Investigating the Impact of Climate and Extreme Weather on Greenhouse Gas Emissions from Irish Soils: An Evaluation of the ECOSSE Model

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Figures

Tables

Glossary

AW: Available Water
BIO: Microbial Biomass
C: Carbon
CH_4: Methane
CO_2: Carbon Dioxide
DPM: Decomposable Plant Material
E_0: Activation Energy
ESM: Earth System Model
ET_a: Actual Evapotranspiration
ET_o: Reference Evapotranspiration
FC: Field Capacity
GHG: Greenhouse Gas
GPP: Gross Primary Production; the amount of chemical energy as biomass that primary producers create in a given length of time
GWP: Global Warming Potential
ha: hectare
HUM: Humified Organic Matter
HWSD: Harmonised World Soil Database
IOM: Inert Organic Matter
IPCC: Intergovernmental Panel on Climate Change
kPa: Kilopascal (1 kPa = 1000 Pa)
Kt: Kiloton (10^9 g)
LAI: Leaf Area Index
M: Million
MRT: Mean Residence Time
N: Nitrogen
N_2O: Nitrous Oxide
NDVI: Normalized Difference Vegetation Index
NEE: Net Ecosystem Exchange; a measure of the net exchange of C between an ecosystem and the atmosphere (per unit ground area)
NO: Nitric Oxide
NO_3: Nitrate
NPP: Net Primary Production; the rate at which all the plants in an ecosystem produce net useful chemical energy (calculated as GPP – respiration by plants)
Pa: Pascal (SI unit of pressure, 1 newton per m^2)
PAR: Photosynthetically Active Radiation
PE: Potential Evapotranspiration
PFT: Plant Functional Type
Pg: Petagram (10^{15} g)
ppm: parts per million
Q_{10}: The rate of increase of soil respiration due to a 10°C increase in temperature
Ra: Autotrophic Respiration
Reco: Ecosystem Respiration
Rf: Soil Fauna Respiration

Rh: Heterotrophic Respiration
Rn: Non-biological CO_2 Production
RPM: Resistant Plant Material
Rr: Root Respiration
Rs: Soil Respiration (Rh + Ra = Rs)
SMD: Soil Moisture Deficit
SOC: Soil Organic Carbon
SOM: Soil Organic Matter
SREX: Special Report on Extremes
SWC: Soil Water Content
T: Temperature
t: Tonne (10^6 g)
Tg: Teragram (10^{12} g)
VPD: Vapour Pressure Deficit
WAS: Water Available at Saturation
WAS: Water Available at Saturation
WP: Wilting Point
WTD: Water Table Depth

Summary

Soil is a complex material capable of storing and releasing large amounts of carbon, making it an integral part of the global carbon cycle. As soil is included in national inventory assessments where countries quantify their emissions, it is important that estimates of the soil carbon flux are as accurate as possible. Measuring the flux of carbon from every surface on the planet is unrealistic, therefore modelling emissions is the next best method of emissions assessment. Among modelling approaches, process-based modelling allows for the highest specificity of input data. Process-based models split soil carbon into pools with different decay rates influenced by environmental (biotic and abiotic) factors and management.

The Estimation of Carbon in Organic Soils – Sequestration and Emissions (ECOSSE) model has previously been recommended as the optimum process-based model for simulating greenhouse gas (GHG) emissions from Irish soils. Results from the site-specific evaluation of the ECOSSE model for an Irish arable site showed a temporal offset between measurements and model outputs which could not be explained by model parameters, motivating further in-depth analysis of the model. This subsequent analysis indicated that the rate modifiers, which control the release of carbon from different pools in the soil, were functioning as intended, but highlighted issues with the model simulation of soil water. The modelled soil dried out fully when in reality it was above field capacity, attributable to erroneous simulation of evaporation on this well-drained sandy soil.

In parallel, a spatial process-based model (GlobalECOSSE) was employed to derive national emissions estimates for multiple GHGs and CO_2 equivalents for designated agricultural land uses on the island of Ireland. The justification for using the spatial process-based model was to provide an assessment of a model that had fewer input requirements and operated on a monthly timescale to simulate areal emissions. Results showed soil carbon emissions are enhanced during warmer months and lessened during colder ones, and showed cropland and grassland to be CO_2 sources on an annual timeframe. The importance of examining emissions holistically is emphasised as some Irish grasslands are GHG sinks when other GHGs such as methane and nitrous oxide are included, and all croplands are GHG sources.

To assess the susceptibility of Irish soils to unusual or extreme weather events, statistical sampling of past weather events was employed to generate inputs for GlobalECOSSE. The response of Irish soils to extreme weather events shows warmer temperatures enhance respiration, while drought conditions restrict it. Warm and wet conditions enhance respiration most as respiration increases with temperature and is not limited by moisture

availability in this scenario. Including all GHGs produces similar patterns with most Irish soils being C sinks under normal climate and hydrological conditions, and more areas becoming sources during hot, very hot and hot & wet conditions (derived from extremes in the observed record). These results are presented in the context of the uncertainties in observations (large ranges across datasets and methods of partitioning fluxes) and in modelling (different models giving different magnitudes and even directions of change). More observations, experiments and modelling studies across land-use and climate types are needed before confident projections can be given. Observational networks should be placed strategically to determine responses from common soil and land-use types, and moisture regimes. Current action should focus on maintaining the carbon already in soils by avoiding disturbance, and promoting sensible sequestration practices such as cover-cropping, minimum/no tillage and incorporation of straw/manure.

1 Introduction

1.1 The Global Carbon Cycle

A key component of life on earth is Carbon (C), the element all known living things are based on. The presence of carbon in our atmosphere as Carbon Dioxide (CO_2) traps and reradiates heat emitted from the Earth's surface; without this natural 'greenhouse' effect, the Earth would be approximately 33°C colder and unable to support complex life (National Geographic, 2019). Our modern industrial society is built around the use of fossil fuels deposited in the earth during the Carboniferous and Permian geological eras over millions of years, and the burning of these hydrocarbons is resulting in an increase in the atmospheric concentration of greenhouse gases (Paul, 2016). It is argued that the anthropogenic increase of greenhouse gases in the atmosphere began around 15,000-12,000 years ago when land-use change and forestry increased the atmospheric concentration of CO_2 from below 200 to ~270 ppmv (Sage, 1995). This allowed for the successful establishment of agriculture as previous concentrations may have been too low for modern crops to thrive, indicating that this increase stimulated the transition from an economic system based on foraging toward a food-producing, agrarian civilisation (*ibid*). There have been advantages to increasing concentrations of CO_2, but these are now significantly outweighed by the negative impacts of climate change.

Figure 1.1 (Le Quéré *et al.*, 2018) outlines the global CO_2 budget for the decade 2007-2016 along with uncertainties for each pool, showing the atmospheric growth of CO_2 in the past decade has been ~4.7 ± 0.1 Pg C yr^{-1} and that the land and oceans are helping to absorb 3.0 ± 0.8 Pg C and 2.4 ± 0.5 Pg C yr^{-1} respectively. The uncertainties associated with these figures reflect the imperfect understanding we still have of our atmosphere and the sources of C emissions.

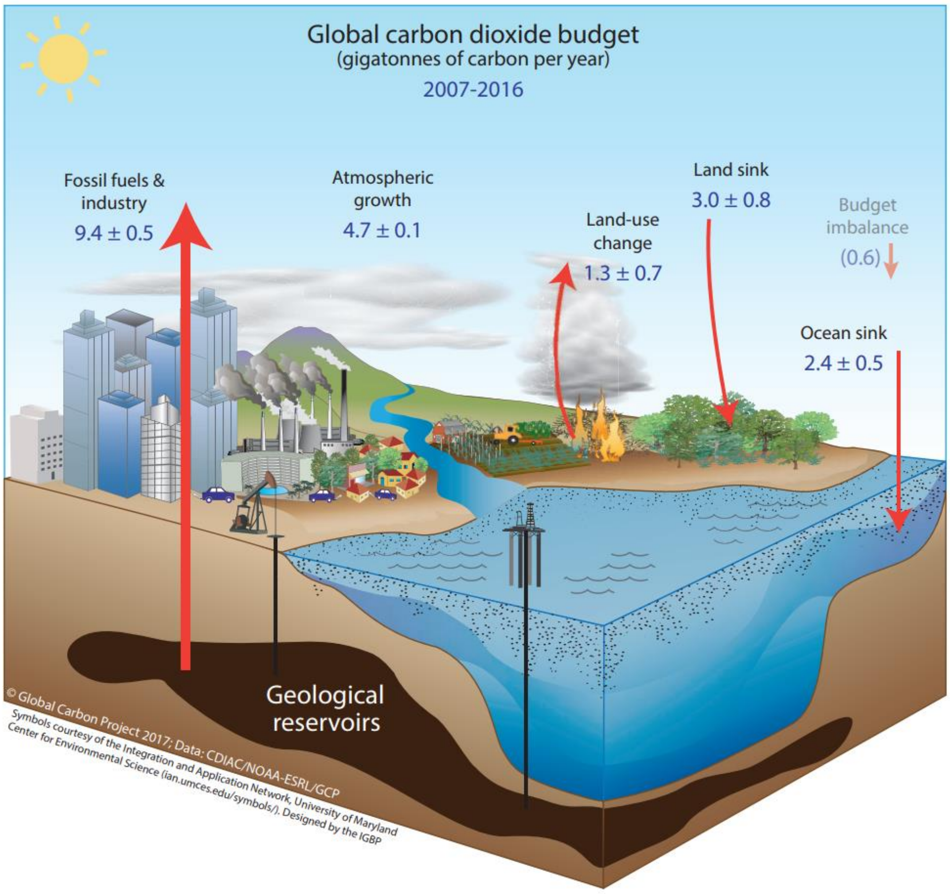


Figure 1.1: The Global CO_2 budget outlining the perturbation of the global carbon cycle from anthropogenic activities for the years 2007-2016, values are in Pg C yr^{-1}, reprinted from Le Quéré et al. (2018). 1 Pg C is equivalent to 1 Gt C.

Ice cores for the past 800,000 years show atmospheric CO_2 levels have remained within a relatively constrained domain (between 170 and 280 ppm), with temperature and CO_2 levels fluctuating in tandem (Parrenin *et al.*, 2013). By 2017, the average atmospheric concentration of CO_2 was 405.0 ± 0.1 ppm, 2.2 ppm higher than the previous year, and the highest atmospheric concentration ever recorded (Blunden *et al.*, 2018). The concentration of CO_2 in our atmosphere gives a radiative forcing (greenhouse effect) of 1.82 ± 0.19 W m^{-2} (Myhre *et al.*, 2013). With CO_2 now over 100 ppm higher than pre-industrial times and increasing at a rate of at least 10 and up to 100 times faster than at any point in the past 420,000 years, human interference in the global carbon cycle has likely driven the earth system outside the glacial-interglacial domains it has experienced for millennia (Falkowski *et al.*, 2000). During these interglacial periods the atmosphere becomes a medium of exchange of CO_2 between terrestrial ecosystems and the oceans. Anthropogenic emissions of greenhouse gases have interfered with the natural global carbon cycle, causing impacts related to heat stress and sea-level rise, and have the potential for triggering irreversible planetary feedbacks which may severely disrupt global temperature and weather patterns (Steffen *et al.*, 2018).

Though estimates vary, the latest research suggests there is approximately 1500 Pg C of organic carbon stored in uppermost meter of terrestrial soils (Scharlemann *et al.*, 2014; Oertel *et al.*, 2016). This makes soil the largest terrestrial carbon pool, roughly equivalent to the atmospheric (816 Pg C) and terrestrial phytomass (469.6 Pg C) pools combined (Scharlemann *et al*., 2014). Soils release carbon to the atmosphere via respiration, the process of soil respiration is complex and dynamic, but can be distilled as follows: larger soil organisms such as earthworms or mites break down soil organic matter (SOM) into small pieces by moving through the soil and feeding on/digesting the SOM itself, while soil fungi perform similar operations as their hyphae can penetrate smaller gaps in the soil, these decomposition processes are assisted by abiotic factors such as freezing and thawing of water, exposing new areas for bacteria and microbes to break down, thus releasing CO_2 (Xu and Shang, 2016). It is estimated that annual soil CO_2 emissions are around 10 times that of current fossil fuel emissions (Bond-Lamberty and Thomson, 2014). Since soils store twice as much C as the atmosphere, understanding the feedback from soils to the atmosphere is crucial (Scharlemann *et al.*, 2014; Heimann and Reichstein, 2008). Soils can sequester and store greenhouse gases like CO_2, CH_4 and N_2O for long periods of time, for example C in soil can have a residence time of ~1200 years, making soils a significant sink for C and other elements (Post *et al.*, 1982). Using a conservative estimate of 300 mg CO_2eq m^{-2} h^{-1} Oertel *et al.* (2016) estimate global annual net soil emissions of over 350 Pg CO_2eq when all GHGs are included.

All of Earth's biomes store large quantities of C in both biomass and soil, this C is vulnerable to being released, and is particularly susceptible to anthropogenic perturbations from land-use change, agriculture, urban growth, industrial and infrastructure development (Lal *et al.*, 2012). Before the industrial revolution in the 1700s, it is estimated that nearly half of the terrestrial biosphere could be considered 'wild', absent of human settlement or land-use, with the remainder (45%) in a semi-natural state with minor agricultural and settlement components (Ellis *et al.*, 2010). By the year 2000 the majority of the biosphere comprised agricultural and settled anthropogenic biomes (settlements, croplands, rangelands and plantations), with 20% semi-natural, and 25% considered 'wild' (*ibid*). These human influences on Earth's natural systems have had a profound effect on the global carbon cycle, and the complexity of these systems makes it difficult to understand and project their dynamics and future states, nevertheless, considerable progress in this regard has been made.

1.1.1 *Understanding the Carbon Cycle*

Scientific attempts to understand the global carbon cycle and its influence on our climate first came to prominence in a paper by Fourier (1824), who discussed the phenomenon of Earth's temperature being higher than it ought to be from the solar radiation budget alone. Fourier's analysis ruled out geothermal effects and allowed for the consideration of the possibility that heat was being prevented from escaping the atmosphere. The experimental evidence to support this was proffered by John Tyndall (Tyndall, 1861) who investigated the radiative properties of gases in Earth's atmosphere, and measured the infrared absorption of greenhouse gases, proving their capabilities to absorb and reradiate heat energy. The introduction of the idea of the climate's sensitivity to CO_2 came from Svante Arrhenius, who investigated the extent to which changes in CO_2 concentrations can affect global temperatures (Arrhenius, 1896). Callendar (1938) was the first to demonstrate the increase of the Earth's land temperature and suggested a link between the increasing temperatures and the artificial production of CO_2 from the combustion of fossil fuels, which became known as the 'Callendar effect' (Hawkins and Jones, 2013). These ideas were advanced further by Plass (1956) who investigated the sensitivity of the climate to increasing concentrations of greenhouse gases and estimated a temperature increase of 3.6°C if the concentration of CO_2 in the atmosphere were to double. Plass (1956) also linked the warming observed in the previous century to the increasing concentration of atmospheric greenhouse gases released from industrial processes and associated human activities and warned of more warming to come for several centuries.

The theoretical basis for modelling the global carbon cycle stems from these seminal research papers, as technology developed it became possible to implement the theory into practice, assessing the significance of humanity's alterations to the global carbon cycle by projecting likely future changes in the climate system due to altered atmospheric concentrations of key GHGs. Early models projected values for climate sensitivity (response of the climate system to a doubling of CO_2) of 2.9°C (Manabe and Wetherald, 1975), remarkably this is in the same range as modern-day estimates (Sherwood *et al.*, 2014). Though these relatively basic models did not incorporate the complexities of the ocean-atmosphere feedbacks, they were very much at the cutting edge for their time, and the outputs from the inaugural Coupled Model Intercomparison Project (CMIP) were used in the first IPCC report (Houghton *et al.*, 1990).

Models have advanced and now incorporate the entire earth system and its feedbacks into their calculations, including dynamic land, ocean and atmospheric components (Flato, 2011). The inclusion of more complexity into models can have a significant effect on projections as exemplified by Mitchell *et al.* (1995) who included sulphate aerosols in their climate model runs and improved the agreement between model outputs and observed temperature changes. Earth System Models (ESMs), which include biogeochemical cycling, are complex and their structures are distinct from one other, leading to uncertainties in outputs but also providing a range of possibilities when no 'perfect' model is available (Alexander and Easterbrook, 2015). The CMIP, now in its 6th phase incorporating 21 Endorsed Model Intercomparison Projects (MIPs), aims to investigate the Earth's response to altered radiative forcings, the origins and consequences of model biases, and assessing future climate change among internal climate variability, predictability and uncertainties in scenarios (Eyring *et al.*, 2015). One of the major sources of uncertainty in projecting future global temperature in relation to CMIP5 is the poor understanding of the terrestrial carbon cycle, as land carbon sinks are uncertain across all four representative concentration pathway (RCP) scenarios giving a large intermodel spread (Friedlingstein *et al.*, 2013). To improve climate model projections, we must enhance our understanding and modelling of the processes which influence land-carbon fluxes; processes which include vegetation, soil carbon storage and turnover time. Most land-carbon components of climate models overestimate photosynthesis and leaf area index, likely due to the exclusion of ozone in parameterisation, while many underestimate primary production in the oceans, and show significant regional variation in their assessments (Anav *et al.*, 2013). Uncertainties around soil carbon-climate feedbacks are present at micro and macro scales due to a lack of observations on the responses of the soil system to external change and ever-changing knowledge about soil C formation and stabilization (Bradford *et al.*, 2016). As our understanding of the complex soil system is improving, it is vital that models incorporate this new knowledge and are fully evaluated and assessed to identify issues and improve model-knowledge integration and better understand the responses of the land-carbon cycle to future changes (*ibid*). As human action is now recognised as the major factor influencing the direction and magnitude of future emissions (IPCC, 2018), the incorporation of human decision making and adaptation into climate models will be a more pressing issue in the future. The integration of earth system models with future human action will be complex and costly, meaning careful assessment of the benefits and drawbacks of incorporating this complexity should be considered, with the overall aim of each individual study in mind (Calvin and Bond-Lamberty, 2018).

1.2 Legal History

Based on the mounting evidence provided by the scientific community regarding the impact of anthropogenic greenhouse gas emissions, regulatory frameworks began to be developed to control emissions.

1.2.1 *IPCC, UNFCCC & COP*

Amid growing concern around the impact human beings were having on the planet, and based on the scientific developments outlined in Section 1.1, the Intergovernmental Panel on Climate Change (IPCC) was formed in 1988 under the patronage of the United Nations Environment Program (UNEP) and the World Meteorological Organization (WMO). The IPCC was assigned the task of assessing the influence of anthropogenic greenhouse gas emissions on climate change, how it affects societies, and forming potential response strategies to future climate change (Devès *et al.*, 2017). Two years after the publication of the first IPCC assessment report in 1990, the United Nations Framework Convention on Climate Change (UNFCCC) treaty was adopted and subsequently ratified in 1994 (UNFCCC, 2018a). Signatories of the treaty (United Nations, 1992) acknowledge that climate change is a problem, developed countries are most responsible, carbon sinks are present on land and in oceans, that immediate global action and cooperation is needed and all states (particularly developed nations) should enact environmental legislation using the most up-to-date science and policy to give developing and low-lying nations the best chance to adapt.

The major development over the course of the IPCC reports is the abundance of evidence showing that human activities are the primary cause of the warming observed on Earth (Jones, 2013). The IPCC reports provide the evidence base for discussions at Conferences of the Parties to the UNFCCC (COP) meetings (Ourbak and Tubiana, 2017); the COP is the 'supreme decision making body of the UNFCCC' (UNFCCC, 2018b, pp. 1) where decisions on compliance and enforcement of UNFCCC guidelines are made. There have been annual COP meetings since 1995 in Berlin, the latest COP 24 occurred during December 2018 in Katowice, Poland.

1.2.2 *Kyoto Protocol*

The Kyoto Protocol, adopted in Japan in 1997, is an extension of the UNFCCC and was signed by 37 industrialised nations and the European Union, which legally committed these parties to reducing emissions to an average of 94.8% of their 1990 emissions by the years 2008-2012 (Aichele and Felbermayr, 2013). Under the protocol, a number of countries could increase their emissions, while others (including the EU, USA, and Canada) agreed to cut their emissions of the six main greenhouse gases (carbon dioxide (CO_2), methane (CH_4), nitrous oxide (N_2O), hydrofluorocarbons (HFCs), perfluorocarbons (PFCs), and sulphur hexafluoride (SF_6)) (UNFCCC, 2018c). Article 25 of the Kyoto Protocol specified that the treaty entered into force 90 days after the date 55 parties to the convention who account for at least 55% of total CO_2 emissions had deposited their instruments of ratification. At the end of the first commitment period in 2012, COP18 in Doha proposed the 'Doha Amendment' which established the 2nd commitment period to the Kyoto Protocol, to commence in January 2013 and end in December 2020, the amendment obliges the EU member states and Iceland to limit GHG emissions from 2013-2020 to 80% of 1990 emissions (European Commission, 2013). As of 30 October 2018, 120 parties to the UNFCCC have deposited their instrument of acceptance, though 144 instruments of acceptance are required for the amendment to be entered into force (UNFCCC, 2018d).

The Kyoto Protocol has been deemed a failure by some due to the small emissions reduction targets, which were not achieved, and the subjection of the world to an ineffective model for solving climate change, potentially setting us back decades (Rosen, 2015). Others have argued that the treaty itself became the goal, rather than the requirements contained within it, as the original intent of significantly reducing GHG emissions was sacrificed for the sake of reaching a deal that many countries would sign (Kutney, 2014). The US indicated that it would not ratify the treaty in 2001, Canada withdrew from the Kyoto Protocol in 2012 (UNFCCC, 2018c), while the EU overachieved its initial target of an 8% reduction by reducing emissions by 18%, on track to meet the 2020 target of 20% (European Commission, 2013). It is worth noting that some countries within the EU did not meet their targets as part of the burden sharing agreement. Emissions increased for most countries over the period, meaning the objectives of the treaty were not realised (Aichele and Felbermayr, 2013). It is difficult to assess the success of the Kyoto Protocol as countries did not meet their targets, but they may have reduced their emissions by more than they would have had the agreement never been signed, perhaps making the treaty somewhat of a success (Grunewald and Martinez-Zarzoso, 2016).

1.2.3 *Paris Agreement*

In anticipation of the second commitment period of the Kyoto Protocol ending in 2020, the 21st COP meeting in 2015 adopted the Paris Agreement. This agreement commits signatories to reducing emissions through Nationally Determined Contributions (NDCs), with the aim of keeping global temperature rise in the 21st century 'well below' a guardrail of 2°C above pre-industrial levels, and to 'pursue efforts' to keep the temperature increase below 1.5°C, while enabling countries to deal with the current impacts of climate change (Ourbak and Tubiana, 2017). Governments agreed that global emissions should peak as soon as possible and undertake rapid reductions after the peak, though the combined NDCs of all nations are not enough to keep global warming below 2°C. Considering this, governments agreed to come together every five years to set more ambitious targets, to report on their progress to achieving their targets, and to track progress towards the long-term goal of emissions reduction through a robust transparency and accountability system (European Commission, 2018a). The European Union was the first to submit its NDC which commits the EU to emissions reductions of 20% by 2020, 40% by 2030, and 80-95% by 2050, with the intention of turning Europe into an energy efficient low-carbon economy which sustains jobs and strengthens Europe's competitiveness (European Commission, 2018b). It is still technically possible for global warming to be limited to 1.5°C, though this is profoundly challenging and depends strongly on immediate collective global action (Peters, 2018), making it highly unlikely to occur.

1.3 Monitoring, Reporting and Verification

There are now 197 parties (196 states and 1 regional economic integration organisation) to the UNFCCC (UNFCCC, 2018a). All parties to the UNFCCC and the Kyoto Protocol are required to report their emissions annually in the form of emissions inventories, and regularly report on climate change policies and measures and progress towards their targets (European Commission, 2018c). Inventories attempt to account for all sources and sinks of GHGs, and serve as a tool to track the magnitude and distribution of emissions over time (Campbell and Paustian, 2015). Monitoring of GHG emissions is not a standard process across countries or emissions sources, while some sources of emissions can be directly measured (e.g. gas meters to measure gas concentration) it is more common for estimates of emissions to be made using accounting based procedures, with emissions derived from indicators such as fuel consumption based on energy bills (Bellassen *et al.*, 2015).

1.3.1 *The IPCC Good Practice Guidelines*

To help countries calculate their national emissions, the IPCC provides a comprehensive and detailed set of guidance and rules for estimating emissions from all sectors of the economy and the biosphere at three levels of detail (IPCC, 2006). Tier 1 methods rely on default emission factors and associated activity data to calculate emissions for a sector or sub-sector, while Tier 3 methods are the most detailed, incorporating country-specific data where available. Tier 2 methods are an intermediary between the two. The most important categories in terms of national emissions and emissions trends for a country are known as 'key categories'; the IPCC encourages the use of tier 2 and tier 3 methods for key categories. When properly implemented, all tiers are intended to provide unbiased estimates of emissions, with accuracy and precision improving when moving from tier 1 to tier 3. The

IPCC (2006) use decision trees to help guide the selection of the correct tier to use based on the national circumstances (available data etc.). Each sector and sub-sector will have different data requirements for each tier, an example from the IPCC (2006) is presented below (Figure 1.2) outlining the method behind choosing the appropriate tier for CO_2 emissions from cropland. The tree shows the process of decision making depending on the importance of the category – i.e. if the category is considered a 'key category' (a significant source of emissions for that country) then it is necessary to obtain data for a tier-2 or tier-3 approach. If reliable data are present or can be collected, and there is a national inventory system allowing for crop management activities to be accounted for, a tier 3 approach can be adopted, if this system is not present an intermediary tier 2 approach is recommended.

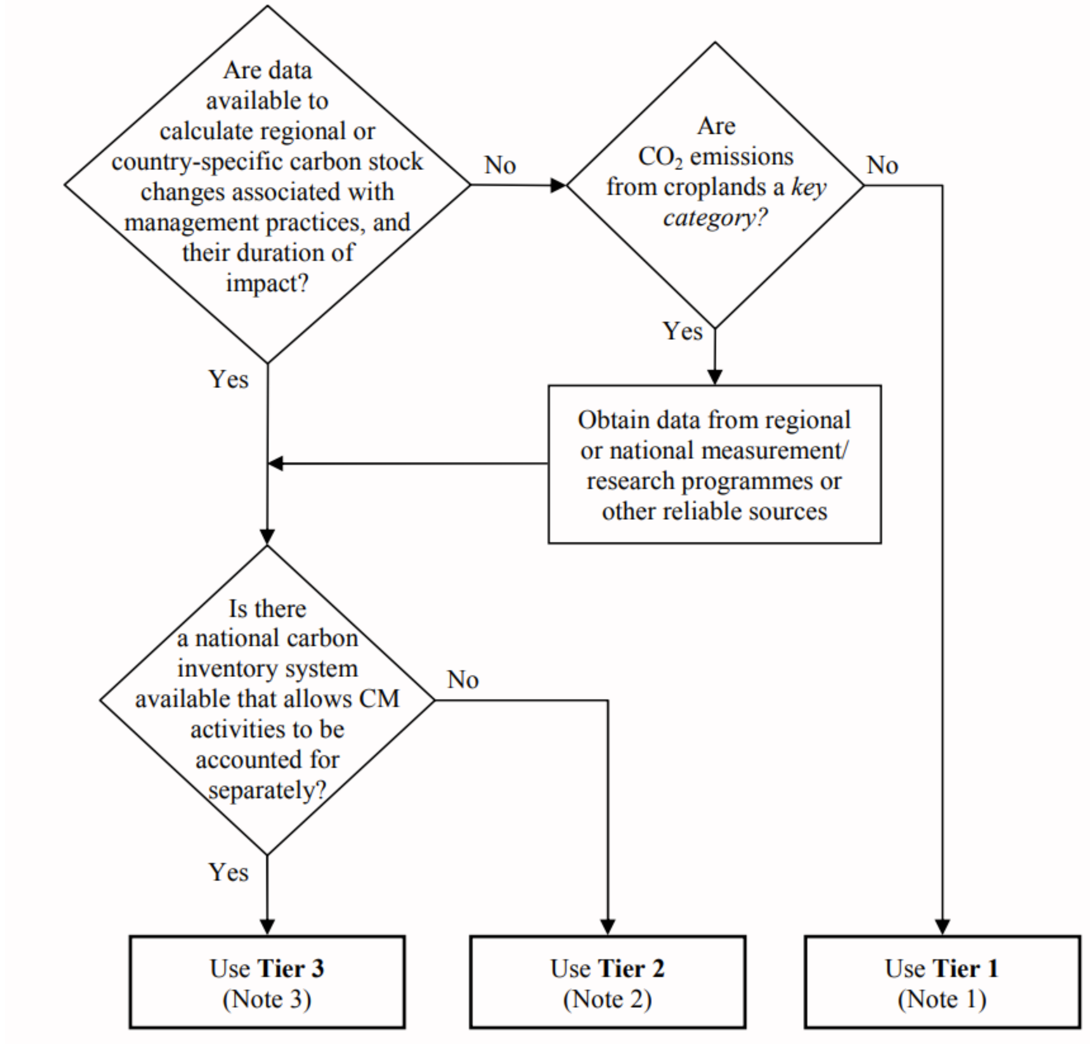


Figure 1.2: Example decision tree for selecting the appropriate tier for estimating C stock changes in mineral soils under cropland (IPCC, 2006). CM: Carbon Management

To derive the 'best' estimate of the emissions from a sector, a country must follow the decision tree to the best of their knowledge, ensuring they choose the most appropriate tier of analysis. Ideally all emissions would be calculated using a tier-3 methodology using as much real or observed data as possible for each country, unfortunately the lack of observed data may make a tier-3 methodology impossible or unwise, as results from this method may introduce errors which give erroneous emissions estimates.

