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

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Abstract

This article evaluates the suitability of the ECOSSE model to estimate soil greenhouse gas (GHG) 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 GHG 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 GHG balance, at site level as well as at national level.

Keywords: ECOSSE model, energy crops, greenhouse gases, land-use change, Miscanthus, short rotation coppice, short rotation forestry

Received 4 June 2015; revised version received 18 July 2015 and accepted 3 August 2015

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 (CO2) 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 failure to take account of GHG emissions following LUC 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 CO2 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 CO2 flux, known as net ecosystem exchange (NEE), includes ecosystem respiration (Reco) which consists of heterotrophic (Rd) and autotrophic (Ra) 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 Reco. A flux-partitioning algorithm that defines a short-term temperature sensitivity of Reco is applied to extrapolate CO2 fluxes from night to day (Reichstein et al., 2005). In a plant removal experiment (Hardie et al., 2009), the total Ra from the whole soil profile was found to be approximately between 46 and 59% of the total Reco. Abdalla et al. (2014) used these values to simulate Ra from selected European peatland sites using a soil process-based model, ECOSSE.

Enclosure methods have been developed to measure CO2 efflux from soil; these methods involve covering an area of soil surface with a chamber and the soil CO2 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 into 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 & Mosier, 1981), or circulating the chamber air through a nondestructive infrared gas analyzer (IRGA) for approximately 2 min (Norman et al., 1992; Smith & 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 Ra and Rd to total soil respiration (Rtot) under different land uses.

Byrne & Kiely (2006) demonstrated that Ra under grassland soil in Ireland accounted for approximately 50% of Rtot during the summer months and 38% during the rest of the year. Pacaldo et al. (2013) reported a contribution of Ra of about 18–33% of Rtot 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 Ra on Rtot 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 Ra/Rtot 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 Ra/Rtot 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 (N2O) emissions compared to agricultural crops because of their lower nutrient requirements, thus reducing the fertilizer requirements, and more efficient nutrient uptake, thus increasing competition with microbial organisms of N2O production (Flessa et al., 1998; Hellebrand et al., 2010; Drewer et al., 2012).

Methane (CH4) is another important GHG that may be a substantial component of the GHG balance from several terrestrial ecosystems (van den Pol-van Dassen et al., 1999). In agricultural systems, soil is typically a small net source or sink for CH4 (Boeckx & Van Cleemput, 2001). Bioenergy crops usually present either a small CH4 sink (Hellebrand et al., 2003; Kern et al., 2012) or a small CH4 source (Gelfand et al., 2011). The magnitude of the CH4 flux is typically much smaller than CO2 and N2O, in both agricultural soils (Boeckx & 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 CH4 emission from bioenergy systems, increasing uncertainty in the direction of this small flux (Zona et al., 2013).

Several factors control the GHG emissions of both bioenergy and conventional crops, such as site management, for example fertilization (Crutzen et al., 2008; Hellebrand et al., 2008, 2010), previous land use (Smith & Conen, 2004) and climatic conditions (Flessa et al., 1998; 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 (CO2, N2O and CH4) 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 parameterize 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 & Smith, 2007).

Although several soil models have been developed for conventional agricultural and forest systems, most of them have not been fully parameterized 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., 2015). Here, we focus on the applicability of the process-based model ECOSSE to predict soil CO2 (heterotrophic respiration), N2O and CH4 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 LUC to SRF (Dondini et al., 2015a), Miscanthus and SRC-Willow (Dondini et al., 2015b), to simulate soil N2O emissions in crop–land sites in Europe (Smith et al., 2010b; Bell et al., 2012) and CO2 emissions from peatlands (Abdalla et al., 2014).

This article evaluates the suitability of ECOSSE for estimating soil GHG fluxes from SRC-Willow, SRF-Scots Pine and Miscanthus soils in the UK after LUC from conventional systems (grassland and arable). Based on previously published recommendations, a combination of graphical techniques and error statistics has 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 this study, the model is evaluated against 2 years of observations at four locations in the UK, comprising one transition to SRF-Scots Pine, three transitions to SRC-Willow and two transitions to Miscanthus. Modelled GHG fluxes from conventional systems have also been evaluated against field measurements (three grassland and two arable fields).

Materials and methods

ECOSSE model

The ECOSSE model includes five pools of soil organic matter, 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 & 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, seminatural, 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 as follows:

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 and
- Soil depth (cm).

Land-use data:
- Land use for each simulation year.

