difference (Kg C/ha/month)	13	-	260	-	-3	-3	-	233	-	-10	-	-104	-	-	-	530		-
***t* = Student's *t* of M**	1.89	-	4.80	-	-0.57	-0.57	-	6.14	-	3.60	-	-2.23	-	-	-	5.54		-
***t*-value (Critical at 2.5% - Two-tailed)**	2.23	-	2.09	-	2.20	2.20	-	2.09	-	2.07	-	2.26	-	-	-	2.20		-
Number of Values	24	24	22	22	13	25	14	21	22	24	23	11	24	24	23	13	22	14

Table 4: ECOSSE model performance at simulating heterotrophic respiration (R_h) at the study sites. Comparison of model outputs with EC-derived and IRGA-derived R_h. Association is significant for t > t-value (at p=0.05). Error between measured and modelled values is not significant for F < F-value (critical at 5%). Mean difference is not significant for t < t-value (Critical at 2.5% - Two-tailed).

Table 5

Land-use system	*Miscanthus*		SRC-Willow			SRF-Scots Pine	Grass			Arable	
Site	Aberystwyth	Lincolnshire	Lincolnshire	East Grange	West Sussex	East Grange	West Sussex	Aberystwyth	East Grange	Lincolnshire	East Grange
r = Correlation Coeff.	0.34	-0.15	-0.13	0.12	-0.02	0.19	0.25	0.06	-0.12	-0.20	0.61
t = Student's t of r	1.72	0.64	0.66	0.48	0.08	0.86	1.24	0.30	0.56	0.97	3.25
t-value at (p=0.05)	2.07	2.10	2.06	2.12	2.06	2.08	2.06	2.07	2.08	2.07	2.10
LOFIT = Lack of Fit											
F	0.37	3.34	54.66	22.62	0.37	40.75	0.62	0.68	312.92	0.43	0.25
F (Critical at 5%)	1.63	1.69	1.59	1.74	1.59	1.63	1.59	1.62	1.63	1.60	1.69
Number of Values	24	20	26	18	26	23	26	24	23	25	20

Table 5: ECOSSE model performance at simulating N_2O fluxes at the study sites. Association is significant for t > t-value (at p=0.05). Error between measured and modelled values is not significant for F < F-value (critical at 5%).

Table 6

Land-use system	*Miscanthus*		SRC-Willow			SRF-Scots Pine	Grass			Arable	
Site	Aberystwyth	Lincolnshire	Lincolnshire	East Grange	West Sussex	East Grange	West Sussex	Aberystwyth	East Grange	Lincolnshire	East Grange
r = Correlation Coeff.	0.31	0.28	0.18	0.53	0.18	0.53	0.27	0.51	0.41	-0.29	0.05
t = Student's t of r	1.52	1.28	0.88	2.51	0.91	2.68	1.40	2.81	1.91	1.44	0.20
t-value at (p=0.05)	2.07	2.09	2.07	2.12	2.06	2.10	2.06	2.07	2.10	2.07	2.10
LOFIT = Lack of Fit											
F	0.33	3.61	6.50	0.53	0.61	2.38	0.30	0.34	4.09	0.66	0.76
F (Critical at 5%)	1.62	1.65	1.60	1.74	1.59	1.63	1.59	1.62	1.63	1.62	1.69
Number of Values	24	22	25	18	26	23	26	24	23	24	20

Table 6: ECOSSE model performance at simulating CH_4 fluxes at the study sites. Association is significant for t > t-value (at p=0.05). Error between measured and modelled values is not significant for F < F-value (critical at 5%).