Typically, the estimation of emissions is performed using the simple equation (IPCC, 2006):

$$\text{Emissions} = \text{AD} * \text{EF}$$

where activity data (AD) (e.g. fuel consumption, number of cattle etc.) is multiplied by an associated emission factor (EF) (e.g. CO_2 emission for fuel type, tonnes of CO_2 equivalent per animal per year). Both activity data and emission factors are not static and change over time, requiring monitoring and updating, though emission factors typically vary less than activity data. Bellassen *et al.* (2015) explain that this monitoring data is then aggregated, recorded and communicated to the relevant authority at individual, company, regional or national scales. Verification of emissions is then undertaken to detect errors resulting from mistakes or fraudulent reporting, typically conducted by an external party who ensures guidelines were followed (*ibid*). Members of the EU are required by law (European Parliament, 2013) to report emissions of greenhouse gases from all sectors: energy, industrial processes, land-use, land-use change and forestry (LULUCF), waste, agriculture etc.; to include projections, policies and measures to reduce GHG emissions; national climate change adaptation measures, low-carbon strategies, and financial and technical support for developing countries (European Commission, 2018c). The emission factors used to calculate sectoral emissions come from the 2006 IPCC Guidelines for National Greenhouse Gas Inventories (IPCC, 2006)

1.3.2 *EU Emissions*

The EU publishes annual GHG inventories reflecting the emissions from two years previously (i.e. the 2018 inventory covers emissions from 2016), allowing countries time to calculate their emissions, and for them to be collated together. The latest report shows how the EU is reducing emissions, with the United Kingdom having the largest reductions in absolute terms (largely due to lower consumption of solid fuels in the power sector) and Poland having the largest increase (mainly due to the road transport sector) (European Environment Agency, 2018a). The EU is on target to meeting its legal obligations under phase 2 of the Kyoto Protocol, though some countries have achieved more than others regarding emissions reduction.

From 2015-2016, Ireland saw the fourth-largest increase in absolute emissions across the EU, behind Poland, Finland and Germany. Depending on the economic prosperity of the country along with other factors which can affect emissions (harsh weather etc.), countries frequently change from increasing to decreasing emissions, for example Irish emissions are estimated to have decreased by 1% from 2016-2017 after their increase in the previous year (European Environment Agency, 2018b). Nevertheless, Ireland is poised to miss its 2020 targets, meaning achievement of targets in 2030 and 2050 is increasingly difficult as there is more ground to make up.

1.4 Agriculture and Land-Use

A growing global population and increasing urbanisation has led to changes in the world's forests, farmlands, waterways and air. The provision of food, fibre, water and shelter to meet global demand is responsible for ~35% of anthropogenic CO_2 emissions since pre-industrial times (Foley *et al.*, 2005), a figure which may be an underestimate as processes including tree harvesting and cultivation shifts increase the percentage (Arneth *et al.*, 2017). The global population is anticipated to reach almost 10bn by 2050, creating an increased demand for agricultural products, leading to the expansion of cropland and grassland areas resulting in increased energy, water and fertilizer consumption (Tilman *et al.*, 2011). Such changes in land-use to date are estimated to have resulted in the emission of 145 ± 16 Pg C over the period 1850-2015 (Houghton and Nassikas, 2017). Land-use changes are currently responsible for ~10% of annual emissions, though this was relatively larger in the past when emissions from other sources like fossil fuels were lower (*ibid*).

Agricultural GHG emissions are increasing annually by 1%, while reductions are difficult to achieve amid growing food demand (Lamb *et al.*, 2016). The nature of agricultural GHG emissions is complex, for example the conversion of grassland to cropland to produce biofuel was initially thought to reduce GHG emissions by 20% due to lower fossil fuel consumption, but analysis showed the impact of the land-use change would cause GHG emissions to double over 30 years (Searchinger *et al.*, 2008).

Land management is strongly linked to GHG emissions from soils, though responses differ across climates and land-use types, sensible management practices serve to enhance soil carbon storage (Ogle *et al.*, 2005). Methods of enhancing soil carbon include the addition of nutrients using fertilizer or by growing certain crops, crop rotation using cover crops, reducing stocking rates, switching to no-till, and optimising the quantity and timing of fertilizer applications (Paustian *et al.*, 2016). Unmanaged grassland and forest soils typically hold more carbon than their managed counterparts, and can lose significant amounts when converted to other uses. Avoiding conversion of land and restoring marginal or degraded lands is important to avoid C losses and enhance C sequestration (*ibid*). The potential for soils to become a significant carbon sink to help mitigate against climate change is highlighted by Smith (2016) who argues that a sequestration potential of 0.7 Pg CO_2eq

(CO_2eq = total effect of all GHGs normalised to CO_2) yr^{-1} is possible, though sink saturation and reversibility are highlighted as limitations. Storing more carbon in soils is seen as a win-win-win strategy for farmers and economies, as it enhances food security, improves the environment and mitigates against global warming (Stout *et al.*, 2016). The complex nature of soil and how it is related to greenhouse gases will be discussed further throughout the thesis.

1.5 The Importance of Soil

The importance of including soil emissions in GHG inventories was recognised by the first iteration of the intergovernmental panel on climate change (IPCC) (Houghton *et al*., 1990). The reporting of greenhouse gas emissions from soils is typically based on the IPCC Guidelines for National Greenhouse Gas Inventories (2006) which allow for estimation of emissions and form the base for mitigation and adaptation practices. While remotely sensed (satellite) data e.g. Sentinel 5 (ESA, 2018) have been assessed, they do not provide accurate enough data to validate these estimations, and data from ground-based experiments and modelling are significantly biased towards northern hemisphere temperate regions where the availability of funding and resources is higher (Oertel *et al.*, 2016). The ground-based estimation of greenhouse gas fluxes brings uncertainties with it, while observed data from chamber and micrometeorological methods can be reliable and highly precise, upscaling these results introduces significant uncertainties as soils are so complex and heterogeneous in their characteristics, depth and distribution.

Soils contain over twice the carbon stored in the atmosphere (Figure 1.1) and are vital for carbon cycling, food production, water quality and nutrient retention (Jackson *et al.*, 2017). Soils release an estimated 350 Pg CO_2eq to the atmosphere, ten times that of fossil fuel burning and the cement industry combined (Oertel *et al.*, 2016). It is important we understand the processes driving emissions from soils to get a complete picture of our national and global carbon emissions.

The importance of soil cannot be understated, most of the world's food supply comes from the soil, and five of the 17 sustainable development goals (UNDP, 2016) make explicit reference to the role of soil. Soils provide a range of ecosystem services including (Creamer & O'Sullivan, 2018):

1. Primary Production – the ability of soil to produce plant biomass, forming the basis of human life in the provision of food, animal feed fibre and fuel.
2. Water Purification and Regulation - providing clean water for both human and animal consumption, and for aquatic ecosystems. As water percolates through soil

layers potentially harmful substances (metals, phosphates) can be adsorbed or transformed, effectively purifying the water. The ability of soils to store water can also prevent flooding and drought as they moderate the release of water into rivers.

3. Carbon storage and sequestration – after the oceans, soils are the largest store of carbon on Earth, as plants photosynthesise and transfer carbon from the atmosphere to the soil for long periods of time as soil organic matter, reducing (or slowing the accumulation) of CO_2 in the atmosphere. Carbon stored in soils is influenced by the soil temperature and water content, which affect microbial activity and the decomposition of soil organic matter. Increasing soil C content not only benefits the climate by reducing atmospheric CO_2, it improves nutrient storage, water holding capacity, aggregation, and adsorption and retention of organic and inorganic pollutants (Kibblewhite *et al.*, 2008).
4. Habitat for intrinsic and functional biodiversity – soils are incredibly complex amalgamations of organisms, so much so that it is estimated that only 1% of soil microorganisms have been identified (Orgiazzi *et al.*, 2016). The organisms within soils aid in their delivery of primary production, water purification and carbon storage.
5. Medium for the cycling and provision of nutrients – soils store minerals and nutrients such as phosphate or lime, they can receive nutrients from agricultural waste products like slurry or manure, and can act as a store and cycling agent for chemical fertilizers.

The physical properties of a soil can strongly influence both its function in an ecosystem and the management practices which will affect it, with the type of vegetation, the movement of water, and the nutrients available to biomass all determined by the properties of the soil itself (Brady and Weil, 2016). Soils and soil organic matter (SOM) are the foundation of life on earth, the amount of SOM (humic and non-humic substances) in a certain location and time depends on biotic (plant inputs and soil food web), abiotic (climate, mineralogy, slope, aspect, frequency of fire) and anthropogenic (fire, N deposition, climate change, land use, land management) factors (Jackson *et al.*, 2017). Crucially, SOM is typically comprised of ~50% organic carbon (Lanigan and Hackett, 2017), though this varies with soil type (Jain *et al.*, 1997) and depth (Westman *et al.*, 2006), this large proportion of carbon emphasises the importance of soil as a significant store in the global biogeochemical cycle.

1.5.1 *Soil Texture*

Often the first (and most important) characteristic of a soil to be determined in a soil survey is *soil texture*, effectively a description of the size of soil particles (when large mineral particles dominate it is a sandy soil, when mineral colloids dominate it is a clayey soil), while *soil structure* defines the manner these particles are aggregated, which in turn determines the pores and channels in the soil (Brady and Weil, 2016). Soil texture influences nearly all soil processes either directly or indirectly (Vos *et al.*, 2016), and can be considered a relatively permanent property of a soil as it is not readily subject to change. Soil texture is typically represented by percentages of sand, silt and clay and can be determined using Figure 1.3, where it is recommended to first identify the % clay in a soil, then % sand, and the % silt can then be calculated as the remainder as the sum must equal 100% (Brady and Weil, 2016). For example, a soil comprised of 10% clay, 60% sand and 30% silt would fit into the 'sandy loam' category. Assessment of soil texture is officially undertaken in laboratories using particle size analysis, but is more commonly carried out in the field by sense of touch, by testing the plasticity, shininess, amount of visible sand and by squeezing the soil between the fingers, a method which turns out to be almost as accurate as laboratory studies (Vos *et al.*, 2016). Though texture can be seen as one of the most basic aspects of a soil, it is even possible to get an idea of soil health from the study of soil texture (Mikhailova *et al.*, 2018).

The large particle sizes of sandy soils means they tend to be porous and allow for the transfer of water, while clay soils are more at risk of compaction and have more pore space, meaning they are more prone to saturation and run-off (Brady and Weil, 2016). Soil texture affects the accumulation of organic carbon, as fine textured soils (high silt and clay content) have a higher water retention capacity (Saxton and Rawls, 2006), which means productivity and subsequent plant (organic carbon) inputs to soil are also high (Colazo and Buschiazzo, 2015).

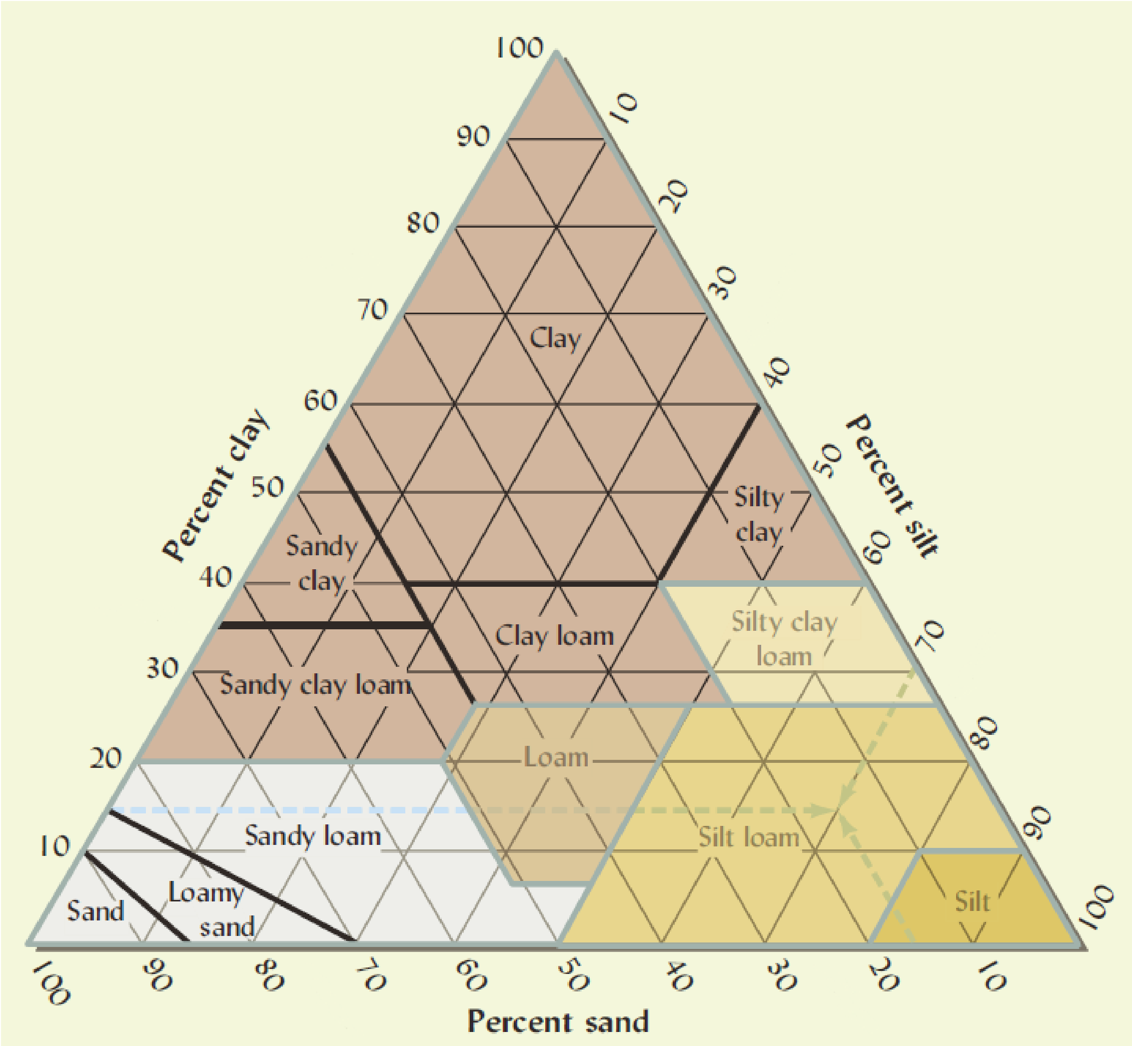


Figure 1.3: Soil textural classes pyramid, from Brady and Weil (2016)

1.5.2 *Soil Structure*

Soil structure can be defined as the "*the size, shape and arrangement of solids and voids, continuity of pores and voids, their capacity to retain and transmit fluids and organic and inorganic substances, and ability to support vigorous root growth and development*" (Lal, 1991 pp. 69). The structure of a soil is determined by the spatial arrangement of particles into complex aggregations, pores and channels. The particles can be considered to be the building blocks of soil, which are held together by microbial glues, roots and fungal hyphae which help stabilise the soil structure, where sand, silt, clay and organic particles becoming aggregated together to form structural units known as peds or aggregates (Brady and Weil, 2016). Strong soil structure is essential for agriculture as it can affect the ability of a plant to absorb water and nutrients (Pardo *et al.*, 2000) and allows for oxygen and water infiltration, and improvement of water storage (Franzluebbers, 2002). The structure of a soil can indicate the functions it is able to provide (Rabot *et al.*, 2018), functions which are vulnerable to management practices that can damage soil structure. Factors such as manuring, composting, fertilizer application, crop rotation and crop management can all positively or negatively affect soil structure, depending how they are implemented (Bronick and Lal, 2005). Soils subjected to tillage rather than no-till practices are found to have poorer pore connectivity (Pires *et al.*, 2017), and soils which do not incorporate plant residues via mulching have poorer structure (Martens, 2000). The aggregation of a soil into its structure is mediated by Soil Organic Carbon (SOC), soil biota, ionic bridging, clay and carbonates, with the SOC acting as a binding agent and nucleus for aggregate formation (Bronick and Lal, 2005). Carbon and other elements related to greenhouse gases will be discussed in-depth in Chapter 2.

1.6 Irish Soils

Irish soils are relatively young, around 15,000 years old, with most soils forming after the retreat of the last ice age, for context, tropical soils in Africa and South America were formed millions of years ago. The soils of Ireland are classified into eleven 'Great Groups' based on their formation, climate and management (Figure 1.4).

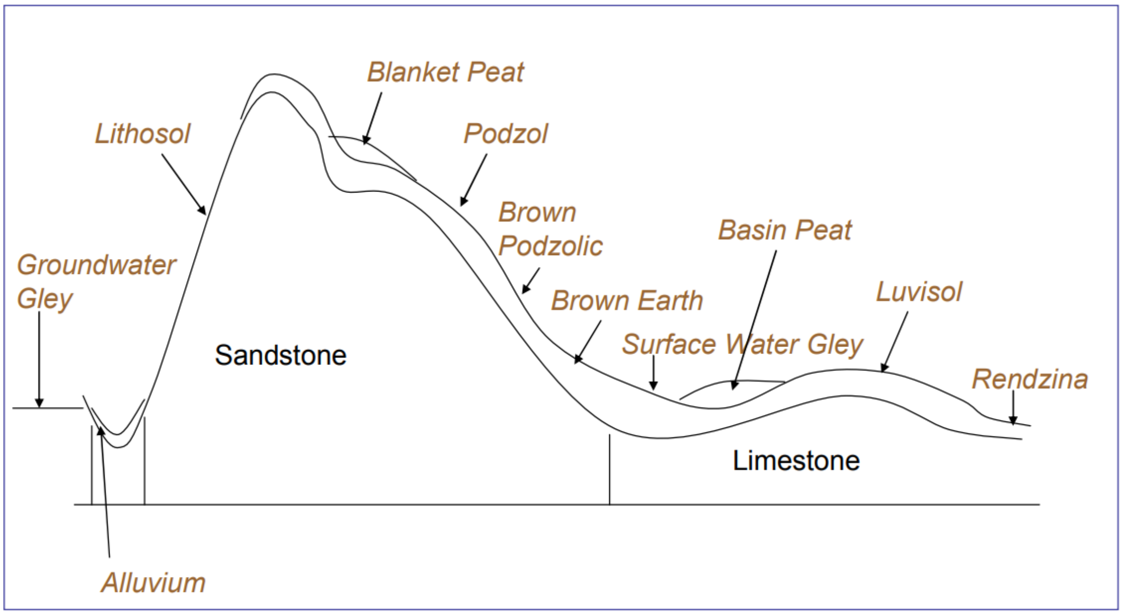


Figure 1.4: Soil Great Groups described across a landscape position (Source: Creamer et al. (2016))

Of the 6.9 million ha of land in Ireland, around 4.5 million ha (65%) is used for agriculture. Of this agricultural land, 81% is grassland (silage, hay and pasture), 11% is used for rough grazing (0.48 million ha), and 8% used for crops, fruit and horticulture (0.38 million ha), while 11% of the total land area is used for forestry (737,904 ha), typically well-drained soils are more suitable for intensive agriculture such as pasture and tillage while waterlogged soils more suited to rough grazing (Creamer & O'Sullivan, 2018).

1.6.1 *Soil Carbon Quantity and Fluxes in Ireland*

Estimates of SOC stock in the Republic of Ireland (ROI) vary across studies due to differing methods of calculation and calculations over different depths. Tomlinson (2005) estimated 1999 Tg C for the entire soil profile, Kiely *et al.* (2009) estimate 1062 Tg C to 50cm, while Eaton *et al.* (2008) estimate 1469 Tg C to 1m for mineral soils, including peatland soils increases this estimate to 2401 Tg C, with 0.55 million ha of arable land making up 65.4 Tg of this total (4.45%) while grassland accounts for 41% of the SOC store and makes up over 50% of total land area (Eaton *et al.*, 2008). Eddy covariance (Jaksic *et al.,* 2006) and chamber techniques (Byrne *et al.*, 2005) suggest that Irish grasslands are moderate CO_2 sinks of -2.52 kg C m^2 yr^{-1}; this is in contrast with the emissions estimates for grasslands under LULUCF which calculate Ireland's grassland emissions in 2016 to be 6889.15 kt CO_2eq, though much of this is likely due to drainage of organic soils, emissions from 'grassland remaining grassland' are assumed to be zero. This assumption is based on previous analyses which indicate Irish grasslands are moderate C sinks (Khalil *et al.*, 2013; Peichl *et al.*, 2011), though uncertainties for the 'grassland remaining grassland' category are reported as 100%, indicating that this is far from a certainty (Duffy *et al.*, 2018).

Measurements of Net Ecosystem Exchange (NEE) fluxes on Irish temperate grasslands found that they are small carbon sinks which are relatively insensitive to variation in precipitation as soil moisture never reached wilting point over two years due to the surface water gley soil (Jaksic *et al.*, 2006). The potential increase in moisture as a result of climate change however, could lead to grasslands requiring extensive instead of intensive management, using more land to produce the same amount of food, which could reduce their sequestration potential (Lawton *et al.*, 2006). Similarly, an intensively managed grassland site in Ireland is found to be a C sink of under 1 kg C m^2 yr^{-1}, but the choice of management regime is the primary control factor on C, water and energy exchanges (Peichl *et al.*, 2012). A study examining ploughing of Irish grassland has shown reductions in GPP and therefore enhanced C loss (rather than enhanced soil respiration) immediately after ploughing (Willems *et al.*, 2011). Attempting to identify the drivers of sequestration is not a simple task, as correlation analysis of environmental variables including air temperature, soil moisture, photosynthetically active radiation (PAR), vapour pressure deficit (VPD) and precipitation showed no correlation with NEE on seasonal or annual scales due to the responses of the components of NEE (GPP and Reco) to the variances of the environmental variables (Peichl *et al.*, 2012). This indicates the influence of other variables is dominating, or that these variables interacting together is affecting the overall signal.

Just under 10% of agricultural land in Ireland is cropland, planting crops disturbs soil and initiates the decay of carbon at greater depths (known as priming), meaning agricultural cropland can have significant levels of soil carbon flux (O'Brien, 2004). Conversion of other land-uses to cropland can cause reductions in SOC content and increased C flux, but Duffy *et al*. (2015) find no evidence that forestry, wetland, settlement, permanent grassland and other land are converted to cropland, the only land-use type which is converted is temporary grassland.

Carbon stock changes in Irish soils are calculated using the Land Parcel Identification System (LPIS) dataset superimposed on the indicative soil map. LPIS contains all parcels of land under the remit of multiple agricultural and rural environmental administrative schemes since 2000 – effectively all agricultural land in Ireland. Under LPIS cropland is defined as lands cultivated in the reporting year, plus lands under temporary grassland which have been recorded as cropland at any point since 2000.

Byrne and Kiely (2008) argue that adequately calibrated models can be used to investigate the effect of changes in management and climate, as well as providing a research tool which can be used to upscale from plot to field and regional level. They find relatively small losses of SOC at farm scale, but highlight that as grassland accounts for 53.3% (3.772 M ha) of land in the ROI, a SOC loss 0.1 t C ha^{-1} yr^{-1} equates to a loss of 0.377 million t C yr^{-1} if all grasslands respond in a similar way. It is therefore important to attempt to quantify the potential changes in soil carbon for all Irish soil types as climate changes. Changes in an area's grass or cropland carbon pools could therefore have a significant effect on the total carbon budget when scaled nationally or globally (Janssens *et al.,* 2003).

Sanderman *et al.* (2017) use a statistical model to assess the influence of land-use and land-cover change (LULCC) on soil carbon over time by simulating past and present SOC stocks and estimate that agricultural land uses have caused the loss of 133 Pg C from soil globally, indicating that further intensification of the Irish agricultural system may result in further SOC losses. Peichl *et al.* (2011) suggest that the drier and warmer summers expected for Ireland under climate change may slightly reduce the uptake potential of Irish grasslands due to a reduction in productivity as a result of drought, yet their position as carbon sinks is expected to continue.

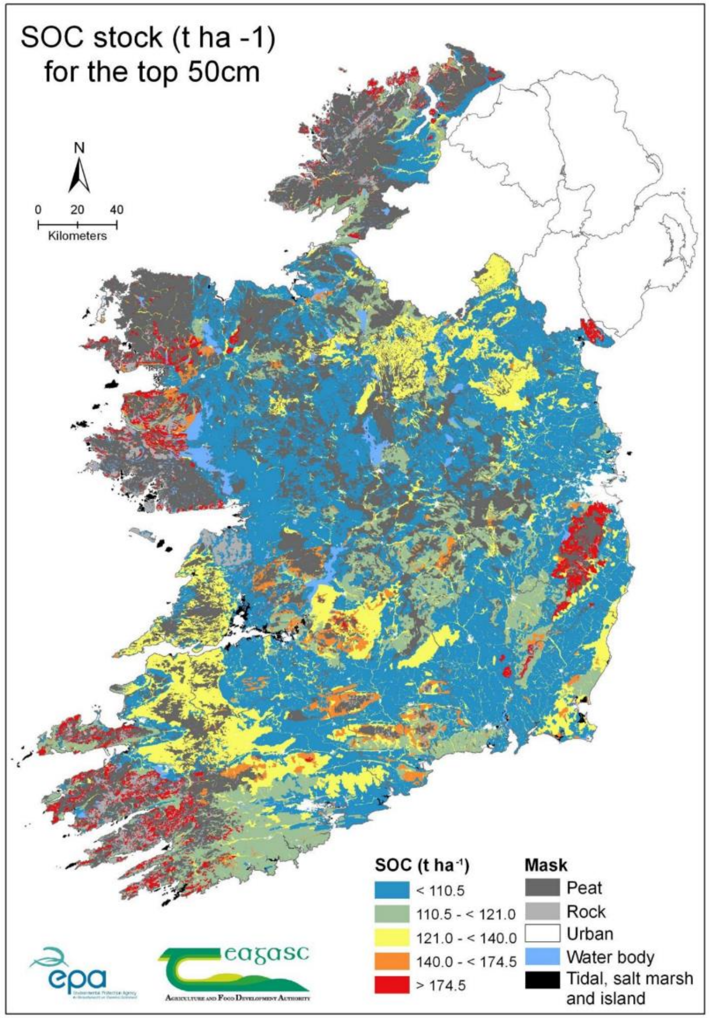
Creamer *et al.* (2016) produced the Irish Soil Information System map which derives estimates of carbon contents for all Irish soils except for peat, which lack data due to an absence of surveying. Two methods for mapping SOC stock were used: A. Mapping SOC based on the lead soil subgroup in the association, and B. Calculating the relative proportions of each subgroup in the association and weighting the SOC of the subgroup constituents, giving the relative SOC (t/ha) for each subgroup within the association, then summing together for the entire soil association. Both methods were tested using two validation models, one which applied indices based on De Vos *et al.* (2005) to establish the predictive quality of SOC mapping using the soil subgroups, and another which directly compared observations to modelled values. This method was only applied to the SOC for the first 50cm as validation data is not available to 1m. The map which gave the most robust confidence results (33.3%) was the 50cm depth using approach B and validation model 2. Maps to 50cm and 1m are presented in Figures 1.5 and 1.6.

While it is useful to get a national estimate of soil carbon quantity, accurate estimation of soil carbon fluxes is vital for national inventory reporting mandated by the United Nations Framework Convention on Climate Change (UNFCCC). As an Annex I party to the convention, Ireland is obligated to report its emissions annually.

1.7 Soil Carbon Sequestration (SCS)

The potential for soils to sequester carbon and offset GHG emissions while enhancing crop yields, food security and water holding capacity has long been understood, and is regarded as a win-win/no-regret scenario for land managers (Lal, 2004b; Lal *et al.*, 2015). Using soils to offset GHG increases is a difficult task as carbon offsets require high certainty and credibility, and SOM dynamics are complex, variable and scientifically uncertain, making it difficult to verify the magnitude of carbon sequestration (Campbell and Paustian, 2015). Nevertheless, SOM models (e.g. CENTURY, DAYCENT, ECOSSE) can and have been used to identify differences between 'business as usual' emissions scenarios and scenarios where changes in management practices are implemented (Dell *et al.*, 2013). These models have been widely implemented (Henderson *et al.*, 2015) including in Europe (Abdalla *et al.*, 2010; Smith *et al.*, 2005), Asia (Cheng *et al.*, 2014), Australia (Scheer *et al.*, 2014) and the USA (Ogle *et al.*, 2010).

After the ratification of the Paris Agreement in 2016, the 4/1000 initiative which was first launched at COP21 gained significant attention. The initiative argued that increasing global SOM stocks by 0.4% per year would compensate for the entirety of anthropogenic emissions for that year. A meta-analysis of the feasibility of this process was undertaken by Minasny *et al*. (2017) who analysed the potential for sequestration on managed agricultural land and found a potential global SOC sequestration of 2-3 Pg C yr^{-1}, 20-35% of global anthropogenic emissions, concluding that SCS is a viable solution to reduce emissions in the short-term. Sanderman *et al.* (2017) simulate past and current SOC stocks globally and estimate a sink potential of ~133 Pg C in total, with 8 to 28 Pg C in cropland and grazing land, but acknowledge that physical, social, economic and technical constraints (Smith *et al.*, 2005b) mean that the amount of the carbon sink that has the potential to be filled is 10-30% globally, and may well be below 10%.



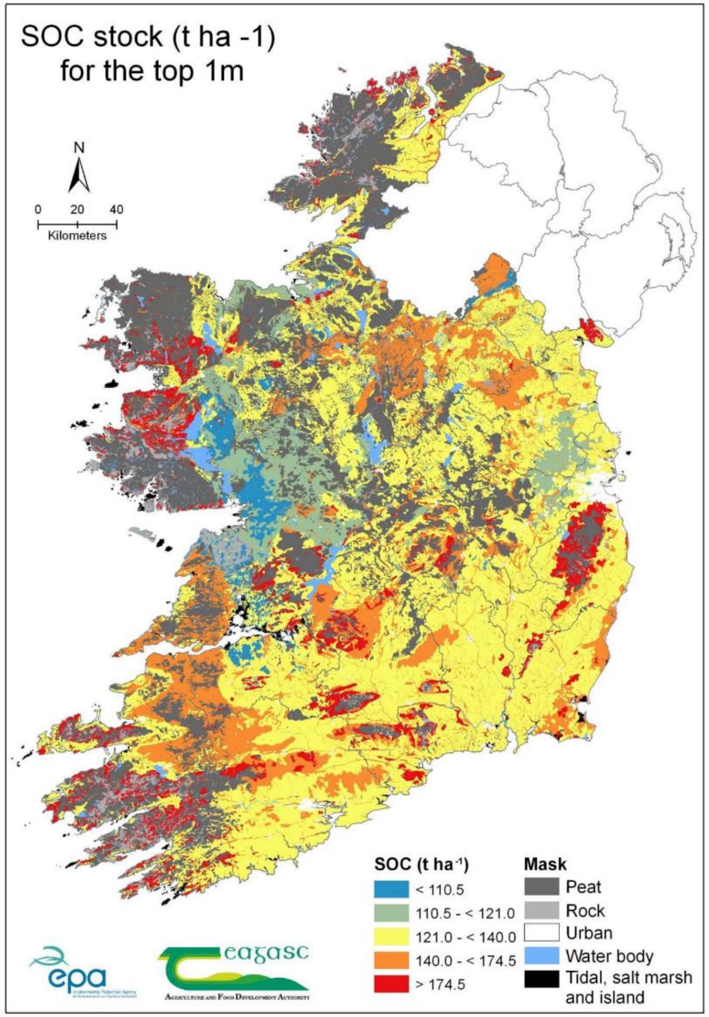


Figure 1.5 (left): Irish SOC stocks to 50cm depth (from Creamer et al. (2016)).