The initialization 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 soil organic carbon (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, 1973), land-management practices of the initial land use and measured above-ground 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., 2015; 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 adja-
cent bioenergy fields (Miscanthus, SRC-Willow, SRF-Scots Pine),
for a total of six transitions to bioenergy at four site across UK
(Table 1). A full description of the sites can be found in Drewer
et al. (2012, 2013); J. McCalmont, N. McNamara, J. Donnison
and J. Clifton-Brown (in preparation); and Z. M. Harris, G.
Alberti, J. R. Jenkins, E. Clark, R. Marshall, R. Rowe, N. McNa-
mara and G. Taylor (in preparation).

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 Reco
(Reichstein et al., 2005).

Soil GHG fluxes were measured on a monthly basis at eight
points randomly distributed within each field. Soil CO2 fluxes
were measured using an IRGA connected to an SRC-1 soil
respiration chamber (PP Systems, Amesbury, MA, USA). Mea-
surements of soil CH4 and N2O fluxes were made using a static
chamber method (approx. 30 l) with the addition of a vent to
compensate for pressure changes within the chamber during
times of sampling. Gas samples were analysed by gas chromato-
graph. All details regarding the chamber data can be found in
Drewer et al. (2012), Yamulki et al. (2013) and Case et al. (2014).

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., 2015; Rowe et al., 2015). Soil
texture was measured for each site up to a depth of 30 cm; val-
ues 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 data set for England and Wales, Scotland and
Northern Ireland. 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). This data set 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 CO2, N2O and CH4 fluxes were
evaluated against monthly chamber measurements. In addition,
the soil CO2 predicted by the ECOSSE model was compared to
estimates of Ra derived from the NEE measured by the EC.

At each site, the ECOSSE model has been run for the refer-
ence 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 LUC, and the length of the simul-
ations 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 LUC to bioenergy crop; the length of
the simulations was based on the time after transition to bioen-
ergy 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 underestimation of the soil CO2 flux
simulations because the ECOSSE model simulates Ra (from
living micro-organisms + decomposition of old C sources, i.e.
saprotrophic), while the CO2 fluxes measured at the sites repre-
sent the total CO2 efflux from the soil profile (Ra + Rw, chamber

| Site          | Land use               | Latitude, longitude | Establishment year | Carbon (%) | Nitrogen (%) | Bulk density (g cm⁻³) |
|---------------|------------------------|---------------------|--------------------|------------|-------------|----------------------|
| West Sussex   | Short rotation coppice (SRC)-Willow Grassland | 50.9, −0.4          | 2008               | 0.63       | 0.17        | 1.50                 |
| East Grange   | Short rotation forestry (SRF)-Scots Pine Grassland | 56.0, −3.6          | 2009               | 0.95       | 0.18        | 1.47                 |
|               | SRC-Willow             | 56.0, −3.6          | 2009               | 1.30       | 0.17        | 1.49                 |
|               | 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                 |

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Table 2 Long-term (30 years) monthly rainfall, temperature, potential evapotranspiration (PET). 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)

| Month   | Aberystwyth | East Grange | Lincoln | West Sussex |
|---------|-------------|-------------|---------|-------------|
|         | Rain (mm)   | Temperature (˚C) | Rain (mm) | Temperature (˚C) | Rain (mm) | Temperature (˚C) | Rain (mm) | Temperature (˚C) |
| 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          |

measurements) or NEE (EC measurements). To compare the modelled and measured Rs, we estimated the Rs as a proportion of the measured CO2 flux, depending on the measurement type (except EC data), vegetation type and growing season.

The EC measurements of NEE were used to derive Reco to our knowledge, only the study by Abdalla et al. (2014) has reported estimates of Rs from Reco. Abdalla et al. (2014) applied the approach proposed by Hardie et al. (2009) for peaty soils and reported a contribution of Rs to Reco of 46–59%.

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

Chamber measurements represent the total CO2 flux from the soil as the sum of Rs and Rn, with the exception of grassland where exclusion of all 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 Rn measured by the chambers under different vegetation types. Additional experiments in the ELUM project were also undertaken to directly quantify Rs and Rn at selected network sites (data not shown); where available, we used the Rs site data to estimate Rs from Rn measured by the chambers (Lincolnshire – Miscanthus, West Sussex – SRC-Willow, Aberystwyth – Miscanthus). An overview of the data source and the monthly proportion of Rs for each vegetation type 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 & 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 & Smith, 2007). The significance of the association between simulations and measurements was assigned using a Student’s t-test as outlined in Smith & 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-test 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 Rs fluxes from eleven fields over four sites, representing the
Table 3 Contribution of heterotrophic respiration ($R_h$) on total respiration ($R_{tot}$) at the study sites