Figure 1.6 (right): Irish SOC stocks to 1m depth (from Creamer et al. (2016)).

1.7.1 *Complexities of the 4/1000 Initiative*

There is a danger that policymakers who do not have the time or knowledge needed to fully analyse the issue of SCS will take the message of the 4/1000 initiative as verbatim and will overestimate the ability of soils to sequester C (Baveye *et al.*, 2018). While the goals of the 4/1000 initiative are laudable and increasing SOC content is widely regarded as a win-win scenario, Chabbi *et al.* (2017) emphasise that we should focus on region-specific implementation options which identify the agroecosystems most suitable to SCS and assess the economic benefits on different soil types, climate zones and farm types. Seeing soil carbon sequestration as a panacea has been warned against for some time, as the quantity of C that can be stored in soil is finite, the process is reversible, and the increase in C sequestration may result in increases in other GHGs such as N_2O and methane, or increases in fertilizer use to encourage plant growth, and associated emissions for production of this fertilizer (Powlson *et al.*, 2011).

Baveye *et al.* (2018) argued against the optimistic goal of the 4/1000 initiative, and were critical of more cautious research which shows that it may be possible for soils to sequester 2-3 Pg C yr^{-1} (20-35% of global GHG emissions, Minasny *et al.,* 2017) as being overly optimistic. Baveye *et al.* (2018) emphasise the fact that this sequestration of C is only effective in the short-term as soils become C saturated (sink-saturation), and that the effectiveness of soils as a sink declines immediately after sequestration is initiated i.e. there are diminishing returns until saturation is reached (Smith, 2016; Franzluebbers *et al.,* 2012). Smith (2016) estimated that global SCS had the potential to sequester 0.7 Pg C eq. yr^{-1}, while an analysis for the potential of French soils to sequester carbon concluded SCS would compensate ~9% of emissions resulting from agriculture, around 1-2% of total emissions (Chenu *et al.*, 2014), much lower than the 4/1000 initiative envisaged. Baveye *et al.* (2018) also warn that Minasny *et al.* (2017) ignore the impact warming will have on soil microbial respiration, citing Crowther *et al*. (2016) who project declines in SOC content as temperatures warm that could be 12-17% of anthropogenic emissions of the period up to 2050, meaning adding 0.4% to soils would merely compensate for the increases in respiration as a result of warming temperatures. Baveye *et al.* (2018) argue that inorganic carbon should be considered in these estimates too, as mobilisation of inorganic C due to temperature increases dissolving carbonates or increasing acidification of soils could result in much more substantial emissions to the atmosphere.

The ambitious nature of the 4/1000 initiative, and the large funding which is now going into soil carbon sequestration research was challenged further by Amundson and Biardeau (2018), who argue that for the 4/1000 initiative to work, it must be immediately implemented on all managed lands on Earth (570 million farms ran by 3 billion farmers), and must be sustained for decades, requiring support from these private landowners. The cultural, economic and physical barriers including conservative mindsets, lack of ownership of the land and a distrust of academic authority mean that soils as major carbon sinks may not be a feasible option, and that it is irresponsible to regard them as a panacea (Amundson and Biardeau, 2018).

Experimental evidence from Poulton *et al.* (2018) find long-term studies at Rothamsted indicate that 4/1000 levels of sequestration (and above) are possible and have been observed in their experiments, with different land-management practices increasing GHG stocks at different rates, but these can be impractical or impossible for farmers to achieve due to a number of reasons including: 1. Insufficient resources available to farmers due to lack of animals for manure or crops for residues (smallholder farmers in Africa), 2. The practice is already widely used (incorporation of crop residues), 3. Widespread adoption would negatively impact global food security (conversion of agricultural land to forest or grassland), 4. Management change would financially harm the farmer or be impractical for some other reason – changes would require alterations in government policies, regulation or subsidies to promote the practice, a factor echoed by Baveye *et al.*, (2018) who call for a financial analysis of SCS to determine what is socio-economically realistic.

While using any methods possible (including soils) to mitigate climate change is admirable and positive, it is recommended that focus be made on increasing SOC by small amounts for the benefits it gives to soil quality as a whole, rather than for its mitigation potential, as the evidence base is stronger for the former (Baveye *et al.*, 2018). Similarly Paustian *et al.* (2016, pp. 44) call for the pursuit of 'all reduction measures that are feasible, cost effective and environmentally sustainable', arguing the inability to quantify and verify soil mitigation activities is a major impediment to implementing SCS strategies on agricultural land. To overcome this, they suggest increasing the acceptance of SCS in compliance and voluntary carbon markets; reducing costs to governments for provision of environment-based subsidies; and meeting consumers demands for low-carbon products. Paustian *et al.* (2016) recommend the strengthening of soil GHG monitoring networks for fluxes and on-farm measurements which can help to illuminate the processes underlying these fluxes in different spatial contexts and informing and involving land-users who will be implementing practices, while taking advantage of their local knowledge.

1.7.2 *Soil Carbon Sequestration in Ireland*

The sequestration potential for Ireland has been assessed by Kiely *et al.* (2017) who examined C deficits for different land-uses and found that croplands are currently at a level of 38% C saturated, grasslands at 48% and forests of 56%, meaning there is significant potential for soils to sequester C. For example, Kiely *et al.* (2010) assessed the C density of Irish soils and found grasslands soils had a density of ~102 t C ha^{-1} for to 30cm depth and 145 t C ha^{-1} to 50cm depth. Taking a conservative assumption that these soils are 75% saturated with C, this gives a potential C deficit of 48 t C ha^{-1}. Ireland has an area of 3.6 million ha^{-1} of grassland, giving a total C sequestration potential for Irish grasslands of 172.8 Mt C.

1.8 Summary & Research Questions

Our understanding of the carbon cycle and climate system has advanced significantly over the past centuries and decades; we better understand the interactions between the surface and the atmosphere, and how greenhouse gases affect these interactions. We know how important carbon is, and the impact carbon emissions are having on our climate. We can now measure and model changes in the carbon cycle, the importance of measuring these changes has been enshrined in international law, compelling us as both nations and citizens to act, with the goal of ultimately reducing our emissions to minimise the harm we are causing to our own species and others.

After Kyoto and subsequent COP meetings, the Paris agreement in 2016 has resulted in the commitment of most (184 of 197) countries to significantly reducing their emissions to avoid 'dangerous' climate change, deemed anything past 2°C above pre-industrial levels, with a target of 1.5°C seen as optimal. Each nation has submitted nationally determined contributions (NDCs) which outline the measures they will take to cut their emissions, from whatever sources they arise. Soil plays a vital role in all of this, storing more carbon than the atmosphere and releasing a significant quantity of that carbon each year, a process exacerbated by agriculture, land-use change, and other human interventions. For this reason, soils are included in national inventory calculations, where their contribution to climate change can be estimated. Soils are also regarded as a potential resource for C sequestration, with Irish soils identified as having strong C sink potential. The land-surface is one of the largest sources of uncertainty in ESMs, meaning we need to improve our understanding of land-surface exchanges to best represent their dynamics.

Emissions reporting is a complex process which has the potential to be improved using models to overcome the absence of measurements. Models can help to move national emissions estimates from a crude tier-1 approach towards a more refined tier-3 methodology, where gaps in knowledge which previously necessitated the use of default emissions factors can be filled. Before models can be used for policy prescriptive purposes it is important that they are fully evaluated and robustly tested. This thesis will provide a comprehensive evaluation and robust analysis of a widely used process based model, and will assess its ability to simulate soil carbon emissions at different scales in Ireland.

Following a discussion of the information which motivated this work (Chapter 2) and an in-depth analysis of modelling GHG emissions from soils (Chapter 3), this thesis will attempt to address the following research questions:

A. Is it possible to use models to improve national emission estimates for soils and move towards a tier-3 reporting methodology?
B. What is the potential impact of future extreme events on emissions of greenhouse gases from soils?

In order to answer these questions, the following aims are outlined:

1. To assess the ability of a model to simulate soil carbon emissions at a selected Irish site (*Research Question A:* Chapters 4 and 5)
2. To upscale site emissions to national scale (*Research Question A:* Chapter 6)
3. To investigate the impact of extreme weather events on quantities and fluxes of greenhouse gases in Irish soils (*Research Question B:* Chapter 7)

1.9 Thesis Structure

Chapters 1-3 of this thesis provide context for the research questions and chapters that follow. Chapter 1 provides a background to our understanding of climate and the carbon cycle, with a summary of the importance of soil and its complexities, which forms the motivation for this work. Chapter 2 details how soils relate to climate, how humans have attempted to understand the interactions between soil and climate through theory and measurement, how we quantify these emissions at national and global scale, and how we have attempted to understand what may happen in the future. Chapter 3 provides an in-depth discussion of process-based modelling of greenhouse gas emissions from soils and details the modifiers and methods used. The following chapters are presented in the form of academic papers though only one is published at this stage, Chapter 4 outlines the process of running the ECOSSE model at an Irish site and comparing outputs to observations, along with an evaluation of the model parameters (*aim 1*). Chapter 5 provides an assessment of the rate modifiers employed by ECOSSE to identify the potential sources of issues uncovered in the model simulations (*aim 1*). Chapter 6 outlines the process of upscaling the model from site to regional scale (*aim 2*). Chapter 7 outlines the potential response of soils to extreme events in the future (*aim 3*), finally Chapter 8 unites the previous chapters in discussion, and outlines directions for potential future work. Figure 1.7 illustrates this thesis structure.

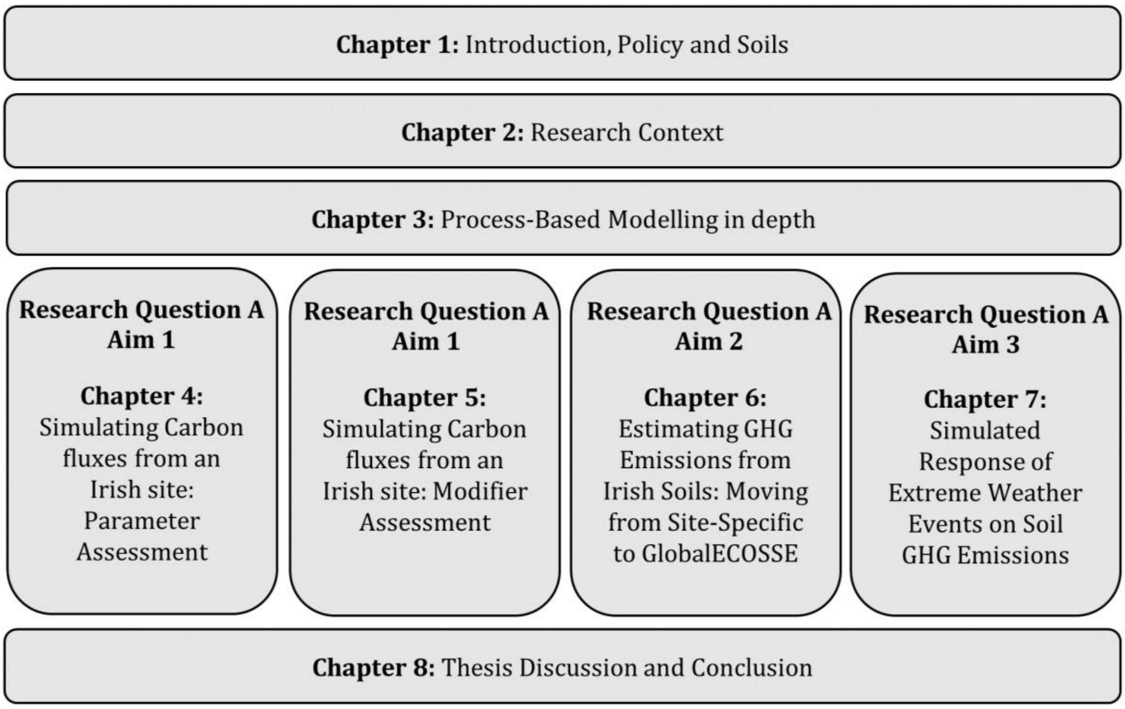


Figure 1.7: Thesis Structure

2 Research Context & Framework

This chapter will outline the nature and properties of soils, their relationship to greenhouse gases, the factors which influence GHG fluxes from soils, and the history of modelling these fluxes. As chronologies overlap across topics, the chapter first describes the theory underlying the interactions between soil and greenhouse gases, then the observations and methods of soil GHG measurement are discussed, followed by the processes involved in modelling GHG fluxes, and a discussion of global soil carbon quantity.

2.1 Theoretical Understanding of Soil and Soil Fluxes

2.1.1 *Soil and Greenhouse Gases*

Over the past 500 million years, carbon in plant and animal life has decayed and been deposited in geological reservoirs, which humans have exploited since the industrial revolution to provide fuel and energy for our development as a species, leading to an increase in the atmospheric concentration of CO_2, and an imbalance in Earth's relative homeostasis. The impact of this human development on our planet has even led to calls for a new geological era called the 'Anthropocene' to be recognised, as human actions are driving widespread changes to the life-supporting infrastructure of Earth (Lewis and Maslin, 2015).

Figure 2.1 illustrates the major global pools of carbon showing the largest C pool is the deep ocean, where 37,000 Pg C has been absorbed and stored for a long time. The soil pool holds a significant amount of carbon, an estimated 2300 Pg C. The amount of C stored in the oceans, fossil fuel reserves and soils is vastly larger than that stored in the atmosphere (800 Pg C), yet the exploitation of the fossil fuel reserve, combined with changes to land-use, cause emissions of ~9 Pg C yr^{-1} producing an increase in the atmospheric concentration of ~4 Pg C yr^{-1}. The remaining ~5 Pg C yr^{-1} is absorbed by the oceans and the terrestrial biosphere.

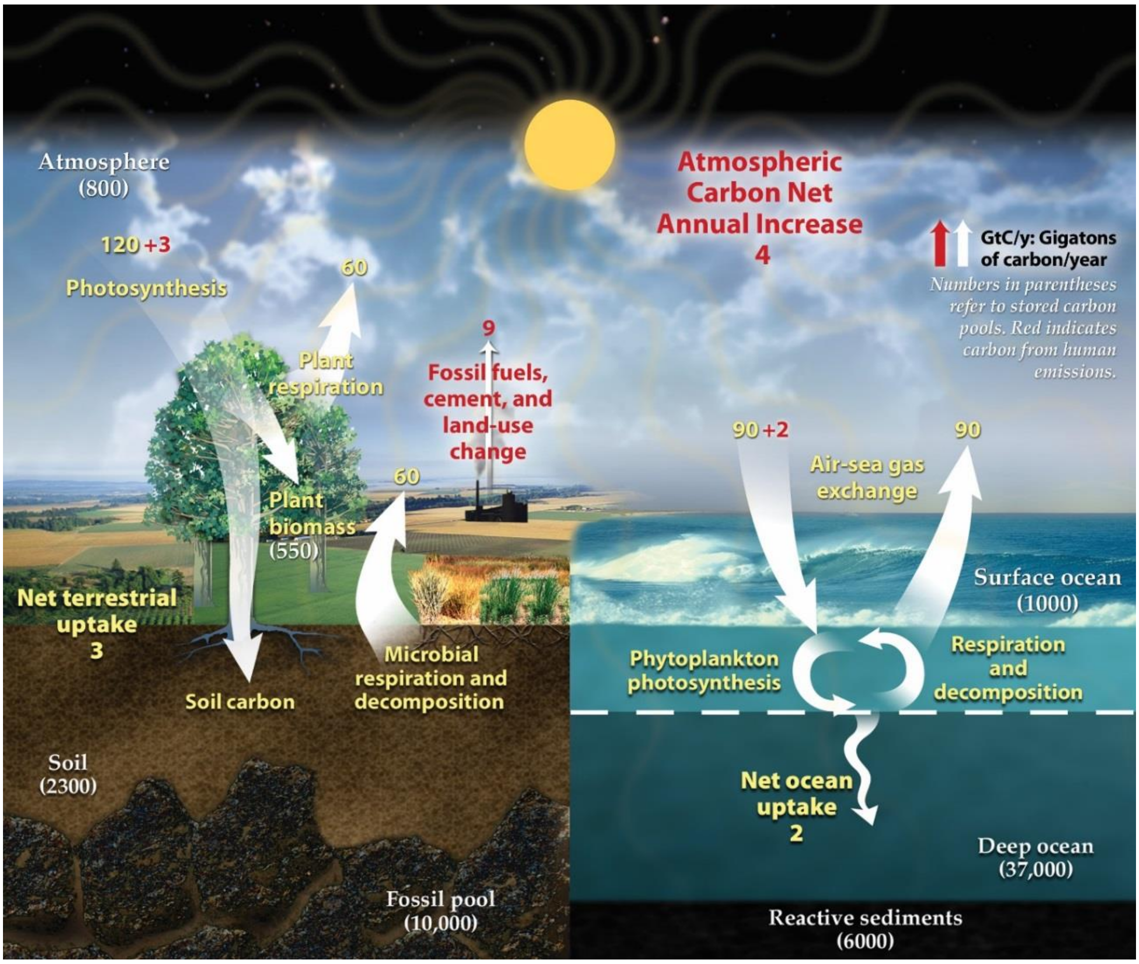


Figure 2.1: The global carbon cycle illustrating the movement of C between land, atmosphere and oceans. Yellow numbers are fluxes while red are human contributions in Pg C yr^{-1} (NASA, 2011).

2.1.1.1 *Carbon*

Carbon (C) enters soils via tissue residues from plants and roots which interact with symbiotic fungi and are then broken down and respired by microorganisms and soil fauna, most of the carbon that enters soil from plant inputs either decomposes and returns to the atmosphere or is leached from the soil over decades to centuries (Trumbore and Czimczik, 2008). If the rate of decomposition is lower than the plant inputs, SOM builds up over time (Paul, 2016). Carbon comprises a significant proportion of SOM, with different levels associated with different soil types, interactions between climate, soil, topography and land-use determine the type of vegetation which grows and subsequently the quantity, location, timing and composition of C inputs to soil (Jackson *et al.*, 2017). C in soils is made up of both inorganic and organic carbon, inorganic carbon is usually found in carbonate minerals e.g. calcite and dolomite, while soil organic carbon (SOC) is the major constituent of SOM and is present in microorganisms, plant and animal residues, humus, and highly carbonised compounds (charcoal, graphite and coal) typically comprising 48-58% of the SOM weight (Nelson and Sommers, 1982). The quantity of carbon stored in soils depends on the balance between organic inputs from living organisms, and carbon losses through heterotrophic respiration (Post *et al.,* 1982, Brady & Weil, 2016). Both organic inputs and the degree of respiration vary depending on the type and productivity of vegetation at a location, as well as the climate, soil management, and the soil texture and structure. Environmental variables like temperature, moisture, oxygen, N availability, phosphorous, pH, space and time all regulate the transformation of SOC, as does litter quality, organomineral properties of SOC, and microbial structure (Luo *et al.*, 2016b). The balance of these fluxes is influenced by temperature and moisture which affect the accumulation and decay of carbon and nitrogen (Jenny, 1980; Oertel *et al.*, 2016). Soils provide essential ecosystem services, giving food, fibre and fuel, filtering water, resisting erosion and being a carbon source or sink in relation to climate change mitigation (Schmidt *et al.*, 2011).

The threats to the terrestrial C pool are well documented; changes from natural to managed land-uses typically result in declines in organic matter (Davidson and Ackerman, 1993), while conversion of land used for cultivation back to natural or perennial vegetation allows soil carbon to accumulate, and increases the soil carbon pool (Post and Kwon, 2000). From 1990-2010 emissions from Land Use and Land Cover Change (LULCC) comprised 12.5% of total anthropogenic C emissions (Houghton *et al.*, 2012), while there are uncertainties associated with this estimate, the vulnerability of the soil carbon pool is clear. The latest global carbon budget indicates that emissions from land-use change released 1.3 ± 0.7 Pg C in 2016, compared to the 9.9 ± 0.5 from fossil fuels and industry, the high uncertainties relative to the total emphasises the knowledge gaps still associated with measuring the land-carbon flux, and the requirement for further research around this vital carbon pool (Le Quéré *et al.*, 2018).

The pools of C within soil that are recognised as sources of CO_2 efflux are 1. the SOM 2. above and below ground plant residues, and 3. organic substances released by living roots, with no distinct boundaries between these three groups as plant residues become humified and part of SOM, and rhizodeposits originating from dead plants or roots (Kuzyakov, 2006). Kuzyakov (2006) suggests the major sources of CO_2 efflux, and the mean residence times (MRT) of each component are:

1. Microbial decomposition of SOM in soil without roots or undecomposed plant remains (basal respiration), MRT = decades to hundreds of years
2. Microbial decomposition of SOM in soil with roots or plant residues present (priming effect), MRT = months to years to decades
3. Microbial decomposition of dead plant litter, MRT = weeks to months
4. Microbial decomposition of rhizodeposits from living roots (rhizomicrobial respiration), MRT = hours to days to weeks

5. Root respiration, MRT = minutes to hours

Soil respiration (Rs) can be disaggregated into its components which include heterotrophic (Rh) and autotrophic respiration (Ra). Heterotrophic respiration is the decomposition of SOM by soil microbes (bacteria and fungi) which aerobically and anaerobically degrade organic matter, producing CO_2 and other greenhouse gases (Xu and Shang, 2016). Autotrophic respiration is dominated by respiration by roots within the soil, which varies in its overall contribution to Rs depending on the time of year and the characteristics of the soil itself (Kuzyakov, 2006). Figure 2.2 illustrates the interactions between plants and soil and the different types of respiration resulting from these interactions.

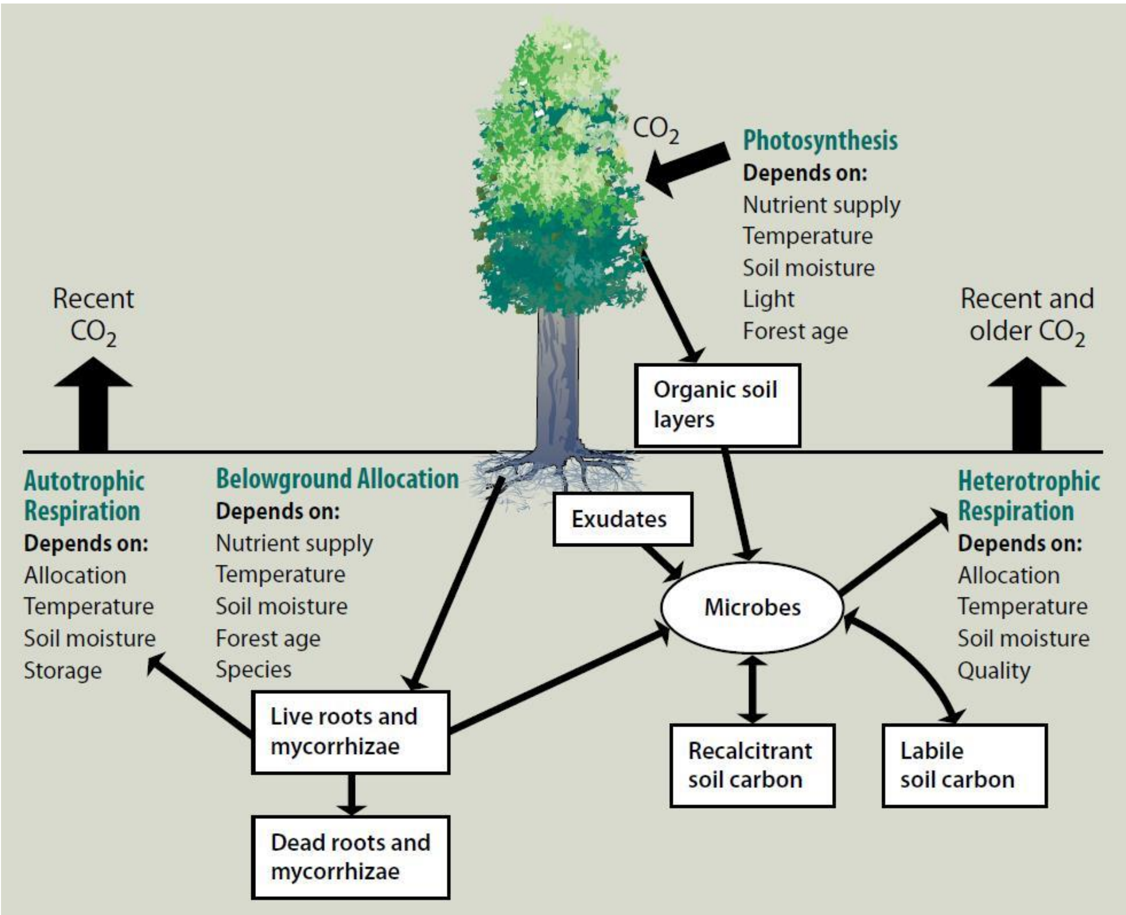


Figure 2.2: Conceptual model of the components of CO_2 flux within soil (Source: r2dkits.com, n,d)

Although estimates of SOC stocks and emissions from terrestrial soils remains highly uncertain (Houghton *et al.*, 2012; Scharlemann *et al.*, 2014; Oertel *et al.*, 2016), there remains a pressing need to improve our understanding of soil C management to minimise soil C losses and increase the C sequestration potential of soils (Scharlemann *et al.*, 2014). Increasing the carbon content in soils is seen as a win-win/no regret scenario as crop yields increase, food security is enhanced, soil structure is improved, surface and groundwaters are purified, and carbon sequestration offsets anthropogenic CO_2 emissions (Lal, 2004a, 2004b).

2.1.1.2 *Methane*

Methane (CH_4) is the second most significant greenhouse gas (after CO_2) accounting for an increase in radiative forcing of 0.48 ± 0.05 W m^2 due to an increased atmospheric concentration from 722 ppb in pre-industrial times, to 1803 ± 2 ppb today (Myhre *et al.*, 2013). Myhre *et al.* (2013) acknowledged that methane has a 100-year global warming potential (GWP) of 28, which has risen from an estimate of 25 in the fourth IPCC assessment report (IPCC, 2007). This estimate has recently been revised upward by Etminan *et al.* (2016) due to the inclusion of short-wave forcing and CH_4's absorption of solar radiation, with the 1750-2011 RF now estimated as being 20-25% higher (from 0.48 W m^{-2} to 0.61 W m^2) than the IPCC value in 2013, giving a new 100-year GWP of 32, showing that there are still uncertainties with even the most basic aspects of climate science, and that it is constantly evolving. There is currently debate about the use of GWP as a metric for short-lived climate pollutants (SLCPs), Allen *et al.* (2018) suggest using a new metric, GWP*, which relates cumulative emissions of CO_2 with the current emissions of SLCPs in order to better meet future emissions targets.

Methane is produced by soil microbial communities, specifically methanogens (a group of Archaea), as a consequence of anaerobic respiration in anoxic environments resulting from the anaerobic degradation of organic matter (fermentation) (Nazaries *et al.*, 2013). Of the total global methane budget of 500-600 Tg CH_4 yr^{-1}, around 35% is from natural sources, with the remainder from anthropogenic activities (Conrad, 2009). Wetlands are the largest natural source of CH_4, comprising 62% of the natural CH_4 budget (*ibid*). The remainder comes from oceans, sediments, plants, termites and geological sources, while anthropogenic methane sources include rice agriculture, livestock, landfills, waste treatment, biomass burning, fossil fuel extraction and consumption and now account for 63% of total global methane emissions – in pre-industrial times they represented less than 10% (Conrad, 2009; Nazaries *et al.*, 2013). As wetlands cover such a small area on the planet this compensates for their relatively high emissions, while data remain scarce and for point locations and are not representative of the larger-scale (Oertel *et al.*, 2016). For most CH_4 sources listed, the actual production is typically higher than recorded emissions, as a large amount of initial CH_4 is consumed by microorganisms before it reaches the atmosphere (Conrad, 2009). The average rate of CH_4 emissions from different land-uses varies in wetlands (0.1-6950 umol CH_4 m^2 h^{-1}) due to the diversity of wetland types and climates, while the average CH_4

emissions from grasslands is <3 umol m^{-2} h^{-1} and either negative or <1 umol m^{-2} h^{-1} for croplands.

Quantities of methane emissions from different wetland types are not identical. Turetsky *et al.* (2014) find that fens are less responsive to temperature than bogs or swamps, with the largest flux observed in bogs after 30 days of dry conditions followed by wet conditions, as fens and swamps record their highest fluxes when antecedent and current conditions are wet, with the exception of drained wetlands which did not show an increased flux in response to warm and wet conditions. These distinct interactions are important as ideally these diverse land-use types should be treated differently by models.

The scale of methane emission across different soil and vegetation types is examined by Levy *et al*. (2011) who use almost 5000 chamber measurements of CH_4 flux for 21 sites to attempt to model the emission process, finding larger emissions for organic over mineral soils (to be expected), with plant species composition giving the highest explanatory power to the model, followed by soil carbon content, peat depth, soil moisture and pH. As methane emissions have recently been increasing at a higher rate than CO_2 and N_2O, likely due to increased emissions from agriculture in Africa and Asia (Saunois *et al.*, 2016), it is important to understand the factors affecting methane release to predict potential changes in climate as methane plays an increasing role as time goes on. This issue has previously been acknowledged in relation to GHG modelling by Bridgham *et al.* (2013) who highlight the inadequate incorporation of factors integral to CH_4 production, consumption and transport into models, along with errors in emission estimates from spatial extrapolations from poorly mapped wetlands, and the paucity of observational evidence of CH_4 fluxes and the environmental variables that may influence them.

2.1.1.3 *Nitrogen*

The quantity of N in soils around the world is estimated at 133-140 Pg N in the upper 1m (Batjes, 1996). Nitrogen fixation is the transformation of un-reactive nitrogen to ammonium compounds and subsequently transformed into amino acids and oxidised compounds by microorganisms, then returned to the atmosphere through denitrification in soils, water and sediments. This process contributes 413 Tg of reactive nitrogen (N_r) to ecosystems annually, with anthropogenic activities responsible for 210 Tg N yr^{-1} which is transformed on land within soils and vegetation where the agricultural use of fertilizer N dominates (Fowler *et al.*, 2013). N_r can be broken down into its constituents as follows: nitrate (NO_3^-) from fertilizer use is leaked from agricultural land and also contributes trace N_r compounds to the atmosphere. Ammonia (NH_3) emissions from land and combustion related emissions of nitrogen oxides (NO_x) emit 100 Tg N yr^{-1} to the atmosphere, which can generate secondary pollutants like ozone and ammonium nitrate (NH_4NO_3) and ammonium sulphate $(NH_4)_2SO_4$, leaching of NO_3 comprises 40-70 Tg N yr^{-1} to the ocean, with a further 30 Tg from atmospheric deposition largely increasing the natural marine biological N fixation of 140 Tg N yr^{-1} (Fowler *et al.*, 2013). Similarly to soil C, soil N concentration depends on the productivity of vegetation, decomposition of organic matter, rainfall, fertilizer input and N fixation, with losses occurring through leaching and denitrification (Post *et al.*, 1985).

Nitrous Oxide (N_2O) is a long-lived atmospheric trace gas, the dominant sources of N_2O in soils come from microbial nitrification and denitrification in managed and natural soils (Butterbach-Bahl *et al.*, 2013). N_2O is 298 times more powerful than CO_2 as a greenhouse gas over 100 years (Ciais *et al*, 2013). N_2O has increased in concentration from 270 ppb in pre-industrial times to 324 ± 0.1 ppb today, increasing total radiative forcing by 0.17 ± 0.03 W m^2 (Mhyre *et al*, 2013). This estimate was recently revised upwards by 2% by Etminan *et al.* (2016), who found N_2O to be more powerful as a greenhouse gas than previously thought. Agricultural soil is the largest source of N_2O emissions, particularly agricultural soils in southern Asia, where the increased use of N fertilizers in developing economies is responsible for the significant emissions increase (Saikawa *et al.*, 2014). Grazing and non-tillage on grasslands have been shown to enhance N_2O emission rates, and grasslands are the largest source of N_2O by land-use as they cover ~25% of global land area, meaning mitigation should be focused at this area (Oertel *et al.*, 2016). N_2O emissions from agricultural soils are strongly influenced by N application rate, crop type, fertilizer type, SOC content, pH, and soil texture, calculations of agricultural emissions of N_2O and NO revealed global annual emissions to be 3.3 Tg and 1.4 Tg respectively (Stehfest and Bouwman, 2006). It is estimated that total global emissions of N_2O from natural and anthropogenic sources have increased from 12 Tg N yr^{-1} in 1500 to 19 Tg N yr^{-1} in 2006, 55% of the latter is attributed to natural emissions and 45% to anthropogenic sources, largely due to food production which makes up ~60% of anthropogenic emissions. The average N_2O emission rate from grasslands is 10 umol N_2O m^{-2} h^{-1}, higher than the <5 umol N_2O m^{-2} h^{-1} from croplands, with a broader range for wetlands of between negative values to 23 umol N_2O m^{-2} h^{-1} (Oertel *et al.*, 2016). A gap remains between terrestrial sources and the atmospheric content, which may be accounted for by uptake of N_2O in the deep ocean (Syakila and Kroeze, 2011).

2.1.1.4 *Uncertainties in Emission Estimates*

As the understanding of the complexities of the relationship between soil and greenhouse gases increases, the uncertainties associated with estimating GHG fluxes need to be understood in order to reduce them. Depending on the question asked, the tools used and the scale chosen for analysis, it is estimated that errors of 10-20% can be present in results (Oertel *et al.*, 2016). The overrepresentation of the northern hemisphere in the global system gives a strong bias to this data over the rest of the world where fewer observations are available (de Caritat and Reimann, 2012). Globally, there is still no standard methodology for estimating the fluxes of GHGs from soil, meaning intercomparisons of results are often difficult or impossible, and upscaling (from site measurements) or downscaling (from remotely sensed data) of data enhances these uncertainties, with associated errors said to 'easily reach' 50% (Oertel *et al.*, 2016, pp. 345). Oertel *et al.* (2016) argue for more experiments monitoring GHG emissions to be set up, over areas which are representative of all global biomes, along with a standardised method of analysis for all soil GHG emissions which homogenises the process of site-selection, methodological set-up of the flux and units, and the way data is displayed in coherent units in order for results to be comparable with one another, all the while reporting the metadata in full to avoid any potential mismatch across studies.

2.1.2 *Factors that Influence GHG Fluxes*

This section outlines the various factors which influence the scale and magnitude of GHG fluxes from soils.

2.1.2.1 *Substrate Quantity, Quality and Availability*

The ability of soil to emit GHGs strongly depends on the quantity and availability of the substrate, for instance, heterotrophic respiration (Rh) is strongly correlated with SOC content as the more C available in the soil, the more sources and reaction sites are available for microbes to decompose and respire the SOM (Wang *et al.*, 2013b). The quality of SOC also affects the degree of respiration, as larger C particles have smaller surface areas for enzymes and microbes to decompose (meaning smaller particles will enhance the rate of respiration), freeze-thaw action in temperate or boreal climates, and the activity of soil fauna such as earthworms, can help to break down C particles into smaller units and increase the rate of respiration (Jennings and Watmough, 2016). The quality of substrate also refers to the chemical composition of the molecules, for example smaller SOC molecules like glucose and cellobiose can penetrate microbial cell walls easier than larger molecules like starch, cellulose and lignin. Larger molecules are therefore recalcitrant, or need to be broken down further before they are available to microbes who prefer labile C sources (Xu and Shang, 2016). The importance of substrate supply as a driver of soil CO_2 emissions on European grasslands is highlighted by Bahn *et al.* (2008) who found reductions in substrate supply at different sites by removing above-ground biomass through grazing and cutting resulted in a significant decrease in soil respiration.

2.1.2.2 *Temperature*

Temperature is a key driver of SOM dynamics, yet the response of soils to changes in temperature is not fully understood, largely due to the fact that temperature effects are difficult to isolate from other factors which may also be temperature dependent (Campbell and Paustian, 2015). It is well established that microbial decomposition processes are strongly influenced by temperature at the micro-scale (Frey *et al.*, 2013), however at ecosystem scale microbial responses may not be as clear cut, as microbes can acclimatise to temperature variations (Tucker *et al.*, 2013). SOM responses to temperature change at landscape level can also become confounded with temperature effects on photosynthesis, transpiration, microbial communities etc. (Bardgett *et al.*, 2008).

Soil respiration is a temperature dependent biochemical reaction, where the temperature drops below freezing, soil respiration is significantly inhibited due to the weak metabolic rate of the roots and microbes (Xu and Shang, 2016). Increasing temperatures have been positively correlated with higher rates of soil respiration, both in experiments and in the extant global temperature record, across all biomes, climate types and land-uses (Lloyd and Taylor, 1994; Bond-Lamberty and Thomson, 2010; Wu *et al.*, 2011). Across the experimental record the global soil respiration (Rs) flux (calculated from a database of worldwide respiration estimations linked to historical climate data) increased by 0.1 Pg C yr^{-1} between 1989 and 2008, giving a Q_{10} (rate of respiration increase as a result of a 10°C increase in temperature) of 1.5 (Bond-Lamberty and Thomson, 2010). This may not mean a direct increase in atmospheric CO_2 however, as the observed increase could result from enhanced plant inputs to the soil, not mobilization of already stored carbon (*ibid*). Nevertheless, the increase is consistent with our understanding of the relationship between temperature and soil respiration.

Q_{10} relationships can be confounded by factors other than temperature, as the seasonality of plant inputs (which themselves are influenced by temperature and radiation) provide different substrate quantity and belowground priming effects depending on the time of year, meaning temperature is not the sole driver of these changes, other (temperature dependent) factors are also at play (Curiel *et al.*, 2004). Most of the available Rs data have been obtained from in-situ measurements, which are confounded with non-temperature factors, meaning the Q_{10} value may over or under-estimate the actual temperature effect on Rs (Xu and Shang, 2016). For example, the confounding effects of soil temperature and moisture on respiration reduced the Q_{10} during hot, dry summers in California as the soil moisture limitation inhibited the temperature response of the soil, making that soil at that time insensitive to changes in temperature (Xu and Qi, 2001). Experimental analysis of soil cores and their response to temperature and moisture found increasing emissions of CO_2, N_2O and NO as a response to increases in temperature (Schaufler *et al.*, 2010). Attempting to control for the temperature variable by performing laboratory experiments confirms that temperature has a strong influence on respiration, but uncertainties remain regarding incubation method and timing, as well as relating the experimental data to actual field conditions (Smith *et al.*, 2008).

Decomposition of SOC in response to temperature has also been linked to the availability of substrate, as soils with high substrate supply exhibited a Q_{10} of 2.5 compared to those with limited substrate supply having a Q_{10} of 1.4 (Fissore *et al.*, 2013). Giardina *et al.* (2014) found that although warming increases the overall carbon flux, this increase is mainly due to enhanced litterfall and increased below-ground carbon flux, which do not influence SOC storage or turnover over centennial and millennial timescales. Most Q_{10} values reported in the literature fall between 1.5 and 3.0 (Xu and Shang, 2016), while it can vary from 1 up to 237, though this extremely high estimate is for frozen arctic soils (Mikan *et al.*, 2002). The sensitivity of different SOC types (high-quality and low-quality) has been questioned before. Previous assumptions based on thermodynamics and Arrhenius kinetics thought that low-quality carbon would cause high losses under warming in future, but this is not replicated in the empirical record (Sierra, 2012). This suggests that different measures used to assess the temperature sensitivity of substrates can give contradictory results even when based on the same principles. The contribution of roots to overall soil respiration was examined by Boone *et al.* (1998) who found that roots are more sensitive to increases in temperature than the bulk soil itself, with Q_{10} values up to 4.6 for roots and 3.5 for respiration by bulk soil. Liu *et al*. (2016) find temperatures above 20°C can turn a soil from a CO_2 sink to a CO_2 source if other factors are kept constant, and that C sequestration of 300 kg SOC ha^{-1} yr^{-1} is achievable in colder environments. High temperatures mainly accounted for differences in SOC changes across sites, and reduced C sequestration despite favourable rainfall (*ibid*).

The reported relationship between soil respiration and temperature has been criticised by Subke and Bahn (2010) who observe that the apparent relationship reported between respiration and temperature is too simplistic and is often confounded with other external effects. In response to this they suggest a move toward modelling entire ecosystem processes, and for experiments to incorporate isotopic tracer studies and environmental manipulations for projections around future climate to be as accurate as possible. Conversely Xu and Shang (2016) emphasise the importance of temperature sensitivity and argue it deserves more attention as it is a critical factor in the link between soil respiration and climate change feedback. Research shows that the contribution of temperature to soil respiration is complex and often confounded by other factors which are themselves temperature dependent, nevertheless it remains a significant driver of soil respiration (Subke and Bahn, 2010).

2.1.2.3 *Vegetation*

The type of vegetation growing in an area can affect the microclimate experienced by a soil, the quantity and quality of litter which reaches the soil, and the rate of root respiration (Raich and Tufekciogul, 2000). Vegetation also affects rhizosphere respiration as it depends on the supply of carbohydrates from photosynthesis, which is a factor of climate and plant physiological and morphological properties (Xu and Shang, 2016). Globally, plant litter production is highly correlated with both SOC content and Rs (Raich and Tufekciogul, 2000; Davidson *et al.*, 2002b; Han *et al.*, 2015), with the species of vegetation being a significant influence on the quantity and quality of litter provided to the soil, and therefore the degree of respiration (Hättenschwiler *et al.*, 2005). A comparison of nine different litter types for 234 cases by Harmon *et al.* (2009) gave decomposition rates ranging from 0.017 to 4.653 yr^{-1}, averaging at 0.353 yr^{-1}. Vegetation type and quantity can affect the microclimate of the area around the soil, and can alter soil temperature and moisture by acting as a barrier to insolation and precipitation (Xu *et al.*, 2004).

Raich and Tufekciogul (2000) collate data from multiple studies to determine the direction and magnitude of the effects of different types of vegetation on soil respiration, and find no discernible differences across crop types, leading them to conclude that other associated factors such as temperature, moisture and substrate supply are more important than vegetation in most cases. However, experimental evidence investigating grassland vegetation on soil microbial structure indicates that removal of aboveground vegetation reduced carbon and nitrogen contents and reduced the rate of respiration (Thomson *et al.*, 2010). Wang *et al.* (2010) undertook a meta-analysis of results from over 100 scientific publications (114 papers and one book) and found significant positive correlation between the seasonal amplitude of the normalized difference vegetation index (NDVI) and the seasonal amplitude of respiration, indicating that seasonal variations in vegetation are a strong modulator of Q_{10} values across sites.

Soil respiration is a process controlled by multiple variables which are all strongly interlinked (e.g. temperature, moisture, soil texture) that it is difficult to control for each one in order attribute responsibility for respiration. Vegetation type can potentially change these abiotic and biotic factors (Fu *et al.*, 2013), meaning it should still be considered as a strong influence on respiration.

2.1.2.4 *Water*

In general, soil respiration is typically low in dry conditions, and is observed to increase with soil moisture until respiration reaches its maximum at an intermediate moisture level, and declines as water content increases to the point where oxygen is excluded (Xu and Shang, 2016). The diffusion of soluble substrates is affected by low soil moisture content while the diffusion of oxygen is affected at high water content, both processes limit soil respiration (Davidson *et al.*, 2006). Reduced soil moisture also limits respiration by reducing the availability and mobility of carbon, causing lowered microbial activity and enzyme production, low levels of moisture also inhibit hydrolytic chemical reactions which break down polysaccharides, slowing the decomposition process (Barnard *et al.*, 2015; Xu and Shang, 2016). The moisture content of soil also influences the oxygen content and subsequent respiration, as the metabolic pathway changes from aerobic respiration to anaerobic fermentation when oxygen is absent, and the outputs change from CO_2 to CH_4 (Kane *et al.*, 2013), while there is a decrease in CO_2 efflux when soils are flooded (i.e. in wetlands) (Xu and Shang, 2016).

The sensitivity of soil respiration to moisture content differs across biomes, and is found to be much more variable and important for regulating respiration in boreal and temperate forests ahead of other land-use types, though there are a paucity of data in other biomes to have strong confidence in this assertion (Hursh *et al.*, 2017). Experimental evidence indicates that respiration decreases with lower soil moisture in forest ecosystems, indicating that drought events reduce the level of respiration from the soil (Jiang *et al.*, 2013).

Moisture and temperature interact with one another also, Wood *et al.* (2013) find the typical response of increased respiration to increases in temperature is constrained by the availability of soil moisture, with a parabolic relationship between moisture and CO_2 flux which peaks at a volumetric soil water content of 0.375 m^3/m^3 (37.5%). In a synthesis of studies, Hursh *et al.* (2017) argue that precipitation and soil respiration are positively correlated at the global scale, but the relationship between soil moisture and soil respiration is more variable, with highest values of soil respiration occurring at around 27% volumetric water content, while respiration is inhibited when soils are dried out or saturated. The 'optimum' value for soil respiration varies across studies, research has shown that the determinant of the value for soil moisture which maximises respiration varies according to clay content, with a positive relationship between the two (Balogh *et al.*, 2011). The seasonal effects of soil moisture changes are often coupled with temperature effects, making it difficult to disaggregate the influence of both on soil respiration (Xu and Qi, 2001). N_2O

emissions are positively correlated with soil moisture, NO and CH_4 oxidation rates are negatively correlated with moisture, while the highest CO_2 emissions have been observed at intermediate levels of soil moisture (Schaufler *et al.*, 2010). Rewetting of dry soil can cause a strong and rapid increase in soil respiration and nitrification, with a 40-fold increase in microbial activity evident following rewetting in one study (Orchard and Cook, 1983). This is known as the 'Birch effect' and is thought to be caused by mineralization of dead microbial biomass or osmoregulatory substances released by soils in response to hypo-osmotic stress (Unger *et al.,* 2010).

The importance of soil moisture is not to be underestimated as climate warms and drought conditions become more frequent, as the positive relationship between warmer temperatures and enhanced respiration is confounded by limited moisture availability (Hursh *et al.,* 2017). Soils do not respond equally to changes at different depths, the factors which influence soil respiration are not equal across the soil profile. Changes in soil temperature, moisture, CO_2 production and diffusion throughout the soil profile are illustrated in Figure 2.3 from Subke and Bahn (2010), where daytime temperatures are higher in the upper soil layers while night-time temperatures and moisture content are higher in lower layers, while respiration is highest in upper soil layers.

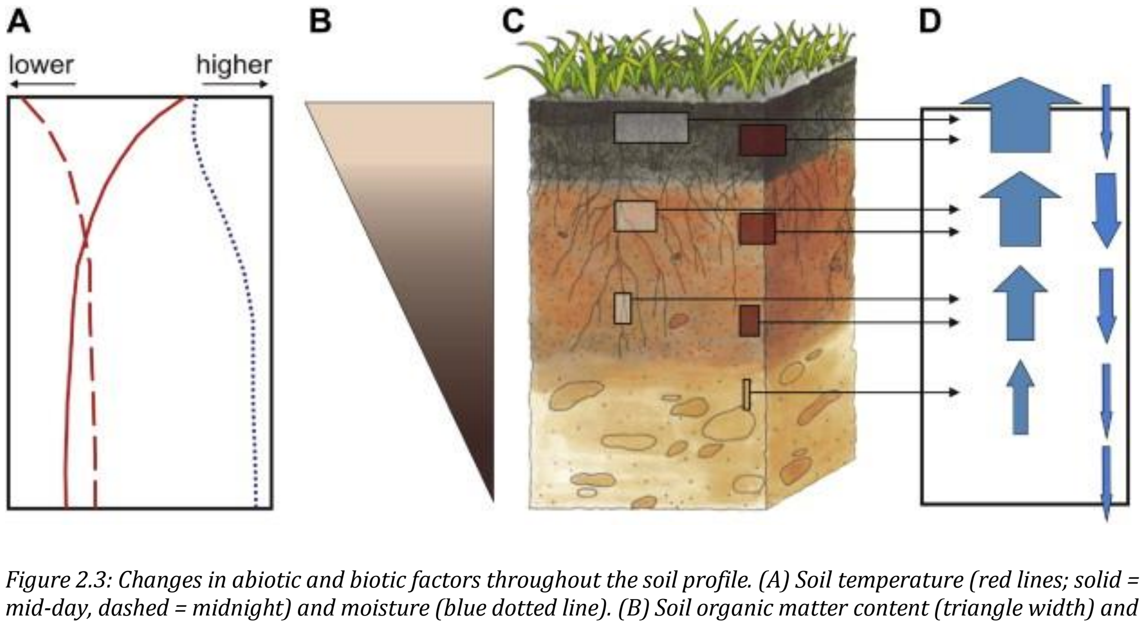


Figure 2.3: Changes in abiotic and biotic factors throughout the soil profile. (A) Soil temperature (red lines; solid = mid-day, dashed = midnight) and moisture (blue dotted line). (B) Soil organic matter content (triangle width) and quality (shading indicates differences in complexity and molecular weight of carbon compounds). (C) CO_2 production (white bars: root and rhizospheric sources, dark brown bars: heterotrophic sources, light brown bar: mineral weathering). (D) CO_2 diffusion between different depths resulting from CO_2 production (Source: Subke and Bahn, 2010)

2.1.2.5 *Management*

Management can affect the factors mentioned above by altering the substrate quantity and quality by planting different types of vegetation and using fertilizers, changing the temperature by using greenhouses, changing the water content using irrigation, and changing the vegetation by planting different crops. Liu *et al.* (2016) use the APSIM-Wheat and APSIM-Agpasture models to simulate SOC changes across nine sites in eastern Australia to investigate how nitrogen fertilisation, stubble management and stocking rate affect SOC levels from sub-tropical to temperate environments. They find that continuously grazed pasture resulted in SOC increases over 60 years, while increasing the stocking rate decreased the rate of SOC change universally. Rotations between crop and pasture indicate that 4 years of pasture reduces declining SOC at low nitrogen application during cropping phases. N fertilization and residue (stubble) incorporation reduced the impact of the stocking rate by lessening the decline in SOC (*ibid*). Improvements in management practices on grasslands can help soils store more C, a meta-analysis of many studies showed improvements in fertilization, grazing management, conversion from cropland to grassland, sowing legumes, improving grass species, introduction of earthworms and irrigation all improved the C sequestration potential of grasslands at rates ranging from 0.105 to over 1 Mg C ha^{-1} yr^{-1}, with the largest increases coming from conversion from cultivation, sowing legumes, and fertilization (organic fertilizers produced enhanced sequestration compared to inorganic) (Conant *et al.*, 2017).

Land management can also affect the degree of soil respiration, the soil structure is altered through land-use change associated with the agricultural processes of ploughing, sowing, fertilizing, irrigating and cultivating crops, or covering the soil surface with our towns and cities, all affect the quantity of soil respiration. Cultivation increases the surface area of soil which is exposed to the air, improving the aeration and moisture leading to higher rates of soil respiration (Xu and Shang, 2016) and a decline in organic matter (Schlesinger and Andrews, 2000).

2.1.2.6 *Soil pH*

The pH of a soil regulates the chemical reactions happening within the soil and within enzymes in microorganisms, many of which are pH dependent (Luo and Zhou, 2006). Most bacterial species thrive within the pH range of 4-9, while fungi thrive between 4 and 6, meaning the pH of a soil has a strong influence on the microbial and fungal communities, and therefore on soil respiration also (*ibid*). A long-term (over 100 year) experiment at Rothamsted in the UK showed that lower pH stimulated a fivefold decrease in bacterial growth and a fivefold increase in fungal growth, however if pH dropped below 4.5 all microbial variables were inhibited (Rousk *et al.*, 2009). Soils with pH values of 3 produce between 2 and 12 times less CO_2 than those at pH of 4 as microbial activity is inhibited, while CO_2 production typically increases until pH 7 and declines beyond 7 (Luo and Zhou, 2006).

pH concentration can change during the agricultural year due to fertilizer addition or liming, and the degree of emission of N_2O can result in a fourfold increase in N_2O emissions from liming a soil with pH 4.5 (Baggs *et al.,* 2010).

2.1.2.7 *Other Factors*

Indirect human impacts from air pollution can cause acid rain which affects respiration in forest ecosystems, with varying outcomes depending on the forest type (Liang *et al.*, 2013). The availability of soil enzymes and microbes also affect the rate of soil respiration, and though knowledge of individual enzymes and their quantity is still limited, they are clearly important to the understanding of soil respiration (Makoi and Ndakidemi, 2008). These enzymes and microbes are principally regulated through biotic and abiotic factors such as climate (Zogg *et al.*, 1997; Barnard *et al.*, 2015), pH (Zhalnina *et al.*, 2015) oxygen supply, nutrient levels and substrate availability (Xu and Shang, 2016), emphasising the interrelationship between the variables previously discussed.

2.2 Observations of Greenhouse Gas Emissions from Soils

Early measurements of ecosystem carbon fluxes began with inventory assessments; measurement, harvest and allometric scaling techniques which assessed changes in above-ground biomass in order to estimate fluxes, these methods have significant limitations due to the intensive nature of the research, with many samples of vegetation types for different species sizes, ages and structure required with information on soil type. These methods only tend to provide an annual snapshot of ecosystem-atmosphere fluxes, rather than capturing complex seasonal dynamics (Baldocchi, 2014). The use of enclosure, cuvette and chamber methods to investigate the gaseous exchanges between different parts of plants and the atmosphere provide an indication of the type of flux to be expected from vegetation, but upscaling this information from leaf to canopy to ecosystem scale is not possible without introducing significant uncertainty, while the use of entire-plant chambers measures the flux from the whole organism, the presence of the chamber alters the microclimate and therefore the flux (*ibid*). To overcome these issues micrometeorological methods of flux measurement came to prominence and grew quickly during the 1990s (Baldocchi *et al.*, 1988; Aubinet *et al.*, 1999; Baldocchi, 2003) coinciding with improvements in personal computer power and data storage. Regional networks of flux towers on different ecosystems have since been developed e.g. AmeriFlux, Fluxnet-Canada, EuroFlux, CarboEurope, OzFlux, ChinaFlux and AsiaFlux, all part of the global FLUXNET network (Baldocchi, 2014).

Soil respiration was initially used as an indicator of soil fertility, and measurements date back to the early 20th century, where the chemical absorption method was used. The method measures respired CO_2 molecules absorbed by alkali solutions, a process which typically underestimates Rs when respiration is high, and overestimates when respiration is low, an effect which seems to cancel itself out (Xu and Shang, 2016). This method was popular until the 1970s, when the infrared gas analyser (IRGA) significantly improved the accuracy of respiration measurements (Norman *et al.*, 1992; Pongracic *et al.*, 1997; Davidson *et al.* 2002b). Gas chromatography has been used by some studies to simultaneously measure multiple GHGs like CO_2, CH_4 and N_2O (Ball *et al.*, 1999; von Arnold *et al.*, 2005). Most studies now use dynamic chambers to measure CO_2 concentration inside the chamber using an IRGA, while the flux is calculated based on the change in CO_2 concentration over time (Xu and Shang, 2016).

Xu and Shang (2016) undertake a meta-analysis of global soil respiration measurements and find that there are currently 6147 soil respiration measurements across 1557 sites around the world, with most measurement sites located in North America, Western Europe and East Asia, and a dearth of measurements in Africa, the Middle East, Eastern Europe and Australia. The land distribution of these sites is biased towards evergreen needleleaf forests (1481), grassland sites (868) and cropland sites (768), with 76.5% of measurements taken using the IRGA method, 11.4% using chemical absorption, 9.7% using gas chromatography and 0.8% using the gradient method. Most measurements were taken in the 1990s and 2000s using IRGA techniques, with only 6.4% of measurements taken before 1990 (Xu and Shang, 2016). Studies which have measurement durations of greater than one year account for 70% of the total measurements in the database. The average global flux of greenhouse gases based on these estimates is 0.845 kg C m^2 yr^{-1} (*ibid*).

The most common methods of estimating GHG emissions from soils include observational methods such as chamber measurement, eddy covariance, remote sensing, and mathematical methods which use empirical or process-based models, each approach has advantages and disadvantages associated with it (Oertel *et al.*, 2016). All of these methods (particularly the modelling) are evaluated using laboratory experiments which take soil samples from multiple locations and investigate influence of parameters such as soil structure/temperature/moisture on GHG emissions by changing single parameters while keeping others constant (Schaufler *et al.*, 2010). While these methods will be discussed in detail below, a number of studies which compare different methods of Rs measurement in more depth are available (Hanson *et al.*, 2000; Davidson *et al.*, 2002b; Pendall *et al.*, 2004; Hibbard *et al.*, 2005; Ryan and Law, 2005).

2.2.1 *Chambers*

Two types of chamber exist, closed chambers which are sealed and allow for the measurement of CO_2, CH_4 and N_2O using various methods of analysis, and open chambers which have two openings drawing in ambient air and calculating the difference between gas concentrations at both ends. Open chambers are more technically sophisticated than closed chambers, which makes them more expensive, closed chamber systems remain the most common (Pumpanen *et al.*, 2004). There are two types of closed chamber, closed static and closed dynamic. Closed static chambers are most common for CH_4 and N_2O fluxes (Pihlatie *et al.*, 2013), and while it is possible to measure CO_2 using these chambers by trapping the gas in an alkaline solution, that method is rarely used as it tends to underestimate CO_2 fluxes (Nay *et al.*, 1994). Closed dynamic chambers analyse gases accumulating within the chamber and are most common for monitoring CO_2, it is possible to measure CH_4 and N_2O with closed dynamic chambers but this method is rarely used compared to static chambers (Oertel *et al.*, 2016). The most popular method for estimating fluxes of CO_2 at the pedon scale are closed chamber measurements from the soil surface, where the closed dynamic chamber method allows for measurement of the flux by analysing the increase of gas concentrations inside the chamber (Luther-Mosebach *et al.*, 2018).

Closed static or dynamic chambers can be either manual or automatic, a manual system requires permanent operation by hand, while automatic chambers can function with less human interference, but are less suited to being moved around, meaning higher material costs are involved as many more automatic chambers placed in different locations are required, while manual chambers can be moved to record gas concentrations at different locations (Oertel *et al.*, 2016). It is possible for chambers to measure NEE if they are transparent (Wang *et al.*, 2013); to measure ecosystem respiration the chambers should be opaque (Sanz-Cobena *et al.*, 2014). Other sources of uncertainty arise from chamber methods as studies typically use measurements between 9 and 11am to represent the mean daily value of their chamber measurements, however this method may not be accurate across ecosystems or for every period of the year, with biases ranging from -29 to + 40%, particularly in trenched plots where roots have been severed, and the bias being more pronounced when fluxes are higher (Cueva *et al.*, 2017).

Experimental analysis of different chamber techniques against known quantities of CO_2 generated by a calibration tank, found over and under-estimation of fluxes across chambers, and even identical chambers with different collar designs showed highly variable results as the different methods of mixing of air within the chamber introduces error (Pumpanen *et al.*, 2004), this highlights the uncertainties prevalent when using chamber measurements, and the difficulties in comparing chamber data across studies. There is still no standardised chamber system in the geosciences, meaning comparison of datasets across space and time is often not possible (Pumpanen *et al.*, 2004; Oertel *et al.*, 2016). As a result of this uncertainty it is difficult to assess which method of chamber measurement is best.

Due to the complex spatial heterogeneity of soil carbon efflux over 30 sampling points are necessary to reliably estimate the soil respiration of an ecosystem (Yim *et al.*, 2003; Adachi *et al.*, 2005), but this may not be possible due to time and budget constraints. Rodeghiero and Cescatti (2008) sample a large number of points and then reduce the points while still maintaining the accurate representation of the ecosystem respiration, and they found this method of stratified sampling reduced uncertainties in forest ecosystems by 55% and 57%, while only reducing uncertainties in grasslands by 12%, again emphasising the complexity of the system and the difficulties in applying similar techniques across ecosystems. Different methods of quantifying chamber measurements can introduce biases, as outlined by Huth *et al.* (2017) who observe a difference between the NEE balances of an agricultural field of between -200 to 425 g CO_2-C m^{-2} depending on the data acquisition or gap-filling strategy, highlighting the importance of correct methodological decision making, and the uncertainties inherent in using chamber data which has been partitioned, motivating the authors to recommend a standard approach to be developed to reduce potential uncertainties.