| Location     | Month   | Arable Koerber et al. (2010) | SRC-Willow Pacaldo et al. (2013) | Grassland Byrne & Kiely (2006) | SRF-Scots Pine Millard et al. (2010) |
|--------------|---------|-------------------------------|----------------------------------|-------------------------------|-------------------------------------|
|              |         | $R_{tot}$                     | $R_{tot}$                        | $R_{tot}$                     | $R_{tot}$                           |
| 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% $R_{tot}$                 | 60% $R_{tot}$                   |                               |                                     |
|              | July     | 82% $R_{tot}$                 | 60% $R_{tot}$                   |                               |                                     |
|              | August   | 82% $R_{tot}$                 | 60% $R_{tot}$                   |                               |                                     |
|              | 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% $R_{tot}$                 | 60% $R_{tot}$                   |                               |                                     |
|              | July     | 36% $R_{tot}$                 | 60% $R_{tot}$                   |                               |                                     |
|              | August   | 36% $R_{tot}$                 | 60% $R_{tot}$                   |                               |                                     |
|              | 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% $R_{tot}$                   | 60% $R_{tot}$                 | 61% $R_{tot}$                       |
|              | July     | 79% $R_{tot}$                 | 25% $R_{tot}$                   | 60% $R_{tot}$                 | 61% $R_{tot}$                       |
|              | August   | 79% $R_{tot}$                 | 25% $R_{tot}$                   | 60% $R_{tot}$                 | 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% $R_{tot}$                       |

*Values derived from direct measurements on root-exclusion plots.
†Where $R_{tot}$ is 60% of measured CO2 to account for plant respiration.
following land-use systems: grassland (permanent), arable (barley), Miscanthus, SRC-Willow and SRF-Scots Pine.

Soil CO\textsubscript{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\textsubscript{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\textsubscript{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,
Table 4  ECOSSE model performance at simulating heterotrophic respiration ($R_h$) at the study sites

| Land-use system | Miscanthus | SRC-Willow | SRF-Scots | Pine | Grass | Arable |
|-----------------|------------|------------|-----------|------|-------|--------|
| Site            |           |            |           |      |       |        |
|                 | Aberystwyth | Lincolnshire | West Sussex | East | Grange | Lincolnshire | West Sussex | Aberystwyth | East | Grange | Lincolnshire | East |
| Measurement type| EC         | IRGA       | EC         | IRGA | EC    | IRGA   | EC         | IRGA       | EC    | IRGA   | EC         | 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 |
| $t$ = 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 |
| $t$-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 |
| LOFIT = Lack of Fit | 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 |
| $F$ (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 |
| $M$ = Mean Difference (Kg C ha$^{-1}$ month$^{-1}$) | 13 | – | 260 | – | –3 | –3 | – | 233 | – | –10 | – | –104 | – |
| $t$ = Student’s $t$ of $M$ | 1.89 | -- | 4.80 | -- | –0.57 | –0.57 | – | 6.14 | – | 3.60 | – | –2.23 | -- |
| $t$-value (Critical at 2.5% - two-tailed) | 2.23 | -- | 2.09 | -- | 2.20 | 2.07 | -- | 2.09 | -- | 2.07 | -- | 2.26 | -- |
| Number of Values | 24 | 24 | 22 | 22 | 13 | 25 | 14 | 21 | 22 | 24 | 23 | 11 | 24 |

Comparison of model outputs with eddy covariance (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).
The simulated CO2 follows the same pattern as the measured values at all sites (Figs 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 CO2 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 CH4 and N2O 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 N2O and CH4 fluxes for each land use. Both N2O and CH4 are very small fluxes and the model outputs were within the

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Fig. 2 Eddy covariance derived (dotted line with diamond markers), IRGA derived (filled triangle) and modelled (solid line with circle markers) monthly heterotrophic CO2 (\( R_h \)) under SRC-Willow plantations during the measurement period.
Fig. 3  Eddy covariance derived (dotted line with diamond markers), IRGA derived (filled triangle) and modelled (solid line with circle markers) monthly heterotrophic CO₂ (\(R_\text{h}\)) under short rotation forestry-Scots Pine plantation during the measurement period.

Fig. 4  Eddy covariance derived (dotted line with diamond markers), IRGA derived (filled triangle) and modelled (solid line with circle markers) monthly heterotrophic CO₂ (\(R_\text{h}\)) under arable plantations during the measurement period.

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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\(_2\)O and from \(-0.29\) to \(0.53\) for CH\(_4\). The high variability of the measured N\(_2\)O and CH\(_4\) fluxes led to a statistically significant error between simulated and measured values at most of the study sites (Tables 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 \((r = 0.29, \text{Table 4})\). The lack of association at this site...
was mainly due to differences between modelled and IRGA-derived Rh 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 CO2 emissions, undetected by the model (May–August 2013 in Fig. 1b) as 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 CO2 emissions under SRC-Willow and SRF-Scots Pine plantations have been quantified using the same sampling methods. At all sites, the modelled Rh 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 CO2 fluxes measured under conventional crops. At all three grassland sites (West Sussex, Aberystwyth and East Grange), the measured CO2 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 CO2 fluxes.