The importance of chamber positioning is examined by Xu and Shang (2016), who highlight the fact that Earth's surface is uneven and that measurements taken from soils on slopes should consider the angle of slope when positioning the chamber, to measure the flux as accurately as possible. There are also uncertainties in relation to post-processing of chamber data, where modelled Reco, GPP and NEE can vary by up to 25% depending on the modelling approach, leading researchers to call for procedures which are clearly defined and universally applicable in order to facilitate comparability between closed chamber CO_2 data (Hoffmann *et al.*, 2015).

2.2.2 *Eddy Covariance Flux Towers*

Taking a direct micrometeorological approach, flux towers use the eddy covariance method which examines vertical turbulences to analyse the heat and gas exchange between the ecosystem surface and the atmosphere (Launiainen *et al.*, 2005). Eddy covariance methods seek to capture the entire ecosystem carbon flux, as vegetation is also included in the footprint covered by the tower, which typically consists of a 2-10m high tower with an ultrasonic anemometer and gas analyser attached, and can measure continuously over areas up to multiple km^2 (Myklebust *et al.*, 2008). Fluxes can be underestimated if near-ground turbulent mixing occurs (Papale *et al.*, 2006), and data must undergo extensive post-processing including gap-filling, energy balance closure and friction velocity threshold estimation (u*) which can also introduce uncertainties in the outputs (Du *et al.*, 2014).

In order to calculate ecosystem respiration (Reco) the method of Reichstein *et al.* (2005) is typically used. This method employs a genetic algorithm which derives short-term temperature sensitivity of Reco from eddy covariance data and applies it to the night-to-daytime flux, the method is not perfect, and it is recommended that alternative flux measurements (such as chamber fluxes) are provided. In order to calculate heterotrophic respiration further partitioning is necessary, with Hardie *et al.* (2009) proposing the Rh fraction is between 46 and 59% of Reco, other methods include running a process based model such as DNDC, and taking the Rh fraction and applying it to Reco (Khalil *et al.*, 2013). The process of partitioning flux data introduces uncertainty, and the further data is partitioned, the potential for error is enhanced (Carbone *et al.*, 2016). Xu and Shang (2016) provide guidelines for new measurement sites where the footprint of the site should be representative of the vegetation, soil, topography and microclimate conditions to match the remote-sensing and climate data as much as possible. The eddy covariance method remains a very popular way of measuring ecosystem fluxes today, despite significant uncertainties associated with partitioning.

2.2.3 *Remotely Sensed Observations*

Satellite observations can provide information on tropospheric (near-surface) CO_2 and CH_4 concentrations by measuring the intensity of reflected sunlight in the visible and short-wave infrared portion of the spectrum (Oertel *et al.*, 2016). The Orbiting Carbon Observatory-2 (OCO-2) is a high-resolution NASA satellite, launched in 2014 which can measure CO_2 at a precision of 1-2 ppm, and performs well when compared to the ground-based observations (Wunch *et al.*, 2017). To follow on from this work, and with plans to be launched at the end of this decade, the European Space Agency's FLEX (Earth Explorer - Fluorescence Explorer) aims to assess the way carbon moves between plants and the atmosphere and how photosynthesis affects the carbon cycle acquiring data in the 500-880 nm spectral range (ESA, 2018). Sentinel-5P is another satellite which aims to provide observations to support monitoring of air quality, ozone UV and climate, and in doing so provides measurements of NO_2 (ESA, 2019).

An alternative method is to use remotely sensed data to determine land-cover types e.g. using landsat data to classify surfaces into distinct land-cover types (Güler *et al.*, 2007) . Specific emissions are then associated with the different categories of land-uses, allowing for the calculation of GHG budgets, however as there is no consensus between different maps, and difference in land-cover maps will have different emissions associated with them, introducing bias into the budget (Oertel *et al.*, 2016). There are issues with accuracy when using remote-sensing to classify land-use, and while no optimum method has been recommended, it is reported that combinations of GIS and remote sensing can improve accuracy (Rozenstein and Karnieli, 2011). It is also possible to measure concentrations of greenhouse gases at different levels of the atmosphere using airplanes, by collecting samples during the ascent and descent of the flight, but this method covers a very short time period and a small area (D'Amelio *et al.*, 2009).

2.3 Estimates of Rs Based on Observations

2.3.1 *Statistical Methods*

Early estimates of global soil respiration come from simple statistical methods of calculation, which estimate soil respiration based on other measurable factors. Beginning with Schlesinger (1977), the initial estimate of global soil respiration flux was 75 Pg C yr^{-1}, a figure obtained by assessing terrestrial detritus and assuming Rs is twice the amount of above and below-ground litter fall. A lower estimate of 50 Pg C yr^{-1} was proffered by Houghton and Woodwell (1989) in their seminal article on global climatic change, recognising soil respiration as a significant source of atmospheric C. Statistical methods also include the approach of Raich and Schlesinger (1992) who compiled published soil respiration data from the literature to generate a database, then calculating the average Rs flux for each biome and multiplying by the area of the biome. Based on extrapolations from 171 measurements from land-biome areas, Raich and Schlesinger (1992) estimated a global Rs flux of 68 ± 4 Pg C yr^{-1}, with a root contribution of 26%. This estimate came with the caveat that arid, semi-arid and tropical regions are vastly underrepresented by experiments. Xu and Shang (2016) combined global Rs statistics with MODIS satellite data to obtain estimates comparable to those resulting from empirical methods.

2.3.2 *Empirical Methods*

Empirical methods of soil respiration estimation involve generating regression models to extrapolate respiration based on observations and other influencing factors such as temperature and precipitation. Early empirical estimates of Rs began with Raich and Potter (1995) who developed a database of 977 monthly Rs flux measurements from 1963-1991 and used corresponding temperature and precipitation data to develop a nonlinear regression model which estimated the global Rs flux at 76.5 Pg C yr^{-1}. This database was updated to exclude most chemical absorption methods of CO_2 flux calculation, and the period measurements were taken from was changed to 1968-2000, giving a revised estimate of 80.4 Pg C yr^{-1} (Raich *et al.*, 2002). Bond-Lamberty and Thomson (2010) incorporated more measurements (1434 from 439 studies) to develop a linear regression model which included temperature and precipitation anomalies, and estimated the global Rs flux to be 98 ± 23.5 Pg C (95% confidence interval). Xu and Shang (2016) include MODIS vegetation map along with a database of respiration measurements and estimate 94.3 ± 17.9 Pg C yr^{-1} (95% confidence interval). Large uncertainties in estimations are due to the spatial and temporal distribution of soil respiration measurements being concentrated in North America, Europe and East Asia, with gaps in Africa, Eastern Europe, North and Southeast Asia and Australia (especially in dry ecosystems) meaning confidence in estimates from these regions is low (Xu and Shang, 2016).

Empirical models have some advantage over the purely statistical methods as they ameliorate the issue of sampling bias, however most regression models have an r^2 value of between 0.3 and 0.6 (Raich and Potter, 1995; Raich *et al.*, 2002; Hashimoto *et al.*, 2015), which could be improved upon by adding more measurements from underrepresented areas of Africa, Eastern Europe, North and Southeast Asia, and the Middle East (Xu and Shang, 2016). In order to improve empirical models, Xu and Shang (2016) point out that the advance of data quality is more important than increasing data points, and that firstly gaps in the temporal sequence should be filled using non-linear regression methods using soil temperature and moisture as independent variables after Xu and Qi (2001).

The use of high-resolution climate data (1km or finer) is recommended to minimise scale-mismatching effects between Rs and climate data, as is the inclusion of more variables which have been shown to improve model performance such as SOC (Chen *et al.*, 2014), LAI (Hashimoto *et al.*, 2015), NDVI and snow cover, along with new techniques such as spatial hierarchical modelling, data mining and machine learning (Xu and Shang, 2016). Xu and Shang (2016) argue for a move toward models which operate at an annual time-step rather than monthly, potentially reducing noise and time-lag effects as monthly Rs fluxes are not independent of monthly temperature and precipitation (Xu *et al.*, 2004).

The empirical estimate of soil respiration with lowest uncertainty is that of Hashimoto *et al*. (2015) who estimate the global Rs flux to be 91 ± 4 Pg C yr^{-1} (95% confidence interval) with 51 Pg C yr^{-1} heterotrophic and 40 Pg C yr^{-1} autotrophic. Hashimoto *et al*. (2015) used the same soil database as Bond-Lamberty and Thomson (2010) and improved their model by allowing Q_{10} to decrease linearly as temperature increased, and allowing antecedent precipitation conditions to affect respiration. Even with uncertainties reduced to 4 Pg C yr^{-1}, this estimation error is still too high to estimate global NEP (2.4 Pg C yr^{-1}), showing that empirical methods require further development (Xu and Shang, 2016).

2.3.3 *Accounting Methods & National Inventory Estimates*

Accounting methods for greenhouse gas emissions, discussed briefly in Section 1.3, provide a means to estimate emissions based on activity data in an economy. Entities from individual to national scale can identify their emissions from their production and consumption of goods and services using known activity data and emission factors. Accounting methods for measuring CO_2 (e.g. Janssens *et al.,* 2003; Ciais *et al.,* 2008) are useful for tracking commercial goods such as fuel crops and timber, but are less good at describing standing biomass and soil carbon accumulation. The methods used by countries to estimate their emissions are outlined in the IPCC Guidelines for National Greenhouse Gas Inventories (IPCC, 2006), and are summarised in Appendix A of this thesis.

As agricultural systems and land-use change are often *key categories,* these areas are frequently targeted for tier 2 and tier 3 approaches (Campbell and Paustian, 2015). If the resources and data are available to develop a tier 3 methodology for agricultural soils, then this method should be employed (using models and/or measurement-based approaches). If the resources and data are not available, a tier 2 method using country-specific data on soil C stock changes due to land-use and management change is recommended. Failing these, if changes in C stocks in mineral soils are not a key category, and land-use and management data are available, then using default emission factors (tier 1 methodology) is recommended. Tier-1 is a crude method of assessment in comparison to others, but may be the only possible method in the absence of data.

For example, Ireland's latest national GHG inventory report (Duffy *et al.*, 2018) indicates that the components of Irish agricultural emissions are enteric fermentation (55.6%), agricultural soils (32.2%), manure management (9.3%), liming (2.7%) and urea application (0.1%). Typically, these emissions are reported using Tier 1 Emission Factors with N emissions reported under the agriculture section and C emissions reported under LULUCF. Tier 1 methods for cropland remaining cropland assumes zero emissions of C where land management practices are well-established (Duffy *et al.*, 2018). Tier 2 methods use the same methodology as tier 1 and incorporate country-specific reference stocks to improve the stock change factors, reference C stocks, climate regions, soil types, and/or the land management classification system, effectively building on Tables 10.1 and 10.2 (Appendix A) to produce country-specific data. A tier 3 approach involves using dynamic models and/or detailed inventory methods to estimate annual stock changes, with multiple models available, model selection should prioritise the capability of the model to represent all the various management practices for croplands, ensuring model inputs are compatible with input data for the country as a whole, and which can be evaluated using independent observations that are representative of the interactions of climate, soil and cropland management on post-conversion change in soil C stocks. It is also noted that a measurement-based approach whereby a modelling network, sampled periodically to estimate SOC stock changes could be employed (IPCC, 2006). Process-based modelling used for tier-3 methods is outlined in detail in Chapter 3.

2.4 Soil Carbon Quantity

As well as estimating the fluxes of greenhouse gases, the measurement efforts outlined in the previous section provide the basis for a major goal of the soil carbon community – to accurately quantify the amount of carbon in Earth's soils. The quantity of carbon stored in soils is not fully agreed upon, as the process of estimation is complicated by the intricacies of the soil system, the inclusion of different forms of carbon in analyses, and the need for extrapolation across ecosystems due to a lack of observation coverage (Govers *et al.,* 2013; Scharlemann *et al.,* 2014; Lorenz and Lal, 2018). This section will outline the consensus around soil carbon quantities, attempt to synthesise the various estimates of soil carbon content, highlight the methods of analysis used, and the sources of uncertainty in estimation.

2.4.1 *Global Soil Carbon Quantity*

Figure 2.4 illustrates the estimated global total soil carbon stock, composed of soil inorganic carbon (SIC) and soil organic carbon (SOC). It is important to note the reporting conventions between these types of soil carbon, for example Batjes (1996) reports total carbon in the first 1 m of soil as 2157-2293 Pg C, and *total SOC* in the first 1 m as 1462-1548. SOC is typically the focus of research as it is more capable of decomposition and therefore rapidly exchanges with the atmosphere and is thus a potential source and sink for CO_2. SOC stocks to 1m depth are estimated as ~1500 Pg C, up to ~2450 Pg C to 2 m depth (Table 2.1), with peatland and permafrost soils containing up to 1400 Pg C more (Hugelius *et al.*, 2014; Yu *et al.*, 2010). When combined with the SIC stocks, the total global C stock estimate increases to 3700-5400 Pg C (Figure 2.4; Lorenz and Lal, 2018).

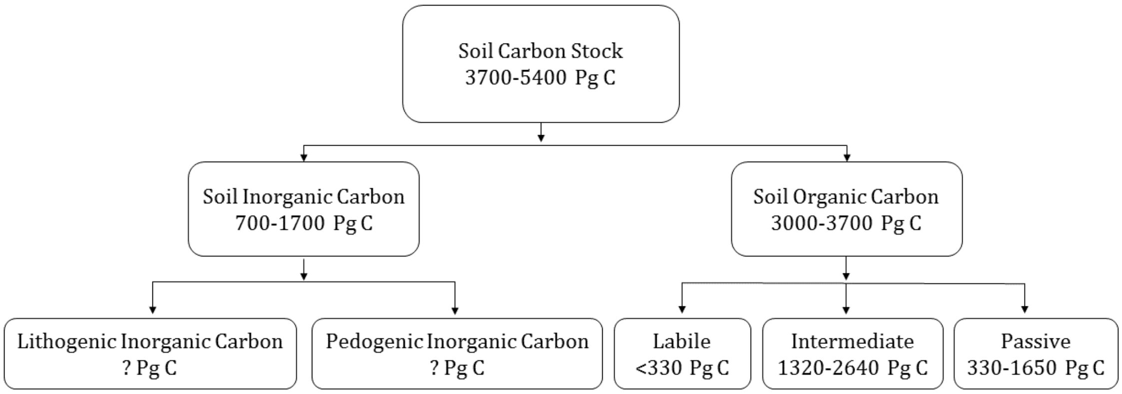


Figure 2.4: Soil carbon stocks (adapted from Lorenz and Lal, 2018) based on estimates for SOC stocks to soil profile depth or 3m depth + permafrost C + Peatland C + SIC to 1m depth from Eswaran et al. *(2000); Jobbágy and Jackson (2000); Yu et al. (2010); Hugelius et al. (2014); Köchy et al. (2015). Data on LIC and PIC stocks were unavailable. Labile, intermediate and passive SOC stocks to 3m depth are based on the conceptual SOM model in Trumbore (1997).*

The earliest recorded estimate of global soil organic carbon content was an extrapolation of measurements of nine soils in the USA and provided an estimate of 710 Pg C globally (Rubey, 1951). This initial estimate was advanced by Bohn (1976) using the FAO-UNESCO soil map with an estimate of 2946 ± 500 Pg C, advanced again in 1982 to 2207 Pg C (Bohn, 1982), and again by Batjes (1996) who used the World Inventory of Soil Emission Potentials (WISE) and estimated stocks at 1462-1548 Pg C in the first 100cm. Figure 2.5 illustrates other studies and shows ranges decreasing over time with estimates converging closer to the median value of ~1500 Pg C.

A more recent estimate of global SOC content based on spatial databases of observed soil carbon content by Tifafi *et al*. (2018) finds values higher than those reported in Figure 2.5 using calculations based on depth and bulk density for the SoilGrids database, and organic carbon content, bulk density, gravel content and layer thickness for HWSD. To highlight the uncertainty in these calculations, SoilGrids estimate a total C content of 3421 Pg C while different methods of bulk density calculation for the HWSD lead to significantly different SOC totals, particularly in northern latitudes, as the SOTWIS method estimates 16% of the total carbon stock at Boreal latitudes (60°N-90°N) and the Saxton method estimates 29% at the same latitude. One method of bulk density calculation using soil type and depth (SOTWIS) gives a carbon total of 2439 Pg C while bulk density calculations using soil texture based on equations from (Saxton *et al.*, 1986) give a total of 2798 Pg C. These estimates are again higher than a revised calculation of the HWSD by Batjes (2016) who used HWSD and WISE to estimate SOC content at 1m depth to be 1408 Pg C and 2m depth to be 2060 Pg C (see Figure 2.6). Notably Batjes (2016) highlights that ~30% of this stock (607 ± 87 Pg C) is in the northern circumpolar region which is particularly vulnerable to increasing temperatures.

Table 2.1: Global SOC estimates (Pg C) in soils across a range of studies (adapted from Masciandaro et al., *2018)*

Source	**0-1 m depth**	**0-2 m depth**	**0-3 m depth**
Post *et al.* (1982)	1395		
Batjes (1996)	1462-1548	2376-2456	
Kasting (1998)	1580		
Jobbágy and Jackson (2000)	1502	1993	2344
Robert (2001)	1500	2456	
Hiederer and Kochy (2011)	1417		
Govers *et al.* (2013)	1400-1600	1990-2460	
Todd-Brown *et al.* (2013)	1260 (890-1660)		
Batjes (2016)	1408	2060	

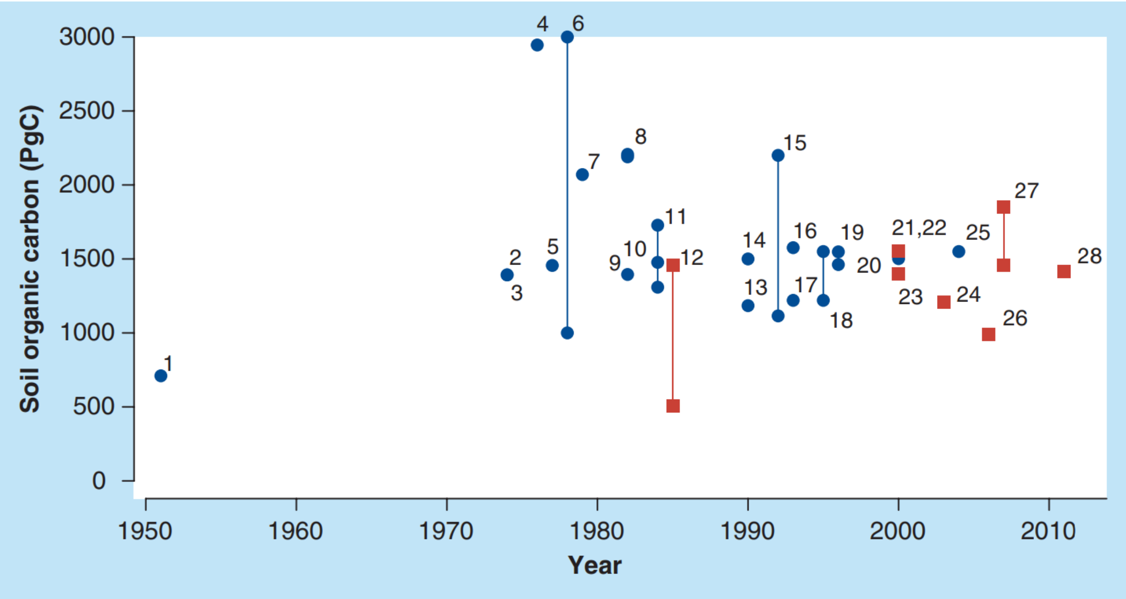


Figure 2.5: Estimates of global SOC stocks through time (from Scharlemann et al. (2014)). Numbers represent different studies and lines connecting dots represent maximum and minimum ranges. The median across all estimates is 1460.5 Pg C with a range of 504-3000 Pg C (n = 27). Red dots denote spatially explicit methods while blue dots represent nonspatially explicit methods.

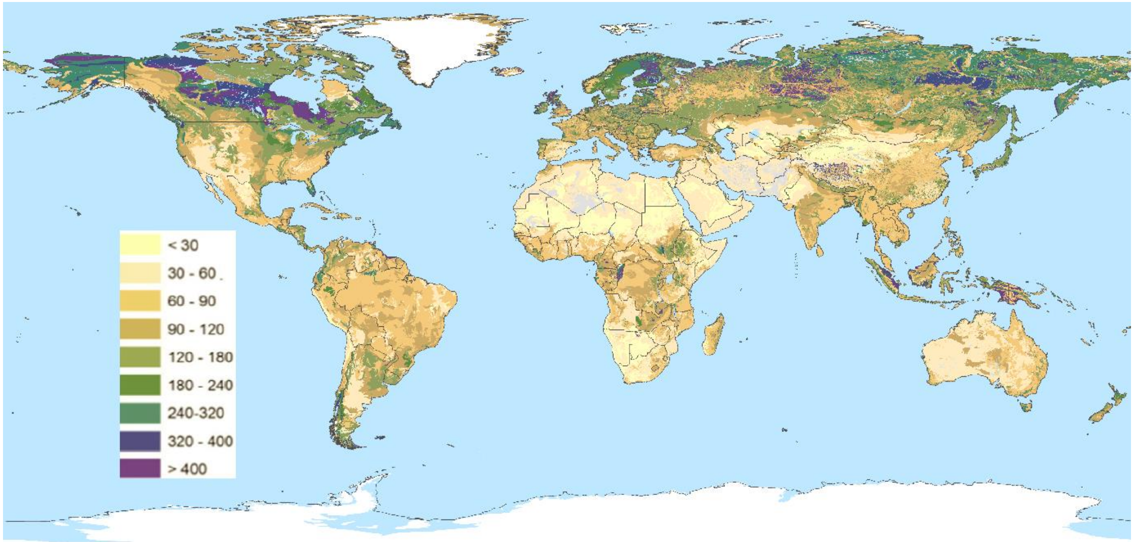


Figure 2.6: SOC content to 1m depth (Mg C ha-1) from a combination of datasets (WISE30sec; Batjes, 2016).

Soil carbon databases which exist globally include SoilGrids, the Harmonised World Soil Database (HWSD) and the Northern Circumpolar Soil Carbon Database. Major discrepancies exist between the total carbon content estimated by these databases, and between the database and field measurements. Tifafi *et al*. (2018) calculate the SoilGrids estimate of total soil carbon stocks at 1m depth to be 3,400 Pg C whereas HWSD estimates the total as ~2,500 Pg C. This estimate is similar to Hiederer and Kochy (2011) who estimated total C stocks from the HWSD to be 2469 Pg C to 1m. Köchy *et al.* (2015) advance the methodologies used to estimate global SOC from the HWSD by adjusting the bulk densities of soils high in organic C and setting the BD of Histosols to 0.1 g cm^3, giving a mass of 1062 Pg C. This is further updated using specific research for the permafrost region (Tarnocai *et al.*, 2009) and the incorporation of tropical peatland carbon which increases the global soil C estimate in the upper 1m from 1062 Pg C to 1325 Pg C, the total mass of SOC at depth is estimated as ~3000 Pg C, with high uncertainties from SOC at depth, and from different estimates of bulk densities. These estimates are higher than the original 2m depth measurement by Batjes (1996) and Jobbágy and Jackson (2000) who analysed over 2,700 soil profiles in three global databases (National Soil Characterization Database (NCSD), WISE, and a Canadian Forest Service database) finding 2344 Pg C to 3m depth, highlighting further uncertainties in calculations and total carbon contents, and indicating that soils may be storing more carbon than previously thought, a claim backed up by more recent, larger estimates (Tifafi *et al.*, 2018). Jackson *et al.* (2017) use a global soil database combined with regional permafrost data and estimate the global SOC stock in the upper 2m (depth of global datasets) as 2273 Pg C with boreal forests comprising 27% of this total and peatlands comprising 26%. Extrapolating the data to 3m gives an estimate of 2800 Pg C, with quantities deeper than 3m assumed to contain 300-500 Pg C in permafrost and up to 50 Pg C in tropical peatlands, and unknown quantities in deltas, floodplains and loess deposits. Uncertainties arise here as ~300 Pg of permafrost region soil C is in peatlands, and care must be taken to not double-count peatlands and permafrost soils. Todd-Brown *et al*. (2013) point out that the HWSD and NCSD do not have an explicit uncertainty estimates, so using them as a benchmark with which to compare models may give incorrect results, as estimated uncertainty could exceed 770 Pg C (similar to the entire atmospheric C pool).

2.4.2 *Uncertainties in Soil Carbon Quantity Estimates*

Typically SOC estimates are performed on a horizontal plane, which may underestimate the impact of slope on soil depth and SOC content. Chen and Arrouays (2018) use the HWSD and the Multi-Error-Re-Moved Improved-Terrain DEM (MERIT DEM, Yamazaki *et al.* 2017) to improve estimates from mountainous regions which vulnerable to climate change by including slope in calculations (calculating on tilted planes), and find increases in SOC from 4.04 to 15% using 90m resolution elevation data. Similarly, Pelletier *et al.* (2016) combine topography, climate and geology to create high-resolution gridded dataset of the average thickness of soil, regolith and sedimentary deposits. When this dataset is applied to inventory methods of soil carbon content calculation it reduces estimates at 2m depth by nearly one third from 2047 to 1354 Pg C, and by ~10% from the 1m horizon (Jackson *et al.*, 2017). These estimates could potentially be improved by adding higher-resolution DEMs e.g. EuroDEM which is available at 60m resolution (EuroGeographics, 2019.)

When comparing these databases to field measurements from the International Soil Carbon Network (ISCN) and others it was found that SoilGrids underestimated field stocks in the USA by 40% while the HWSD underestimated by 80-90%. SoilGrids overestimated by 30% in France and by over 150% for England and Wales. Tifafi *et al*. (2018) argue that the value estimated by SoilGrids is the closest to reality based on underestimation of organic carbon stock in northern latitudes, peatlands and wetlands by previous studies. They also maintain that low SOC values estimated from HWSD can be attributed to poor estimation of C stocks in wetlands and permafrost soils (a large fraction of total SOC stock). This suggests that estimates for non-permafrost or wetland soils are more accurate, but highlights the significant uncertainties prevalent in the calculations, and the importance of work yet to be done. SoilGrids data has recently been updated using machine learning techniques rather than linear regression, at an improved resolution of 250m from 1km, comparisons of the modelled SOC values to measured yielded an r^2 value of 0.64, calling for more local assessments to be combined with their global data to improve estimates all round (Hengl *et al.*, 2017).

Todd-Brown *et al.* (2013) examine total simulated soil carbon from 11 model centres to empirical data from the Harmonised World Soil Database (HWSD) and Northern Circumpolar Soil Carbon Databaes (NCSCD), they find ranges of stocks from 510 to 3040 Pg C from models, significantly different from the HWSD estimate of 1260 (ranging from 890-1660 Pg C). The differences between models and databases are most pronounced at northern latitudes (60 to 820 Pg C for models vs 500 Pg C with a 95% confidence interval of 380-620 Pg C for NCSCD and 290 Pg C for HWSD. At biome level models were relative accurate (mean r^2 of 0.75), this is not the case at 1° resolution. Using seven ecosystem models to simulate global soil C stocks, Nishina *et al.* (2014) find a range of estimates from 1090-2646 Pg C depending on model chosen, Tian *et al.* (2015) compare 10 terrestrial biosphere models and find a range from 425 to 2111 Pg C, with these large ranges attributed to differences in C inputs and residence times.

In an attempt to overcome some of these uncertainties Duarte-Guardia *et al.* (2018) discuss the fragmented global database of SOC stocks and attempt to estimate global SOC using partial least squares regression and multiple geographic datasets describing SOC, climate, organisms, relief, parent material and time to predict SOC stocks. Their model explains 49% of SOC variability, overestimating low stocks and underestimating high stocks. The usefulness of this dataset is primarily in the identification of areas of pristine (untouched) ecosystems which may have the potential for C sequestration as these estimates can be compared with observations indicating their potential C storage may not have been reached.

These uncertainties within and across studies emphasise the nascent nature of the discipline and highlight the significant work remaining to reduce uncertainties and improve the accuracy of our estimates of soil carbon quantity and GHG fluxes. In order to improve these estimates, we must improve the models used to simulate fluxes. The next chapter will discuss the current state of modelling GHG emissions from soils.

2.5 Summary

Globally, it is estimated that approximately 1500 Pg C of organic carbon is stored in uppermost meter of terrestrial soils (Scharlemann *et al*., 2014; Oertel *et al*., 2016). This represents the largest terrestrial carbon pool, roughly equivalent in sum to both the atmospheric (816 Pg C) and terrestrial phytomass (469.6 Pg C) pools (Scharlemann *et al.*, 2014). Although estimates of SOC stocks in terrestrial soils and their emissions remain highly uncertain (Houghton *et al.*, 2012; Scharlemann *et al*., 2014; Oertel *et al*., 2016), there remains a pressing need to improve our understanding of soil carbon management in order to minimise soil carbon losses and increase the carbon sequestration potential of soils (Scharlemann *et al*., 2014).

This chapter outlined how soil sequesters, stores and releases the main greenhouse gases, namely carbon, methane and nitrogen. The release of these gases depends strongly on the quantity of substrate supply, temperature, moisture, vegetation, soil characteristics and land-management. In order to model these processes successfully, it is essential that observations of these fluxes are recorded. Fluxes are measured in several ways including chambers placed on the soil, eddy covariance measurements from flux towers, and using satellites for remote sensing. These methods have led to various estimates of the global soil carbon flux, the latest estimates are ~94 ± 17.9 Pg C yr^{-1}. The high uncertainties are associated with a lack of measurements in Africa, Eastern Europe, and parts of Asia, along with discrepancies in the methods used for measurement. Along with the carbon flux, it is also important to estimate global soil carbon quantity. Studies estimate global soil carbon content to be ~1500 Pg C to 1m depth, though these estimates also have significant uncertainties associated with them. These uncertainties stem from sparse sampling and the method of extrapolation chosen and highlight the difficult nature of estimating the emissions and stocks of carbon derived from highly complex processes within soils. The next chapter will outline the process of modelling the GHG emissions from soils, and how the observations outlined in this chapter are used to evaluate model outputs.

3 Modelling Greenhouse Gas Emissions from Soils

This chapter outlines the methods of process-based modelling of GHG emissions from soils. Simpler methods of estimating GHG emissions such as statistical and empirical methods which estimate/derive emissions based on observations are outlined in Chapter 2. This chapter focuses solely on process-based methods which are more complex. The chapter begins with a brief history of soil modelling and an outline of the different approaches used to assess soil respiration. This is followed by an in-depth analysis of process-based models, outlining their typical structure and the modifiers used to simulate soil respiration.

3.1 Introduction

Attempts to quantify the biogeochemical processes within soils using models have been occurring since the 1930s when the first mathematical models to represent carbon fluxes were employed (Salter and Green, 1933). Since then with the advancement of computers, the quantity and variety of models developed highlights the ongoing effort to describe and quantify the complexities of soils and their biogeochemical interactions (Manzoni and Porporato, 2009). After decades of research on the topic, there remains an incomplete understanding of soil carbon processes, as soils are the most complex biomaterial on the planet and are heterogeneous at both molecular (Young and Crawford, 2004) and regional/continental scales (Ettema and Wardle, 2002). Soil dynamics occur on multiple different time and space scales, ranging from hourly responses to changes in the environment (Schwinning and Sala, 2004), to decadal responses of soils to ecosystem and climatic change, and timescales longer still for the development of soils themselves (Brady and Weil, 2016). All of these factors are further complicated by both climatic and anthropogenic forcing factors such as extreme events and agriculture (Manzoni and Porporato, 2009). In the 80 years of modelling reviewed by Manzoni and Porporato (2009), around 250 mathematical models from the highly-used stalwarts to less-known theoretical analyses of soil dynamics have been published, this number includes soil sub-models to ecological or hydrological models (Figure 3.1).

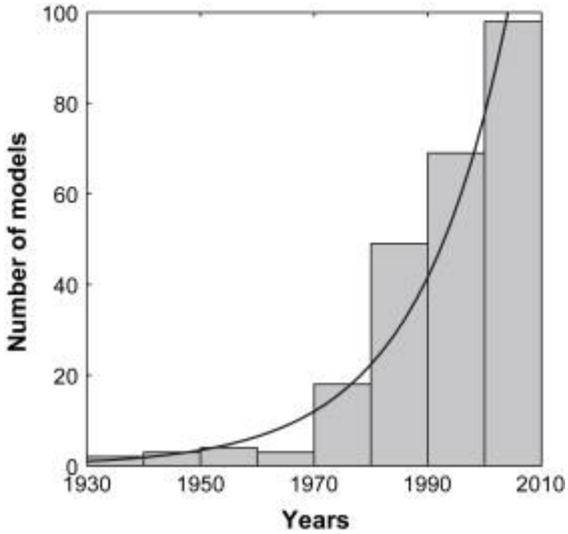


Figure 3.1: The number of soil C and N models over time (solid black line is exponential least square regression of the data, showing a 6% annual increase (from Manzoni & Porporato, 2009).

Most of these models describe a system which includes characteristics of the SOM such as the substrates which are available to decomposers, and the nature of the decomposers themselves, and how they relate to inorganic compounds, environmental variables, and external inputs and outputs (Manzoni and Porporato, 2009). Nikiforoff (1937) split SOM into pools with different turnover times, a method still employed by models popular today (Coleman and Jenkinson, 1996; Smith *et al.* 2010a). Models advanced to represent the processes of decomposition at different depths by splitting the soil into layers which include water flow components to influence the advection of dissolved compounds along the profile (Kirschbaum and Paul, 2002; Jenkinson and Coleman, 2008). This is a simplification of reality as soils are heterogeneous at depth, however it is necessary to reduce model complexity. Most models currently describe SOM dynamics over time using ordinary differential equations for each pool, a method first proposed by Hénin and Dupuis (1945). Though some models have advanced to include multiple complex biogeochemical reactions (Shaffer *et al.*, 2001), 90% of models include less than 30 variables, and 70% include 2-10 variables, with most incorporating a dynamic microbial biomass component, and including soil moisture and temperature as dynamic components (Manzoni and Porporato, 2009).

Process-based models attempt to represent physical and chemical processes happening at field, pedon or point scale, and their interactions with abiotic factors such as temperature and rainfall, to estimate their production/sequestration of GHGs. Simulation models allow us to assess complex interactions between biogeochemical cycles and the processes driving these cycles (Burke *et al.*, 2003). Soil heterotrophic respiration is primarily influenced by the decomposition of organic matter, which itself is dependent on substrate quality and quantity (Janssens *et al.* 2001; Hartley and Ineson, 2008), soil temperature (Lloyd and

Taylor, 1994; Kätterer *et al.*, 1998; Conant *et al.*, 2011), soil water content (Davidson *et al.*, 1998; Leirós *et al.*, 1999), microbial community (Holland *et al.,* 2000; Whitaker *et al.,* 2014) and acidity (Walse *et al.*, 1998; Schmidt *et al.*, 2011). Typically, soil respiration models simulate pools of carbon with different substrate qualities and quantities and therefore different decay rates, which are then further attenuated using temperature, moisture and other edaphic factors (Del Grosso *et al.*, 2005). While statistical, empirical and accounting based methods are outlined in the previous chapter, process-based methods are outlined in detail below.

3.2 Process-Based Models: An Overview

Process-based models integrate major ecosystem processes including respiration, photosynthesis, decomposition, evapotranspiration, nutrient cycling and phenology (Running and Hunt, 1993; Parton *et al.*, 1993). They are initialised and parameterised using site-based observations and produce outputs based on the knowledge of the ecosystem and the interactions between different processes. Most ecosystem models and Earth System Models (ESMs) simulate Rh and root respiration (Rr), with few actually reporting Rr, making it difficult to compare global Rs estimates from empirical models with those from process-based models (Xu and Shang, 2016).

An important purpose of process-based soil carbon models is to provide predictions of the size of SOC stocks for different soil types, with the potential to perturb the parameters of the model to incorporate differing management practices (grazing, crop rotation, fertilizer application) and changing climate variables including temperature, precipitation and evaporation (Stockmann *et al.*, 2013). The most popular models in terms of citations from literature where models are used are CENTURY, the Rothamsted Carbon Model (RothC), DeNitrification-DeComposition (DNDC), Environmental Policy Integrated Climate (EPIC), Decision Support System for Agrotechnology Transfer (DDSAT) and DayCent (a daily version of the CENTURY model) (Campbell and Paustian, 2015). These are all process-based models which attempt to simulate processes involved in SOM transformation. They split SOM into conceptual C pools which differ by decomposition rates, typically with a number of SOM compartments including an 'active pool' with a mean residence time (MRT) of 1 year, a 'slow pool' with MRT of 100 years, and a passive/inert pool with an MRT of 1000 years. The models are based on first-order kinetic decay rates on daily, weekly or monthly timesteps and typically simulate the top 30cm of soil at field and regional scale. Since most models only simulate the top 30cm of soils, processes occurring below the 'plough layer' are not explicitly incorporated (Trumbore, 2009).

Process based models have been widely applied to a number of ecosystem and land-use types (Abdalla *et al.*, 2010; Bell *et al.*, 2011; Smith *et al.*, 2010a; Stockmann *et al.*, 2013). Smith *et al.* (1997) analysed the performance of nine SOM models across different land uses and climatic conditions; most showed good abilities in representing SOM dynamics, and their study highlighted the importance of model calibration in achieving accurate results.

3.2.1 *CENTURY & DayCent*

The most widely used model based on the literature is CENTURY, a model designed to simulate long-term SOM dynamics, plant growth, as well as N, P and S cycling (Campbell and Paustian, 2015; Parton, 1996). Initially developed for grassland it has been extended to include arable, forest and savanna ecosystems (Parton, 1996). The model runs on a monthly timestep, and includes two forms of litter, metabolic and structural, splitting SOM into active (1-5yr MRT), slow (25 yr MRT) and passive (1000 yr MRT) pools (Stockmann *et al.*, 2013). DayCent (Parton *et al.*, 1998) is a daily version of the CENTURY model which allows for simulation of CH_4, N_2, N_2O and NO_x gas fluxes, plant production dynamics, soil N dynamics, soil NO_3 leaching and SOM dynamics (Stockmann *et al.*, 2013).

3.2.2 *RothC*

The Rothamsted Carbon (RothC) model (Coleman and Jenkinson, 1996) was developed using data from long-term experiments at the Rothamsted Research centre in the UK, it is parameterised for arable land but has been applied to temperate grasslands and forest soils. RothC runs on a monthly timestep and splits SOM into decomposable plants, resistant plant material, microbial biomass, humified organic matter (all with MRT of 50 yr and comprising 80-90% of SOC) and inert organic matter (MRT of 10,000 years, 5-15% of SOC) (Stockmann *et al.*, 2013). These pools are broken down using first-order kinetics to give CO_2 output, and the pools are recharged from plant inputs which are typically split in a DPM/RPM ratio of 1.44, meaning 59% of the plant material is decomposable, and 41% is resistant to decomposition (Coleman and Jenkinson, 1996). RothC calculates decomposition rates, microbial biomass and the ratio of humus based on the clay content of the soil, and is similar in structure to CENTURY (Stockmann *et al.*, 2013).

3.2.3 *DNDC*

The DeNitrification-DeComposition model (DNDC) (Li *et al.*, 1992) is a daily timestep model consisting of two components, the first component consists of soil, climate, crop growth and decomposition sub-models to predict soil temperature , moisture, pH, redox potential and substrate concentration, while the second consists of the nitrification, denitrification and fermentation sub-models which predict NO, N_2O, N_2, CH_4 and NH_3 fluxes based on changes in environmental factors, and has been widely employed internationally including in the

NitroEurope EU project (Giltrap *et al.*, 2010). DNDC has advanced over the past 20 years to have versions applied all over the world for different ecosystem types and applications (Gilhespy *et al.*, 2014).

3.2.4 *ECOSSE*

The ECOSSE model is similar to RothC in that it separates SOM into five pools decaying at specific rate modifiers. Decomposition within the model is further modified by temperature, moisture, vegetation, soil texture, pH, bulk density and clay content while land-use and management data can also be inputted, and the model simulates C and N emissions for six vegetation categories: grassland, arable, forestry, seminatural, short-rotation coppice (willow) and *Miscanthus* (Dondini *et al.,* 2015). The model was initially developed for organic soils, but has recently been used to simulate C and N cycles on mineral soils also (Dondini *et al.*, 2016). The ECOSSE model is discussed in-depth in the following chapters.

Multi-model inter-comparison studies are yet to identify the model which performs best, some models perform better than others at simulating different components of the soil system, or work better at different locations (Campbell and Paustian, 2015), suggesting that model performance ought to be assessed before a model is chosen. Burke *et al*. (2003) point out that temperature modifiers across biogeochemical models are based on a few imperfect data sources from experiments on litter decomposition and soil respiration, with a lack of field data to validate many models. Xu and Shang (2016) describe differences in ESM outputs and highlight the imperfections of current process-based models, which produce different results due to the alternative model structures, reinforcing the need for further measurement and modelling of Rs to improve the model accuracy and provide the best estimate of soil respiration for global carbon budgets.

To illustrate how discrepancies across models arise, the following section will outline the current state of knowledge in relation to process-based soil respiration modelling and will examine common modifiers and their effects.

3.3 Process-Based Modelling

3.3.1 *Decomposition Rates*

Nutrients in plant material are broken down and consumed by soil microorganisms during the transformation of plant material into humus, this process of respiration releases 50-60 Pg C yr^1 to the atmosphere, which in its simplest form can be expressed as:

$$M = M_0 e^{-kt}$$

where M_0 is the original mass, k is an annual decay rate, and t is time in years (Bonan, 2015; pp 361). The larger the decay rate, the less organic material accumulates on the ground e.g. k = 1 means 37% of litter remains after one year (a humid tropical climate) while k = 0.1 means 90% of the original litter mass remains after one year (representative of cold climates) (*ibid)*. It is then possible for this simple decomposition rate can be further modified by both soil temperature and soil water content. A similar simple single pool model is outlined by Campbell and Paustian, (2015), shown in Figure 3.2, where hypothetical data used to formulate (A), calibrate (B), drive (C) and evaluate (D) model functions.

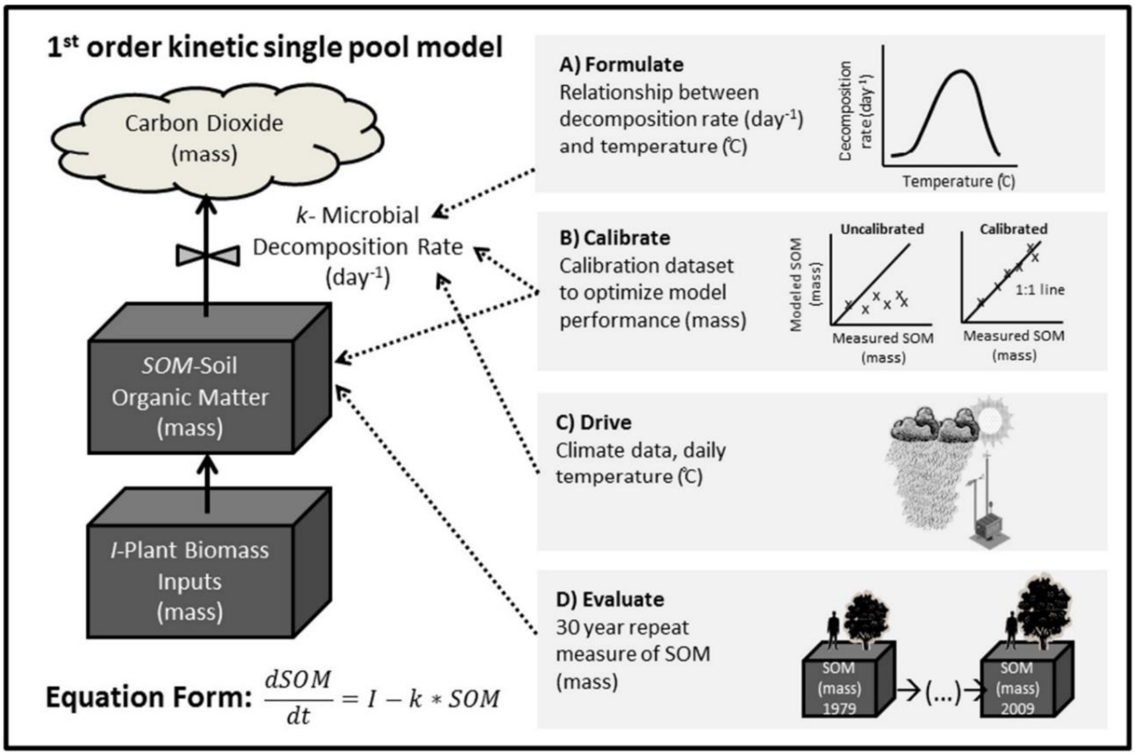


Figure 3.2: A single pool SOM dynamic model which simulates decay over time. Models which incorporate climate (or other driving variable) variability and models with greater structural complexity require much more detailed computer functions and therefore lead to increases in complexity and computational time (from Campbell and Paustian, 2015).

The heterogeneous nature of SOM calls for more complex mathematical representation of the decomposition process. Henin *et al.* (1959) first attempted to represent different decomposition rates for labile and stable material, and the transfer of material from the labile to the stable pool using the following basic model:

$$\frac{dX_1}{d_t} = L - k_1 X_1$$

$$\frac{dX_2}{d_t} = \alpha k_1 X_1 - k_2 X_2$$

Where X_1 is the C content of the labile pool and X_2 is the C content of the stable pool, L is the input of organic matter, k is a decay constant, α represents the transfer rate between pools (humification).

To account for the effects of external factors on decomposition rates, biogeochemical models which simulate decomposition can be represented by systems of differential equations thus:

$$\frac{dX_1}{d_t} = f_1(\theta_1 k_1 X_1, \dots, \theta_m k_m X_m)$$

$$\vdots$$

$$\frac{dX_m}{d_t} = f_m(\theta_1 k_1 X_1, \dots, \theta_m k_m X_m)$$

Where θ is a parameter set modifying the decomposition rate - k, and m - the total number of compartments of the system (typically less than 10; Manzoni and Porporato, 2009) which can be modified by temperature, moisture and/or other edaphic conditions (Sierra *et al.*, 2012). The partitioning of SOM into different pools according to their decomposition rates reflects the different residence times of C compounds in the soil, respiration is therefore affected by the stability of C in each pool combined with environmental factors related to the soil type and the ecosystem (Delogu *et al.*, 2017).

The widely-used RothC model uses five pools, two representing plant material in the litter layer and three representing active, slow and passive material in the soil, with residence times varying from months to hundreds of years (Delogu *et al.*, 2017). The decomposition rates of these pools are then modified further by climatic and edaphic factors. RothC then partitions SOM into decomposable plant material (DPM), resistant plant material (RPM), microbial biomass (BIO), humified organic matter (HUM) and inert organic matter (IOM), with a ratio of DPM:RPM of 1.44 (59% DPM, 41% RPM), DPM and RPM then decompose to BIO and HUM and release CO_2 with 46% BIO and 54% HUM and the amount released as CO_2 dependent on the clay content of the soil, and the decomposition rate of each pool fixed based on comparison of the model to experiments (DPM:10.0, RPM:0.3, BIO:0.66, HUM:0.02), while modified by temperature, moisture and crop cover (Coleman and Jenkinson, 1996). Models which divide organic matter into multiple pools have C transfer methods which can be summarised as follows (Yiqi Luo *et al.*, 2016):

$$\begin{cases} \dfrac{\mathrm{d}X(t)}{\mathrm{d}t} = Bu - A\xi(\mathrm{t})\mathrm{KX}(\mathrm{t}) \\ X(t=0) = X_0 \end{cases}$$

Where X(t) is a vector of pool sizes at time *t*, *B* is a vector of partitioning coefficients among plant pools, *u* denotes C inputs, A is a square matrix of transfer coefficients, ξ(t) is a diagonal matrix of environmental scalars, K is a diagonal matrix of exit rates and X_0 is a vector of initial pool sizes, with the exit rate being the first-order decomposition rate. Summing all column elements for each row of matrix A multiplied by -1 gives the mineralization of decomposed C to CO_2, effectively the respiration for each pool.

Inert Organic Matter (IOM) is often calculated using the Falloon method which uses radiocarbon data to derive IOM from SOC using Equation 3.1 with units t C ha^{-1} (Falloon *et al.*, 1998):

$$IOM = 0.049 \times SOC^{1.139} \qquad \text{Equation 3.1}$$

The equation was tested using additional variables (clay content, soil type, pH, land-use, C input, mean precipitation and mean temperature) which did not improve the model predictions (Falloon *et al.*, 1998).

3.3.2 *Temperature*

Soil respiration is commonly predicted by expressing respiration as an exponential function of soil temperature using a Q_{10} temperature coefficient representing the change in respiration due to a 10° C increase in temperature (Delogu *et al.*, 2017). The use of a constant Q_{10} equation which responded linearly to changes in temperature was advanced by Lloyd and Taylor (1994) who collated measurements of respiration from multiple ecosystems and proposed an Arrhenius-type equation explaining the temperature sensitivity of soil respiration, as the Q_{10} method is too simplistic over wide temperature ranges. Kätterer *et al.* (1998) supported this and find linear Q_{10} functions are not as accurate as others in temperatures below 5°C across a range of experiments.

Multiple temperature modifiers (often denoted as f(T)) are employed by different studies for various reasons, this section will outline modifiers commonly used in biogeochemical models, with equations adapted from Sierra *et al.* (2015). The Lloyd and Taylor (1994) temperature modifier is shown in Equation 3.2 where the effective activation energy for respiration varies inversely with temperature (Lloyd and Taylor, 1994).

$$f(T) = \exp\left(308\left(\frac{1}{56.02} - \frac{1}{(T+273)-277.13}\right)\right) \qquad \text{Equation 3.2}$$

Where T is average air temperature (°C). Similar temperature modifiers from popular ecosystem models include the RothC model temperature modifier (Equation 3.3; Coleman and Jenkinson, 1996):

$$\mathrm{f(T)} = \frac{47.91}{1+e^{\left(\frac{106.06}{T+18.27}\right)}} \qquad \text{Equation 3.3}$$

The CENTURY model has two iterations of temperature modifiers, Equation 3.4 (Burke *et al.*, 2003) and Equation 3.5 (Adair *et al.*, 2008)) shown below.

$$\mathrm{f(T)} = \left(\frac{T_{max}-T}{T_{max}-T_{opt}}\right)^{0.2} \exp\left(\frac{0.2}{2.63}\left(1-\left(\frac{T_{max}-T}{T_{max}-T_{opt}}\right)^{2.63}\right)\right) \qquad \text{Equation 3.4}$$

$$\mathrm{f(T)} = 3.349 \exp\left(\frac{0.2}{2.63}\left(1-\left(\frac{T_{max}-T}{T_{max}-T_{opt}}\right)^{2.63}\right)\left(\frac{T_{max}-T}{T_{max}-T_{opt}}\right)^{0.2}\right) \qquad \text{Equation 3.5}$$

Where T_{opt} is mean temperature. The DAYCENT model (a daily version of the CENTURY model) also has two iterations (Equation 3.6 (Kelly *et al.*, 2000) and Equation 3.7 (Del Grosso *et al.*, 2005)).

$$\mathrm{f(T)} = 0.8 \exp(0.095Ts) \qquad \text{Equation 3.6}$$

$$\mathrm{f(T)} = 0.56 + (1.46 \arctan(\pi 0.0309(Ts - 15.7)))/\pi \qquad \text{Equation 3.7}$$

Where T_s is soil temperature. Other popular temperature modifiers include that of Kirschbaum (1995) (Equation 3.8) who exclusively used laboratory based experimental data to form the temperature modifier.

$$\mathrm{f(T)} = \exp(-3.764 + 0.204T(1 - 0.5T/36.9)) \qquad \text{Equation 3.8}$$

Demeter-1 (Foley, 1995) (Equation 3.9) which aimed to simulate the terrestrial carbon budget.

$$\mathrm{f(T)} = \exp((\ln(Q_{10})/10)(T - 20)) \qquad \text{Equation 3.9}$$

StandCarb (Harmon and Domingo, 2001) (Equation 3.10) was developed to simulate the carbon stored in forest stands.

$$\mathrm{f(T)} = \exp(-(\mathrm{T}/(\mathrm{T_{opt}} + \mathrm{T_{lag}}))^{\mathrm{Tshape}})\mathrm{Q}_{10}^{(\mathrm{T}-10)/10} \qquad \text{Equation 3.10}$$

These varying methods for modifying the degree of soil respiration as a response to temperature have been formulated as part of the SoilR package (outlined in Sierra *et al.* (2012)), where the temperature modifiers from Kirschbaum (1995), CENTURY (Parton *et al.*, 1989; Parton *et al.*, 1994), DayCent (Parton *et al.*, 1998), Lloyd and Taylor (Lloyd and Taylor, 1994), Demeter (Foley, 1995), StandardCarb (Harmon and Domingo, 2001) and RothC (Coleman and Jenkinson, 1996) are included as functions, the software allows for the inclusion of other modifiers as user inputs. SoilR allows for an evaluation of the different modifiers and their effect on soil respiration. The responses of the modifiers to a range of increasing temperatures are illustrated in Figure 3.3, where the large range across modifiers is evident, particularly as temperatures increase, and change over time is considered.

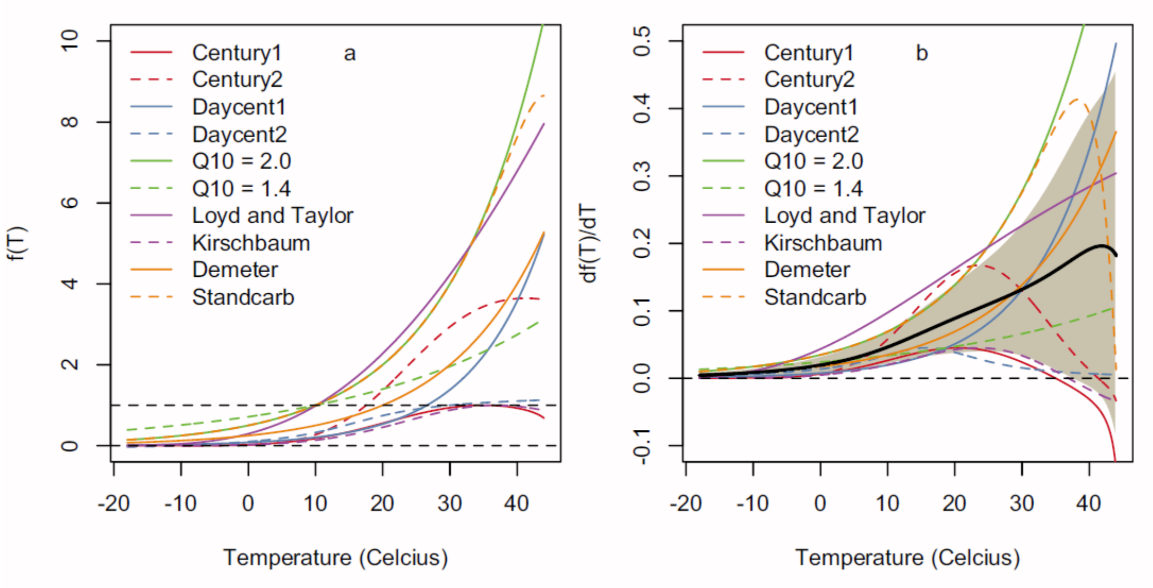


Figure 3.3: Modifiers used in biogeochemical models which predict the effects of temperature on decomposition rates. (a) shows dependence while (b) shows sensitivities to temperature, the thick black line shows the average across models, and grey areas show the standard deviation across models (from Sierra et al. (2015)).

The choice of modifier will clearly have a significant impact the outcome of the study, and the importance of comparing the modelled results to observed data is therefore emphasised. This echoes research undertaken by Burke *et al.* (2003) who find variations in decomposition rate up to fivefold across different models, with models agreeing that decomposition increases with temperature, but none agreeing on the magnitude or rate of change. Sierra *et al.* (2015) outline the various temperature and moisture modifiers commonly used in studies and argue that the addition of new modifiers is not currently necessary, what is necessary is the critical assessment of the current modifiers to reject those which are not useful to reduce the uncertainty among models. It has been noted that widely used models such as CENTURY and DNDC may misrepresent the temperature sensitivity of different SOM pools, as they use kinetically-defined SOM pools and Q_{10} functions (Campbell and Paustian, 2015), an approach which has been strongly criticised as it may overestimate the response of soil C stocks to warming (Tang and Riley, 2015).

3.3.3 *Water*

In addition to the temperature modifiers listed previously, models also typically modify decomposition rates using water/moisture modifiers (often denoted as f(W)). The moisture modifier for the RothC model (b) is shown in Equation 3.11.

$$\mathrm{f(W)} = \textit{if acc. TSMD < 0.444.}\ \text{max.}\ \textit{TSMD,}$$

$$b = 1.0$$

$$\textit{otherwise,}$$

$$b = 0.2 + (1.0 - 0.2)\,\frac{\text{max. } TSMD - acc.\ TSMD}{\text{max. } TSMD - 0.444\ \text{max. } TSMD} \qquad \text{Equation 3.11}$$

Where TSMD is topsoil soil moisture deficit and is calculated as

$$\text{Maximum TSMD} = -(20.0 + 1.3\ (\%\text{clay}) - 0.01\ (\%\text{clay})^2)$$

For the site in Rothamsted where clay content is 23.4%, TSMD = -44.94. The effect of the modifier is illustrated in Figure 3.4.

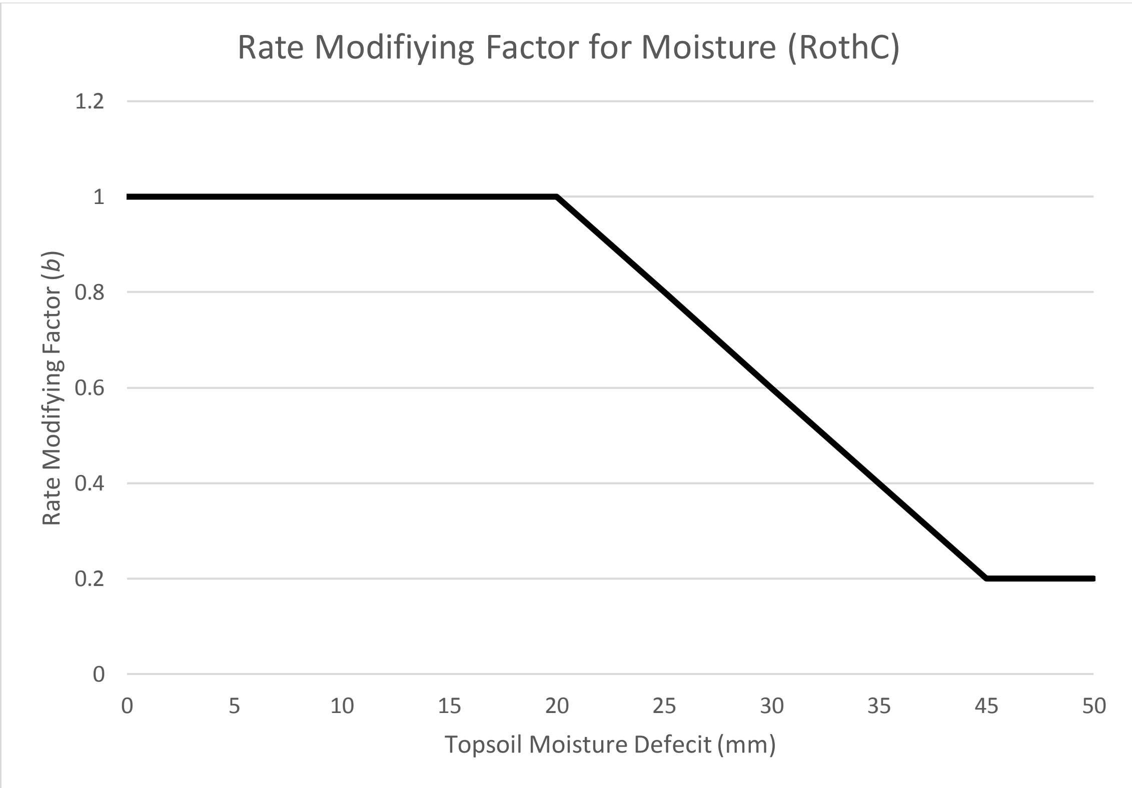


Figure 3.4: RothC Rate modifying factor for soil moisture, adapted from Coleman and Jenkinson, (1996).