Under grassland, Rh 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 the respiration of the vegetation included in the chamber. When deriving Rh from grassland, we estimated that 60% of the measured CO2 can be attributed to plant (leaf) respiration, as reported by Byrne & Kiely (2006), but this crude estimate does not always reflect the field conditions. For an accurate quantification of field respiration would be needed to explicitly quantify plant respiration and biomass. The analysis of the soil Rh fluxes from the arable fields reveals reasonable model performance at the Lincolnshire site, while at the East Grange site, correlation coefficients show a high degree of accuracy.

Table 5  ECOSSE model performance at simulating N2O fluxes at the study sites

| Land-use system | Miscanthus | SRC-Willow | West Sussex | East Grange | Aberystwyth | East Grange |
|-----------------|------------|------------|-------------|-------------|-------------|-------------|
| Site            |            |            |             |             |             |             |
| Aberystwyth     | 0.34       | -0.13      | -0.12       | 0.19        | 0.25        | -0.12       |
| Lincolnshire    | -0.15      | 0.12       | 0.02        | 0.06        | -0.20       | 0.61        |
| r = Correlation Coeff. | t = Student’s t of | t-value at (P = 0.05) | LOFIT = Lack of Fit |
|                 | 1.72       | 0.66       | 0.48        | 0.08        | 0.86        | 1.24        |
|                 | 0.64       | 2.06       | 2.12        | 2.06        | 2.08        | 2.06        |
|                 | 2.07       | 2.10       | 2.06        | 2.08        | 2.06        | 2.08        |
|                 | 0.37       | 3.34       | 54.66       | 22.62       | 0.37        |
|                 | 3.44       | 22.62      | 40.75       | 0.62        | 0.68        |
| F (Critical at 5%) | 1.63       | 1.69       | 1.74        | 1.59        | 1.63        |
|                 | 1.59       | 1.59       | 1.63        | 1.59        |
| Number of values | 24         | 20         | 18          | 26          | 24          |

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%).
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 three sites (for a total of four 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 data set; 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

| Land-use system | Miscanthus | SRC-Willow | SRC-Willow | Miscanthus | Miscanthus | Miscanthus | Miscanthus | Miscanthus | Miscanthus | Miscanthus |
|----------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|
| Site           | Aberystwyth| East Grange| Lincolnshire| West Sussex| East Grange| East Grange| Lincolnshire| East Grange| East Grange| East Grange|
| \( r \) Correlation | 0.31 | 0.28 | 0.18 | 0.53 | 0.27 | 0.51 | 0.27 | 0.51 | 0.41 | 0.76 |
| Coeff. \( t \) | 1.52 | 1.28 | 1.28 | 2.51 | 2.81 | 1.39 | 1.39 | 1.39 | 2.07 | 2.07 |
| \( t \)-value at \( P = 0.05 \) | 2.07 | 2.09 | 2.09 | 2.07 | 2.09 | 2.07 | 2.07 | 2.07 | 2.07 | 2.07 |
| \( F \) Critical at \( 5\% \) | 2.10 | 2.10 | 2.10 | 2.10 | 2.10 | 2.10 | 2.10 | 2.10 | 2.10 | 2.10 |
| Number of values | 24 | 24 | 24 | 24 | 24 | 24 | 24 | 24 | 24 | 24 |

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%).

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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 CO₂ fluxes under five land-use systems.

Model simulations of N₂O and CH₄ fluxes resulted in low correlation and association at most of the study sites (Tables 5 and 6), which is expected with such low fluxes, and does not represent a failure of the model. In fact, the measured N₂O and CH₄ 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 N₂O and CH₄ 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 N₂O (e.g. Oenema et al., 1997; Skiba et al., 2013; Cowan et al., 2015) and CH₄ 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 & Smith, 2007) and low correlation is expected.

Measured fluxes of CH₄ were shown to be negligible across all land uses and their contribution to the total GHG balance, when converted to CO₂ equivalent, was on average <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 CH₄ production and there was little seasonal trend associated with the measurements. In general, CH₄ production or consumption was negligible also for this field.

Across all land uses, measured fluxes of N₂O 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 2 years measurement period at both fields). Due to technical issues and issues regarding access to sites for sampling, the data set 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 CH₄ and N₂O 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.

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-EPF project ENSEMBLES (http://ensembles-eu.metoffice.com) and the data providers in the ECA&D project (http://www.ecad.eu).

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