Other moisture modifiers include CENTURY (Equation 3.12; Parton *et al.*, 1989; Parton *et al.*, 1994; Adair *et al.*, 2008).

$$\mathrm{f(W)} = 11 + 30\exp(-8.5\mathrm{W}_i) \qquad \text{Equation 3.12}$$

Where W_i is the water content at each timestep. DAYCENT (Equation 3.13; Kelly *et al.*, 2000)

$$f(W) = \left(\frac{W_i - b}{a - b}\right)^{d\left(\frac{(b-a)}{a-c}\right)} \left(\frac{W_i - c}{a - c}\right)^{d} \qquad \text{Equation 3.13}$$

Where a-d are constants. The Demeter water modifier (Foley, 2011) is shown in Equation 3.14.

$$f(W) = 0.25 + 0.75(W_i) \qquad \text{Equation 3.14}$$

The Standcarb water modifier (Harmon and Domingo, 2001) is shown in Equation 3.15.

$$f(W) = (1 - \exp(-(3/W_{min})(W_i + a)))^{b} \exp(-(W_i/(M_{\max} + c))^{d}) \qquad \text{Equation 3.15}$$

SoilR also outlines these modifiers and more which calculate the effect of saturation/drought on soil respiration, these modifiers are applied to a moisture index from 0 (totally dry) to 1 (saturated) in Figure 3.5.

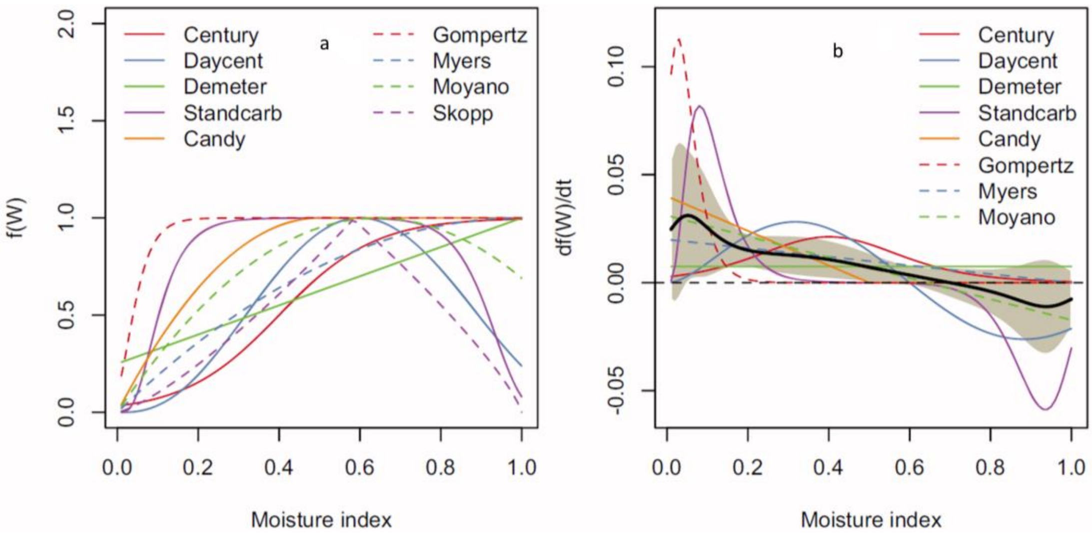


Figure 3.5: Modifiers used in biogeochemical models which predict the effects of moisture on decomposition rates. (a) shows dependence and (b) shows sensitivity to moisture, the thick black line shows the average across models, and grey areas show the standard deviation across models. From Sierra et al. (2015).

The choice of water modifier can therefore also have a significant effect on the outcome of a study, as is shown by the significant variation in values at different levels of moisture. These modifiers are then applied to the decomposition rate and can therefore inhibit the degree of respiration significantly, depending on the modifier and the wetness of the soil.

3.3.4 *Model Uncertainty*

Burke *et al.* (2003) examined a suite of popular soil carbon models and concluded that the decomposition and temperature relationships which the models are based on are built on a limited number of imperfect data sources, that rates across models vary significantly due to a lack of knowledge about the temperature-decomposition relationship, and that this uncertainty results in a high degree of variability in model outputs. This is echoed by Campbell and Paustian (2015) who acknowledge that the quality of SOM modelling is dependent on the quality of measured data which support the modelling efforts. Uncertainties in modelling are also emphasised by Wieder *et al.* (2013) who note the inclusion of microbial process modelling in soil carbon models improves their simulation of carbon stocks under future change, as the adaptation of microbes to changes in temperature is crucial to the ability of the soils they dwell in to accumulate carbon. Many of the process-based approaches are incorporated into the land surface models employed by climate models, Yiqi Luo *et al.* (2016) find that the incomplete use of observations in model parameterization is a large source of differences between models; CMIP5 model projections of global soil C stock range from 510 to 3040 Pg C. Moyano *et al.* (2013) highlight the questionable predictive capacity of current models due to the mechanisms determining the response of soil respiration to moisture availability, and recommend the inclusion of further soil moisture responses to develop a unifying model whereby the relationship between soil respiration and moisture can be quantified across soil types and biomes.

Studies have shown that climate change feedback effects from enhanced soil respiration may significantly increase atmospheric CO_2 concentration and subsequently global temperatures (Cox *et al.*, 2000; Heimann and Reichstein, 2008). The magnitude of this feedback depends strongly on the Q_{10} of soil respiration, and there is still no consensus among modelling communities about how to best improve the Q_{10} function (Xu and Shang, 2016). Future projections of the response of soil to climate change are also uncertain, as higher CO_2 concentrations will increase C supply due to the carbon enrichment effect, it has been speculated that the rise in temperatures will also stimulate increased decomposition, leading to the effects to modulate one another, however the indirect effects of moisture availability will further complicate this process (Pendall *et al.*, 2004). Tian *et al.* (2015) call for improved validations of NPP, C allocation and Rh against field observations toward more accurate simulation of global SOC dynamics, urge caution when interpreting model outputs due to the large range in estimates from different models.

Increased detail regarding microbial biomass and activity has been incorporated into some models, yet more efforts in this direction are necessary such as the inclusion of stochiometric theory at all scales to link decomposer activity, nutrient availability, vegetation growth and climate dynamics (Manzoni and Porporato, 2009), and the inclusion of C dynamics when N is limited (Manzoni *et al.*, 2008). The widespread idea that soil fauna are principally decomposers who assist in mechanical degradation (Smith *et al.*, 1998a) may need to be advanced to include all of the interactions of the specific whole soil food-web dynamics (Osler and Sommerkorn, 2007), though this requires detailed models which are only practical at the site scale, meaning calibration is difficult, leading modellers to use simpler representations of soil biota and microbes, though it is recommended that the potential errors from not introducing food-web interactions are quantified (Manzoni and Porporato, 2009). Recent advances have identified alternative drivers of soil respiration in response to warming, namely the changes in mineral reactivity and resulting nutrient availability in the soil strongly impacts soil respiration in response to warming as the mineral changes alter the microbial community composition, the carbon inputs and enzyme activity, meaning biogeochemical alteration of the soil matrix controls the composition of the soil microbial community, rather than short-term warming (Doetterl *et al.,* 2018). The knowledge of this subject area is constantly advancing and models need to reflect this, although more complex approaches are not always matched by improved performance, as simple models often provide similar or better results than complex ones (Manzoni and Porporato, 2009). Overall, a better connection between advances in SOM research and SOM model applications is needed (Campbell and Paustian, 2015).

Amid these significant uncertainties, a combination of top-down (atmospheric) and bottom up (process-based) methods which complement one another is recommended to get a fuller picture of soil carbon processes (Peters *et al.*, 2010).

3.3.5 *Improving Global Soil Carbon Modelling*

As plant-soil interactions are such a significant part of the carbon cycle and therefore strongly linked to climate change, the importance of including them in global carbon cycle models is highlighted by Ostle *et al.* (2009) who point out that the intricacies of biological and ecological analysis at field level are not represented in large-scale climate models, and call for these processes to be represented in models while not overly complicating the models themselves. Incorporating processes which are important at the local level is central to this goal. Recently, the inclusion of priming (adding fresh organic carbon as a result of litter input or root exudation of carbohydrates) in models has led to improved simulations of SOC content, with research finding that the inclusion of priming in models leads to improved model performance (Guenet *et al.*, 2018).

Wieder *et al.* (2013) find that inclusion of microbial processes in soil C models matches closer to observations than traditional models, as the microbial model includes the consumption of additional inputs to the soil by microbes. When adaptive microbial processes are included in the Community Land Use (CLM) model the results indicate large soil C losses under future climate change, higher than the modest losses traditional models project (*ibid*) (Figure 3.6). This recommendation is echoed by Suseela *et al.* (2012) who call for simulation of the response of microbes to temperature resulting from the outcome of their experiments investigating the response of soil respiration to warming. Frey *et al.* (2013) find microbial breakdown of organic matter depends on both substrate quality and temperature, but efficiency declines as temperatures increase for more recalcitrant substrates, suggesting climate change and warming could affect stable organic matter compounds and their decay dynamics, enhancing the positive feedback to climate change in the short term, shifting to a more efficient microbial community in the long term. The importance of microbial interactions and a proposal for assimilating these interactions into ESMs is proposed by Xu *et al.* (2014) who find changes in vegetation will impact soil C storage more than climate effects on microbial activity. While improving models across scales by including microbial processes is desirable, it is not always sensible or feasible due to the cost of increased model complexity, and the lack of data on microbial processes needed to drive the models (Jackson *et al.*, 2017).

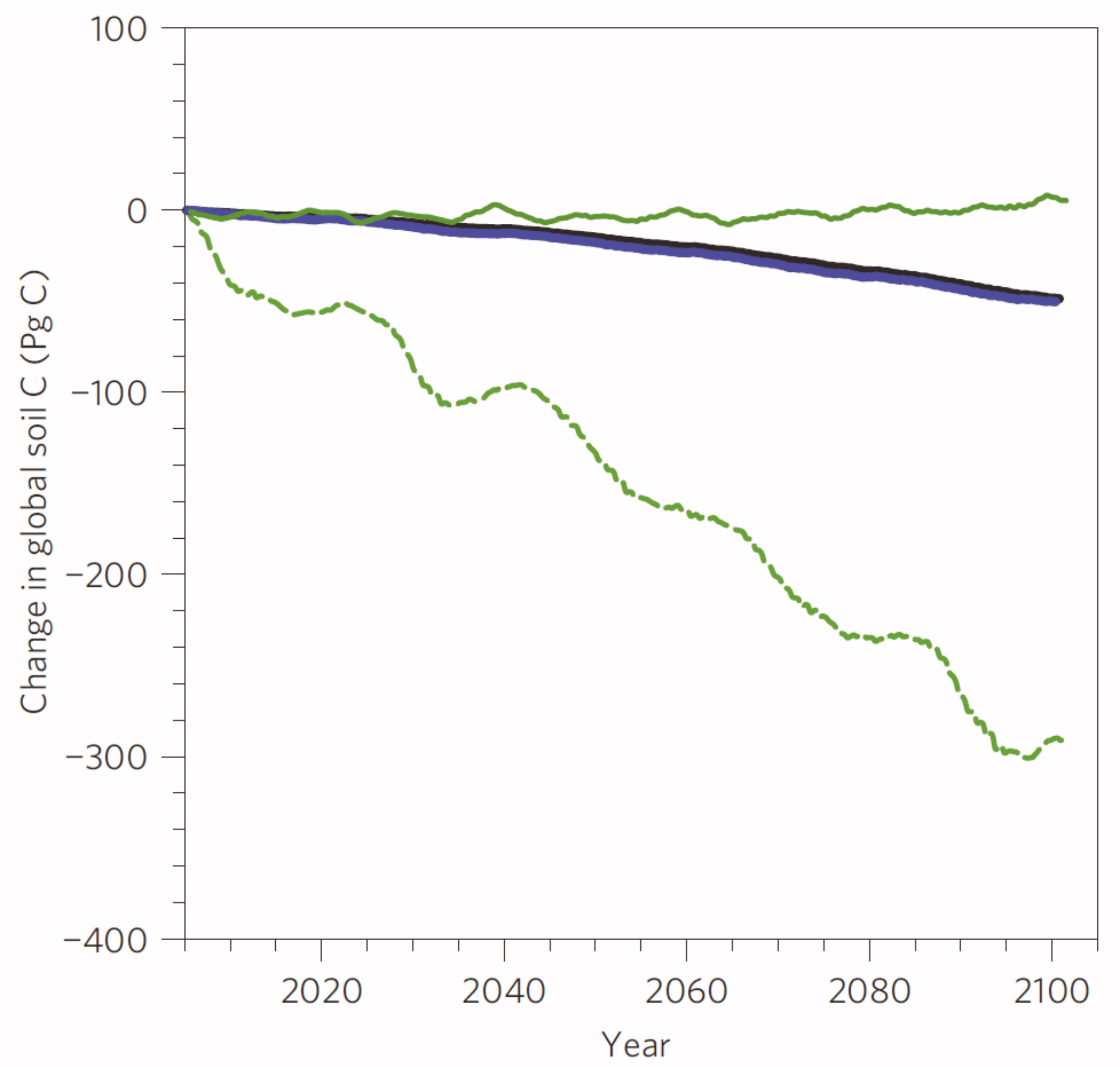


Figure 3.6: Response to a 4.8°C increase in mean global temperature by 2100 based on RCP 8.5 from 2006-2100 where conventional models (CLM4cn, black; DAYCENT, blue) are compared to the CLM microbial model where microbial growth efficiency (MGE) changes with temperature (solid green line), or microbial communities adapt to increasing temperatures without changing MGE (dashed green line) from Weider et al. (2013).

While global estimates of SOM and SOC distributions are rapidly improving partly due to the analysis of soil profiles in global databases, uncertainties remain regarding wetlands, peatlands and permafrost soils as definitions of what exact conditions constitute these categories are different across countries and scientific disciplines (Jackson *et al.*, 2017). Zhou *et al.* (2018) examine CMIP5 models and find those which include a nitrogen module have lower NPP and therefore lower C storage and C storage capacities due to the productivity of the ecosystem (plant productivity) being limited by lack of reactive N, and the CO_2 fertilization effect being dampened by N limitation. Models which include an N module project decreasing global C stock trends compared to increasing trends in those that do not. It is recommended that future assessments take place at regional rather than global scales, to incorporate more region-specific factors and uncertainties (Zhou et al., 2018).

Smith *et al.* (2015) summarise global modelling research thus far and highlight that the knowledge gaps in modelling which require further study are: to aim for similarity in measured and modelled SOM fractions (after Zimmermann *et al.*, 2007), to improve modelling in the subsurface soil layers, to develop spatially and temporally improved observational networks with which to validate models, to resolve representation of soil C in global models, and to further investigate the response to climate extremes. Todd-Brown *et al* (2013) call for the improvement of empirical datasets, model driving variables and parameterisation to improve the relationship between modelled and measured values. Keenan *et al.* (2013) investigate the most valuable data in improving model performance and conclude that fast-moving processes (NEE, soil respiration) combined with slow moving processes (turnover rates of soil carbon pools, monthly/annual cumulative fluxes, litter from wood/leaves) improve performance most, and that carbon stock sizes were of little value when other more informative measurements were available – therefore they suggest prioritising collection of these data in future to avoid wasting scarce money and resources. Omuto *et al.* (2013) in a state-of-the-art assessment of global and regional soil information call for the unification of the soil science community at global, regional and national scales to plan activities in the short, medium and long term to best satisfy the needs of communities and stakeholders. The combination of both flux- and pool-based data is recommended to improve biogeochemical models to constrain C input and residence times (Yiqi Luo *et al.*, 2016). In order to improve the modelling of soil respiration it is essential that data-sharing among the soil respiration community is encouraged and facilitated, as is the publication of Rs fluxes estimated by ecosystem and earth-system process-based models, advancements in computing and big data technologies like data mining and cloud computation could also help to improve soil carbon measurements (Xu and Shang, 2016). Recent meta-analyses (Stockmann *et al.*, 2013; Campbell and Paustian, 2015) have called for improved measurement data to improve model calibration and validation, along with an inclusion of the entire soil profile, and deeper understanding of the soil system itself.

Uncertainty in modelling regional fluxes is investigated by (Xiao *et al.*, 2014) who use a simple model to estimate C fluxes based on vegetation and advise against using a single site to parameterise a plant functional type (PFT) as it may introduce biases to the flux estimates and not capture the ecological and biophysical properties within a PFT. It is recommended to use multiple observations where possible to parameterize the PFT used by the model, it is also noted that uncertainty assessment at regional scales can be computationally expensive, even for their simple model, as compromises in spatial or temporal resolution are necessary. These complexities show that there is currently no ideal modelling structure and trade-offs must be made due to limitations in observational data, computation and memory.

Despite the uncertainties and imperfections in modelling soil GHG stocks and fluxes, remarkable progress has been made in an incredibly complex area. The increased understanding of the role soil can play as a source or sink of GHGs along with the feedback processes is moving us toward a more complete understanding of the soil system, where geodatabases outlining the stocks and fluxes of soil GHGs around the world which are accurate, open and verifiable are the ultimate goal (Oertel *et al.*, 2016). Smith *et al.* (2015) emphasise the importance of focusing on what we do know and making decisions on this basis, rather than focusing on what we do not know. Jackson *et al*. (2017) foresee decades of research ahead in experiments, synthesis and modelling of SOM.

4 Simulating Soil Carbon Fluxes at an Irish Arable Site: Parameter Assessment

Following the review of observations and models in chapters 1-3, this chapter outlines the process of simulating soil carbon fluxes using the ECOSSE model at an arable site in Co. Carlow, Ireland. The ECOSSE model is described in detail, the data which are used to drive it are outlined, along with any partitioning of the data. Results of the investigation into the model parameters are presented, and findings are discussed.

4.1 Introduction

The ECOSSE (Estimating Carbon from Organic Soils – Sequestration and Emissions) model is a biogeochemical model originally developed to estimate the stocks and fluxes of greenhouse gases in organic soils, and has subsequently been employed on mineral soils for national inventories (Smith *et al.,* 2010b). ECOSSE has been applied for multiple land-use types including European cropland (Smith *et al.*, 2010b; Bell *et al.*, 2011; Khalil *et al.* 2013; Dondini *et al.*, 2017), peatland (Abdalla *et al.*, 2014), land under Miscanthus and Willow (Dondini *et al.*, 2016a) and bioenergy cover crops (Dondini *et al.*, 2016b). ECOSSE has been used for national estimates of soil C using limited inputs, and to inform national inventories (Smith *et al.*, 2010b), it has also been coupled with JULES (Joint UK Land Environment Simulator) in the latest Met Office Unified Model (Ostle *et al.*, 2009); and forms an integral part of the Ecosystem Land Use Model (ELUM) project (Richards *et al.*, 2016).

ECOSSE differs from RothC in that it can scale to national level (Chapter 6) by making use of the limited available information by using measurements of soil C to interpolate the activity of the SOM and the plant inputs used to achieve those measurements. Other data inputs such as information on plant inputs, nutrient applications, and timing of management operations can also be included to improve the understanding of the factors driving SOM activity. If these data are unavailable the model can still provide simulations of SOM dynamics, though the accuracy will be lower due to the reduced detail of the inputs (Smith *et al.,* 2010a). The full details of the ECOSSE model are outlined in Smith *et al.* (2010c).

ECOSSE has been employed previously in Ireland at this site in the past (e.g. Khalil *et al.*, 2013), and has been recommended ahead of other similar models as it outperformed both DailyDayCent and DNDC in simulating N_2O fluxes on Irish soil (Khalil *et al.*, 2016). Based on an assessment of a selection of process-based models (DNDC, DailyDayCent and ECOSSE) on Irish soils, Khalil *et al.* (2016) found both the ECOSSE and DNDC models useful at estimating surface soil nitrate (0-10cm), while ECOSSE outperformed all other models when estimating N_2O fluxes. DNDC underestimated total heterotrophic respiration by 50%, DailyDayCent underestimated by 24%, while ECOSSE underestimated by just 7%. The model inherits some characteristics from RothC (Coleman and Jenkinson, 1996) and SUNDIAL (Bradbury *et al.*, 1993) which have been widely used in the literature, with RothC recommended along with CENTURY as the most suitable model for simulating SOC stock changes in Irish grassland soils (Byrne and Kiely, 2008). The model (described in detail below) was employed in site-specific mode for a field location where flux data was recorded over the period 2004-2006, model outputs were subsequently compared to observed data in order to evaluate the model.

4.2 The ECOSSE Model

Motivation for the development of the ECOSSE model came from drawbacks in previously existing methods for predicting fluctuations in soil C and N, which were largely based on mineral soils, and do not satisfactorily describe the processes and turnovers in organic soils resulting from land-use or climate change (Smith *et al.,* 2010a). Accurate quantification of the effects of climate and land use change on all soils is vital for informing land-use policy, as soil can be either a carbon source or carbon sink under certain conditions (Scharlemann *et al.*, 2014). The ECOSSE model was originally developed and applied in Scotland, to predict the responses of both organic and mineral soils to external changes in climate and management (Smith *et al.*, 2010b). Its ability to simulate emissions from organic soils is important, as around 20-30% (~600 Pg C) of total terrestrial carbon is held in 3% of the land area in peatlands, most of which has accumulated since the last glacial maximum (Yu *et al.*, 2010). The organic soil ecosystem is clearly a significant store and potential sink of CO_2, but it is also a vulnerable landscape, with estimates for Scotland indicating that 15% of the country's total emissions result from land-use changes on high C soils (Smith *et al.,* 2007). In order to get meaningful projections for national emissions, it is therefore important that the uncertainties regarding C storage and flux are minimised, and that all soil types are included.

The aim of ECOSSE is to simulate the impacts of land-use and climate change on GHG emissions from organic, mineral, and peat soils. The model is driven by meteorological data and requires descriptions of soil characteristics and predicts the impacts of land-use and climate change on C and N stores. The model can function at both field (Chapter 4 and 5) and national (Chapter 6) scales, allowing results to inform national inventories and policies.

4.2.1 *Model Structure*

The ECOSSE Model has developed from concepts initially implemented by the RothC (Coleman & Jenkinson, 1996) and SUNDIAL models (Bradbury *et al.,* 1993). RothC measures carbon turnover in mineral soils while SUNDIAL incorporates nitrogen dynamics, with parameters fitted from observing long-term field experiments at Rothamsted, where experiments have been running since 1843 (Johnston and Poulton, 2018). The pool type approach used in both RothC and SUNDIAL is also used in ECOSSE. This approach delineates SOM into pools of inert organic matter (IOM), humus (HUM), biomass (BIO), resistant plant material (RPM) and decomposable plant material (DPM), where processes and turnover rates of C and N are simulated using simple equations driven by common input variables such as soil characteristics and climate data. The decomposition process is described by first order rate equations (with specific rates for each pool) which are modified according to external factors such as temperature, moisture, crop cover and soil pH.

4.2.1.1 *Temperature*

The ECOSSE model describes the decomposition of SOM and associated soil respiration using first-order rate equations based on temperature, moisture, crop cover and pH (Dondini *et al.*, 2017). The temperature modifier in ECOSSE (m_t), inherited from SUNDIAL and RothC for both aerobic and anaerobic decomposition, is shown in Equation 4.1:

$$m_t = \frac{47.9}{1 + \exp\left(\frac{106}{T_{air} + 18.27}\right)} \qquad \text{Equation 4.1}$$

where T_{air} is the mean daily air temperature (°C). ECOSSE also assumes a Q_{10} constant (rate of change of a system due to a 10°C temperature increase) of 2.0.

4.2.1.2 *Water*

Soil water in the ECOSSE model also inherits its characteristics from the SUNDIAL model where water passes through soil layers via piston flow, once the first layer reaches field capacity the water then transfers to the second layer (Smith *et al.*, 1996); this method assumes aerobic decomposition proceeds at its maximum rate as the soil dries from field capacity to the amount of water held at -100 kPa, with decomposition being increasingly inhibited until the soil reaches permanent wilting point as shown in Equation 4.2:

$$m_w = 1 - \frac{((1 - m_{w0}) \text{ x } (\Psi_{\mathrm{f}} - \Psi_{\mathrm{c}} - \Psi_{\mathrm{i}}))}{\Psi_{\mathrm{f}} - \Psi_{\mathrm{i}}} \ ; (\text{if } (\Psi_{\mathrm{f}} - \Psi_{\mathrm{c}}) < \Psi_{\mathrm{i}}, m_{\mathrm{w}} = 1) \qquad \text{Equation 4.2}$$

where m_{w0} is the rate modifier at permanent wilting point (0.2), Ψ_{c} is the water held above permanent wilting point, Ψ_{i} is the water held between field capacity and -100 kPa, and Ψ_{f} is the water held between field capacity and permanent wilting point (all units in mm/layer^{-1}). This is calculated for each 5 cm soil layer to the specified depth in ECOSSE, leaching between layers is by simple piston flow. Saturated conditions are also known to inhibit aerobic respiration (Reichstein and Beer, 2008) and ECOSSE includes a modifier for soil water conditions between field capacity and saturation. Each 5cm soil layer in ECOSSE is filled until it reaches field capacity, where it then drains to the next layer or is evaporated. At field capacity decomposition is assumed to be at its maximum, decomposition is reduced due to dry conditions below field capacity, and oxygen limitation above field capacity. When the soil is saturated, decomposition is 20% of the field capacity, and losses of methane dominate ahead of CO_2 (Smith *et al.*, 2010a). Any water remaining when all layers have been filled to field capacity is partitioned between drainage and excess, and either leaves the soil profile or fills each layer (from the bottom) to saturation. This process uses the inputted water table depth, available water at saturation and weather data to calculate 'restriction to drainage' (Richards *et al.*, 2016). Figure 4.1 (adapted from Smith *et al.,* 2010c) describes the rate modifier graphically.

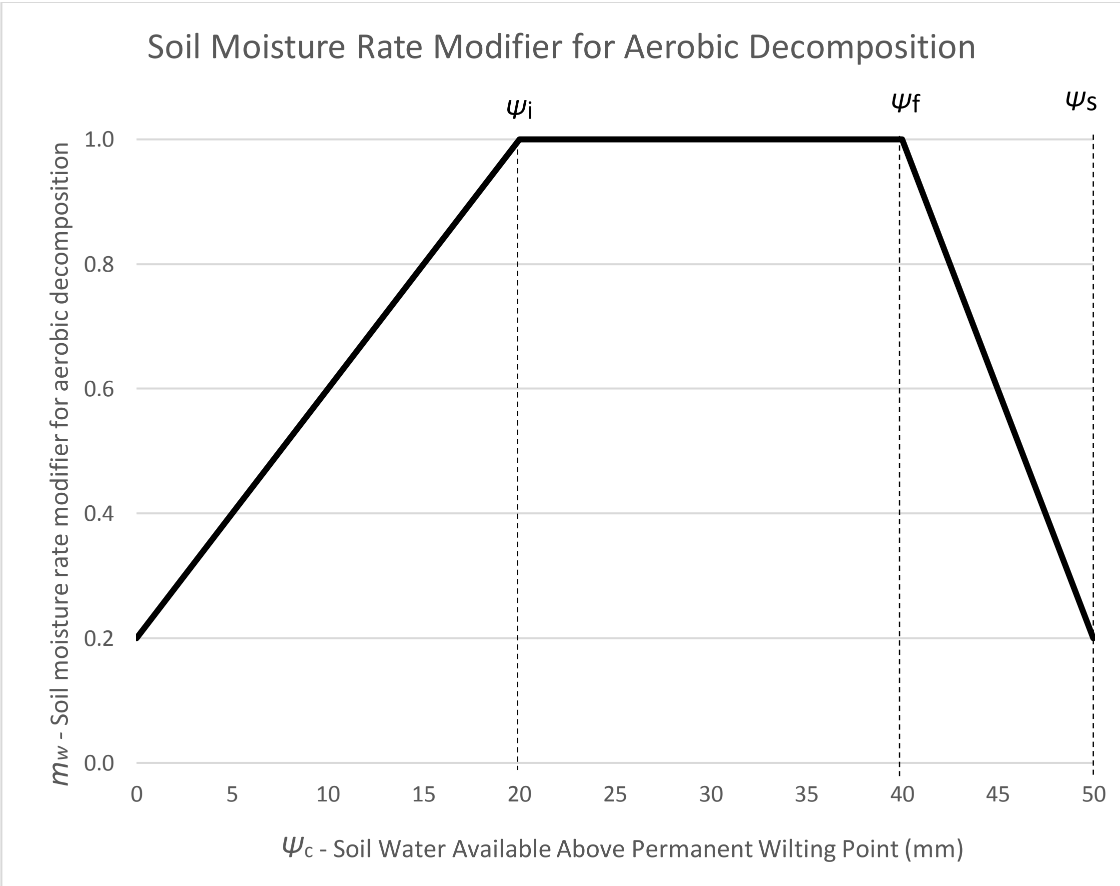


Figure 4.1: ECOSSE soil moisture rate modifier for aerobic decomposition of SOM (Adapted from Smith et al. (2010c))

4.2.1.3 *Crop*

ECOSSE simulates the modifying effect of crop cover on soil respiration using a crop modifier inherited from RothC. While the selection of the threshold is somewhat arbitrary, it is based on findings from a number of studies (e.g. Sommers *et al.,* 1981; Sparling *et al.,* 1982). The crop modifier (m_{crop}) is set as

m_{crop} = 1 if the soil is bare (no effect), and

m_{crop} = 0.6 if the soil is vegetated.

This has the effect of reducing soil respiration during the growing season by 40%.

4.2.1.4 *pH*

ECOSSE also incorporates a pH modifier, introduced for simulating decomposition in organic soils where pH is more variable. It is defined as shown in Equation 4.3:

$$m_{\mathrm{pH}} = m_{\mathrm{pH,min}} + \left(1 - m_{\mathrm{pH,min}}\right)\left(\frac{pH - pH_{\mathrm{min}}}{pH_{\mathrm{max}} - pH_{\mathrm{min}}}\right) \qquad \text{Equation 4.3}$$

where aerobic decomposition proceeds at an optimum rate (m_{pH} = 1) until the pH falls below a critical threshold (pH_{max}) and the minimum rate of decomposition is set as,

$m_{\mathrm{pH,min}}$= 0.2, pH_{min} = 2, pH_{max} = 4.5

If the soil pH is closer to neutral (~7) this modifier is assumed to be 1, similar to RothC and SUNDIAL (Coleman and Jenkinson, 1996; Bradbury *et al.,* 1993) for well managed arable soils, thus having no impact on the estimated soil efflux.

4.2.2 *Decomposition in the Model*

The IOM pool does not decompose as the C is excluded from soil processes due to either its inert chemical composition or protected physical state. The HUM pool decomposes relatively slowly as it represents matter which has been stabilized due to earlier decomposition processes. The BIO pool decomposes quickly as it is still physically active and has not yet become humus. DPM and RPM pools consist of undecomposed plant material with DPM being readily decomposable and RPM being more recalcitrant. The ratio of DPM to RPM depends on the land-use type with DPM:RPM typically being 1.44 for arable land and grassland, 0.25 for forestry and 0.67 for semi-natural land (values taken from RothC model). The decomposition process results in losses of CO_2 from the soil to the atmosphere under aerobic conditions, and mainly losses of CH_4 under anaerobic conditions. Decomposition rate constants (k) in years for each pool (taken from RothC (Coleman & Jenkinson, 1996)) are set at:

- DPM: 10
- RPM: 0.3
- BIO: 0.66

- HUM: 0.02

These values are based on long term field experiments at Rothamsted. The amount of N in the soil follows the decomposition of the SOM at a stable C:N ratio defined for each pool at a given pH, with N being either mineralised or immobilised to maintain the ratio. N released from decomposing SOM as ammonium (NH_4^+) or added to the soil can be nitrified to nitrate (NO_3^-). Nitrification is the conversion of ammonia to nitrate which involves interactions with oxygen and two types of bacteria, nitrosomonas (ammonia oxidisers) and nitrobacter (nitrite oxidisers) which are collectively known as nitrifiers. C and N can be leached from the soil in the form of NO_3^-, dissolved organic carbon (DOC) and dissolved organic nitrogen (DON). Other routes for C and N loss include denitrification, volatilisation or crop offtake. C and N can be returned to the soil (or transferred from the atmosphere) via plant inputs, inorganic fertilizers, atmospheric deposition (from precipitation) or organic amendments.

Ideally the model would calculate the sizes of the SOM pools quickly using the inputs about plants and organic amendments, in the same way as RothC. The relative proportions of these pools then determine the rate of decomposition of the SOM, if there is a more rapidly decomposing pool then decomposition will be higher and vice versa. However, data on plant inputs are rarely available, even at field scale, as the amount of litter, debris and root exudates in the soil is difficult to quantify. Consequently, an iterative process is used which allows for the comparison of simulated and measured values based on default values outlined by Falloon *et al.* (1998). The model iterates until it reaches a steady state and the simulated and measured values are within 0.0001kg C ha^{-1} $layer^{-1}$. The model is assumed to reach a steady state when the SOM pool sizes and plant inputs closely match the observed soil C measurement, and the model can then be perturbed to calculate the impact changes to soil, land use and climate have on SOM turnover. Factors which are not defined as inputs are then estimated according to the relative pool sizes. If soils are likely to become saturated it is important to include water table depth explicitly as an input factor as otherwise the model will overestimate total soil C due to aerobic decomposition, under anaerobic decomposition the rate is slower, and the estimate is likely to be closer to reality. This serves to highlight the limitations of the model and the importance of having relative but not absolute confidence in simulations. If N limitation is being included as a factor, a more time-consuming initialization procedure is needed to stop SOM accumulating instead of reaching a steady state.

4.2.3 *Model Equilibrium*

When total organic inputs to the system are balanced by the total losses of soil C, the model is considered to be at a steady state. Simulations begin with zero SOM in all pools, RothC default values for plant inputs based on land-use type are used to calculate organic inputs, and weather conditions (rainfall and air temperature) are taken from a 30-year average of long-term weather data on a monthly time step. The simulation continues until the total soil C in each layer differs to that of the previous year by less than 0.0001 kg C ha^{-1} layer $^{-1}$. When this happens the spin-up is stopped and the organic inputs are adjusted according to Equation 4.4:

$$C_{\mathrm{in}} = C_{\mathrm{in,def}} \text{ x } \frac{C_{\mathrm{tot,meas}}}{C_{\mathrm{tot,sim}}} \qquad \text{Equation 4.4}$$

Where C_{in} is he annual organic input, $C_{\mathrm{in,def}}$ is the default organic input, $C_{\mathrm{tot,meas}}$ is the measured total soil C, and $C_{\mathrm{tot,sim}}$ is the simulated total soil C (all in kg C ha^{-1} layer $^{-1}$). This calculation is iterated until the simulated and measured values are within 0.0001 kg C ha^{-1} layer $^{-1}$. This methodology can also be adjusted to accommodate sites which are accumulating or losing carbon at constant rates.

4.3 Data and Methods

4.3.1 *Site Description*

The experimental field site, located at Teagasc Oak Park Research Centre, Co. Carlow, Ireland (52.8588N, 6.9178W; Figure 4.2) is an arable field which had been under cropland for over 50 years with sugar beet, spring barley, maize and oil seed rape planted in rotation until 2000, since then spring barley has been the major crop. This study initially focuses on the years 2004-2006 due to the availability of suitable data.

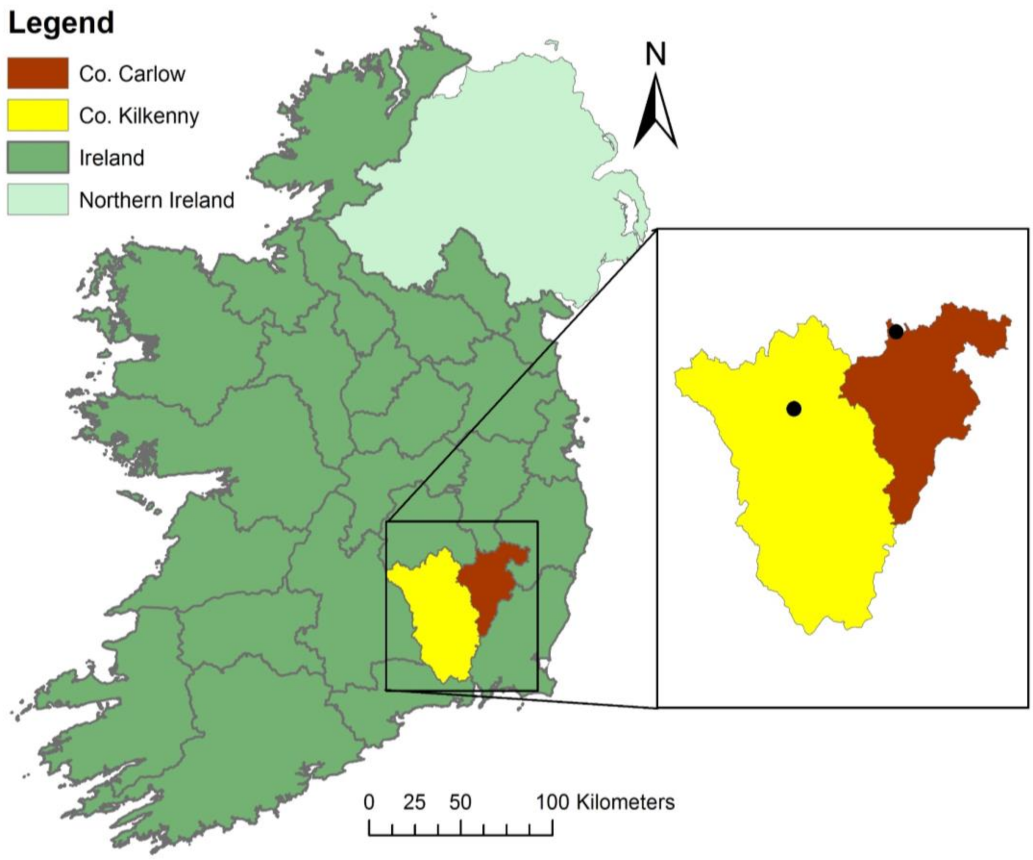


Figure 4.2: Republic of Ireland showing Kilkenny (yellow) and Carlow (brown) with black points denoting Kilkenny synoptic station and the case study location at Oak Park, Co. Carlow.

Full details of the site and soil characteristics are listed in Table 4.1. Land management details for the period including fertilizer applications are outlined in Table 4.2. A map of the field in relation to its surroundings is shown in Figure 4.3.

Table 4.1: Oak Park Site Characteristics (adapted from measured and observed data, Abdalla et al., *(2009); Davis* et al*., (2010); Khalil* et al., *(2013))*

Site Characteristics	
Climate Data	
Latitude / Longitude (decimal)	52.8588 / -6.9178
Elevation (m)	58.208
Mean annual temperature	10.04
Annual accumulated precipitation	822.7
Land-use history	Heavily cultivated for 40 years with a mix of oil seed rape, cereals and sugar beet, was previously under pasture. Spring barley since 2000.
N concentration in rainfall (mg N l^{-1})	0.001*
Atmospheric CO_2 concentration (ppm)	380*
Annual atmospheric N deposition (kg/ha^{-1}):	11
Soil Properties	
Vegetation cover	Spring Barley
Soil type	Euteric Cambisol/Grey Brown Podzolics

Soil texture	Sandy Loam
Bulk density (g cm^{-3}): 0-10/0-25cm	1.42/1.48
Clay (%) 0-10/0-25cm	15.13/14.73
Silt (%) 0-10/0-25cm	25.63/33.73
Sand (%) 0-10/0-25cm	59.24/51.55
Total SOC (kg ha^{-1}): 0-10/0-25cm	19,912/42,888
Total IOC (kg ha^{-1}): 0-10/0-25cm	1478/3543**
Organic C content at surface (kg C kg^{-1})	0.019
Soil pH 0-10/0-25	7.24/7.35
AW at field capacity (mm): 0-10/0-25cm	22.69/55.13
Water content at saturation (%): 0-10/0-25cm	47.21 (AW=29.51mm)/ 45.56 = 133.87mm (AW = 71.17mm)
Water content at field capacity (%): 0-10/0-25cm	40.39 (AW= 22.69mm)/ 38.97 = 97.43mm (AW = 54.73mm)
Water content at wilting point (%): 0-10/0-25cm	17.70 (AW= 17.70mm)/17.08 (AW = 42.7mm)
NH_4 and NO_3 (kg N ha^{-1}): 0-10/0-25cm	2.8/6.92 and 9.5/23.17
Harvest	Grain harvest, mulch/till
Tillage	Conventional and reduced
WFPS at field capacity (0-10cm depth)	0.68
WFPS at wilting point (0-10cm depth)	0.12
Depth of water retention layer (cm)	100
Depth of impermeable layer (cm)	>150 (drainage class high)

*Default values from Abdalla *et al.* (2009)
**Total IOC was calculated using the Falloon method (Falloon *et al.,* 1998), however the value reported here differs from that reported by Khalil *et al*. (2013). The IOM values listed here are calculated using t/ha, as required by the equation, rather than kg/ha, giving significantly smaller values than those reported elsewhere.

Table 4.2: Management Timeline for the observations site growing Spring Barley fertilized with CAN NitroSulphur

	2003	**2004**	**2005**	**2006**
Crop 1 sow	20/03/2003	26/03/2004	14/03/2005	20/03/2006
Crop 1 harvest	23/08/2003	26/08/2004	08/08/2005	01/08/2006
Fert 1 Date	15/04/2003	27/04/2004	16/04/2005	12/04/2006
Fert 1 (kg N / ha)	137	140	109	89.91
Fert 2 Date	-	-	10/05/2005	11/05/2006
Fert 2 (kg N / ha)	-	-	55	50
Crop 2 type	-	-	Mustard Cover	-
Crop 2 sow	-	-	12/09/2005	-
Crop 2 harvest	-	-	21/02/2006	-

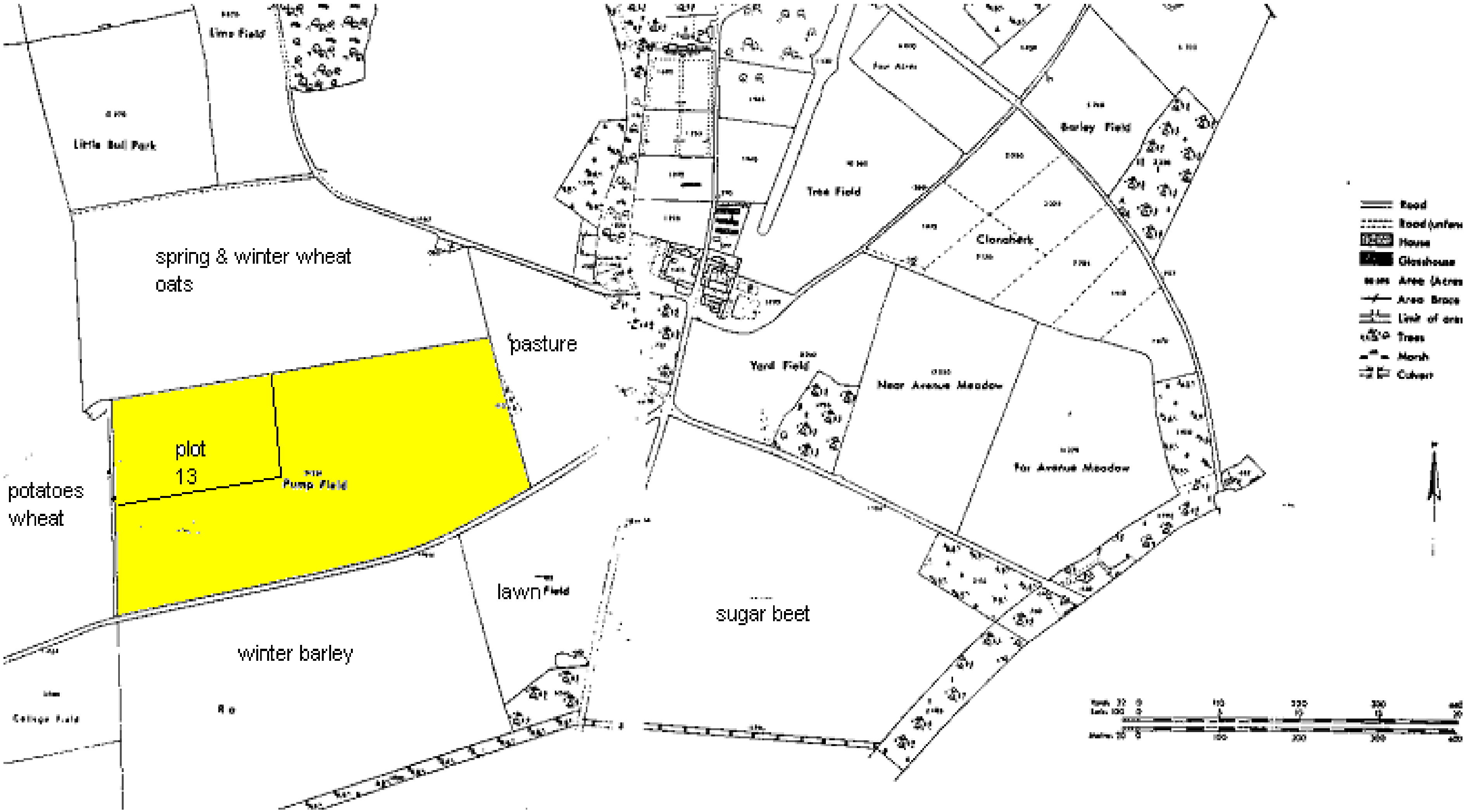


Figure 4.3: The pump field location (highlighted in yellow) where Plot 13 is the CARBOEurope verification site. Source: Provided with flux tower observation data.

4.3.2 *Meteorological Data*

Daily meteorological data were obtained from two sources: the Irish meteorological service, Met Éireann, who provided data from the nearby weather station located on the grounds of the Teagasc Oak Park Research Centre, and the nearest synoptic station located in Kilkenny approximately 30km away, the second source is the flux tower stationed in the experimental field, covering the period from 2004 to 2006. As ~7% of the data from 2004-2006 were missing from the Oak Park meteorological station, gaps were subsequently infilled using either the meteorology recorded at the flux tower or Kilkenny synoptic station data, in that order. As long-term data were not available from Oak Park, data from the nearby Kilkenny synoptic station were obtained to derive the 30-year averages used for model spin-up (in which soil C is brought to equilibrium – see Section 4.2.3). Meteorological and climatological information used for the study is shown in Figure 4.4.

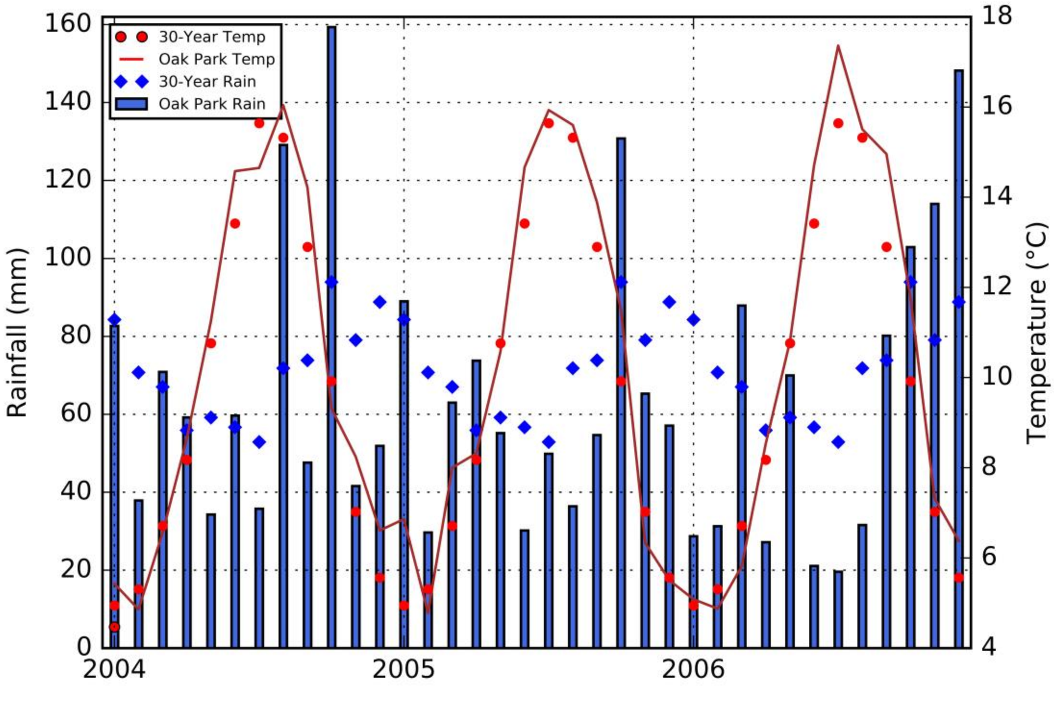


Figure 4.4: Meteorology for 2004-2006 for Oak Park and 30-year climatology from 1974-2003 from Kilkenny synoptic station (~30km from Oak Park).

Reference evapotranspiration (ETo) values were unavailable for the Oak Park site for the years 2004-2006. Consequently, daily values for ETo for the period of interest were initially estimated using the Hargreaves method (Hargreaves and Samani, 1985). Since 2008 when the weather station was upgraded, Met Éireann calculate estimates of ETo using the FAO-56 Penman-Monteith method, facilitating an evaluation of the Hargreaves method over the period 2008 to 2016. This evaluation indicated a significant overestimation of ETo values derived using the Hargreaves approach when compared to the Met Éireann calculated values. A linear calibration was derived from the 2008 to 2016 period and subsequently applied to the Hargreaves estimated values for the 2004 to 2006 period, resulting in modified ETo values which were used as input to the model. Figure 4.5 illustrates the cumulative sums for the years 2008 to 2010 based on the original Hargreaves method, the modified Hargreaves estimates and the Met Éireann derived ETo values. A difference in annual accumulations of ~100mm is evident between the pre- and post- modified Hargreaves values. r^2 values are over .99 (significant at $p = 0.01$) for both the Hargreaves method and the SPSS modified PE when compared to Met Éireann observed values, but MAE and RMSE values are much lower for the modified PE data than for Hargreaves, indicating it is much closer to the Met Éireann derived estimates (Table 4.3).

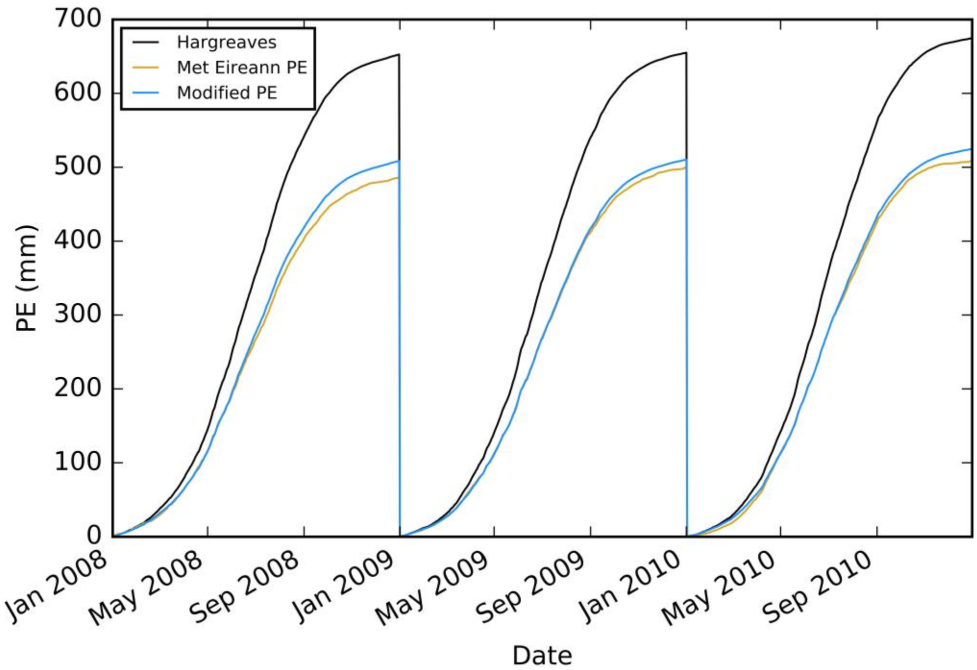


Figure 4.5: Cumulative PE illustrating the overestimation derived using the Hargreaves calculation, compared to Met Éireann PE and PE modified, using calibration equation.

Table 4.3: MAE and RMSE values for different PE calculation methods when compared to Met Éireann PE

	Hargreaves	**Modified**
MAE	82.37	6.43
RMSE	103.34	9.10

4.3.3 *Flux Data*

The study site used in this analysis contributed to CARBOEurope, a member of the FLUXNET project, a network of flux measurement sites which record daily information on soil and meteorological characteristics (Baldocchi *et al.*, 2001). The site hosted an eddy covariance flux tower (Figure 4.6) over the study period providing net ecosystem exchange (NEE) measurements (Davis *et al.*, 2010). Data available from the flux tower included meteorology, radiation, soil temperature, volumetric soil water content, latent heat and NEE, from which Reco (and subsequently Rh) were derived. NEE is typically presented in units of g C m^2 yr^{-1}, representing the amount of elemental carbon, not CO_2 (Kiely *et al.*, 2018).

Figure 4.6: Eddy covariance equipment on a trolley, located in the study field facing west. Source: Provided with flux tower observation data.

The model validation process is complicated by evaluation data which are not directly comparable to one another. The ECOSSE model simulates heterotrophic respiration (Rh) while the measured Eddy Covariance (EC) data allows for the calculation of Ecosystem Respiration (Reco), a combination of autotrophic and heterotrophic respiration from the ecosystem. As Reco represents the combined auto- and hetero- trophic respiration, the daily Reco values were partitioned between the gross autotrophic (plant) and heterotrophic (soil) components. This was achieved by running DNDC (DeNitrification-DeComposition; Giltrap *et al.,* 2010), using the same inputs and weather data outlined previously, to derive ratios of Rh to Reco, following the method of Khalil *et al.* (2013). Alternatively, Hardie *et al.* (2009) propose that Rh is between 46-59% of Reco; Abdalla *et al*. (2014) split this seasonally so that Rh is assumed to be at its lowest at 46% during summer (JJA), 59% during winter (DJF) with a mean value (52.5%) for the rest of the year. Both these methods produced a similar temporal signal (Figure 4.7), but the cumulative fluxes were found to be higher for the seasonal method.

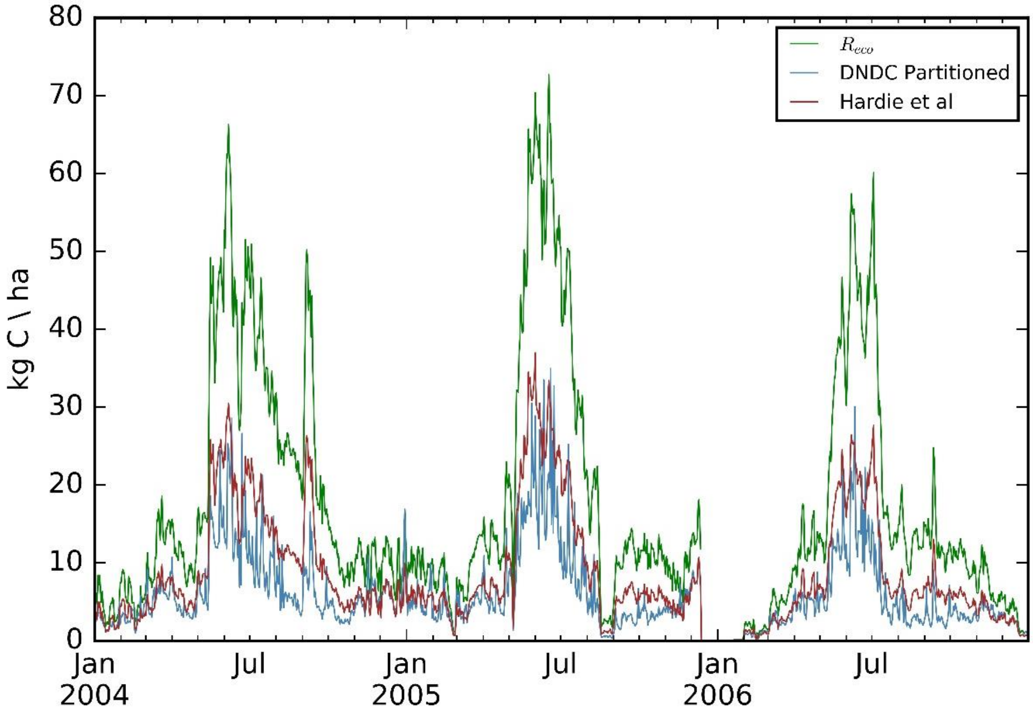


Figure 4.7: Comparison between Reco, estimated from measurements at the flux tower, Rh partitioned using relative proportions (Rh/Reco) from DNDC (following Khalil et al. 2013), and Rh partitioned using the method of Hardie et al. (2009).

4.3.4 *Soil Chamber Data*

Due to the complexities regarding partitioning flux tower data into autotrophic and heterotrophic components, soil respiration measurements using soil chamber data were also incorporated into the analysis. Comparison of chamber to eddy covariance flux measurements on blanket bogs in Ireland has previously indicated that, despite differences on a sub-daily and daily level, the results from both methods on larger scales gave similar estimates of the fluxes (Laine *et al.*, 2006). However, soil respiration from chamber data was only available at this site for 2004. These chamber measurements of CO_2 fluxes, obtained from Jones *et al.* (2010), were measured using a CIRAS 2 infra-red gas analyser coupled to static chambers (SRC-1 soil respiration chamber, PP Systems, Hitchin, Herts, UK). The system allowed automated in-field soil CO_2 flux measurements every 20-90 min. Twelve collars were inserted to a depth of 5cm into the soil 12 days before measurements began to alleviate the effect of soil disturbance on the fluxes. It is likely that the measurements from the soil chambers include both components of heterotrophic (Rh) and autotrophic (Ra) respiration, the chamber data is therefore also partitioned to be comparable with model outputs.

4.3.4.1 *Chamber Flux Partitioning*

Measured soil respiration (Rs) incorporates both Rh and Ra, both processes which respond differently to environmental changes, however, chambers placed on soil are unable to separate the two, therefore it is necessary to partition the Rs data into its autotrophic and heterotrophic components to compare with ECOSSE model output which represents heterotrophic respiration. Soil respiration can be further disaggregated into root respiration (Rr), soil fauna respiration (Rf) and non-biological CO_2 production (Rn) (Xu and Shang, 2016), however, for the purposes of this analysis the focus will remain on Ra and Rh. The partitioning of Rs into Ra and Rh has been widely discussed in the literature (e.g. Hanson *et al.*, 2000; Subke *et al.*, 2006) with ranges for the contribution of Rh to Rs from under 10% to over 90% across different soil and climate types, and a common trend being the higher the total respiration, the higher the autotrophic contribution to the total respiration (Bond-Lamberty *et al.*, 2004). Studies that integrate root contribution to soil respiration give average annual values of 60.4% for the root contribution to respiration for non-forest vegetation (Hanson *et al.*, 2000). Uncertainties abound in this type of research, as the trenching method of root exclusion (whereby respiration is recorded at a 'normal' site and at a site where the root system has been severed, to isolate the heterotrophic portion of respiration) can introduce errors as trenched plots may have reduced water uptake, the elimination of roots may reduce the 'priming' effect roots have on respiration, or the decaying roots may increase the substrate available to microbes, thereby increasing overall respiration, overestimating Rh and underestimating Ra (Savage *et al.*, 2012). Kuzyakov (2006) discusses the advantages and disadvantages of methods of partitioning total soil CO_2 efflux into root and SOM derived CO_2, along with isotopic techniques for tracing the source of CO_2, non-isotopic techniques such as root exclusion, shading and clipping, tree girdling, regression, component integration, excision of roots, and on-site measurements of root respiration are discussed, with no method coming out as distinctly 'best', a suggested approach for partitioning should:

1. Minimise or eliminate disturbance to the ecosystem
2. Incorporate root, rhizomicrobial, plant residue, priming and basal respiration
3. Be universally applicable to multiple ecosystems
4. Generate reproducible reliable results
5. Be inexpensive to set up, maintain and analyse.

Regarding the choice of manual or automated systems to measure CO_2 fluxes, Savage and Davidson (2003) found that weekly measurements using a number of manual flux chambers which are spatially distributed can adequately describe seasonal fluxes and characterise spatial variation very well, while automated chambers provide insight into the effects of rapid changes in water content and temperature. Ideally both manual and automatic chamber approaches could be combined and used to inform and test each other, though this would be expensive.

The potential contribution of Rh to Rs ranges from 3% to 99% in the literature across biomes, land-use types and seasons, and the values taken from temperate arable and grassland land-uses range from 27 to 90% (Subke *et al.*, 2006), these values are chosen to illustrate partitioning ranges as this is the land-use type which most closely resembles the site. A popular method of partitioning fluxes employed by Dondini *et al.* (2016) is that of Koerber *et al.* (2010) who estimate the contribution of Rh to total respiration to be 32% in January, February, March, April and May, 79% in June July August and September, and 67% in October, November and December. Clearly there is no universally applicable process of partitioning chamber data, and the method chosen can significantly alter the results of a comparison, as the large potential ranges show. Amid these uncertainties it is difficult to ascertain a proportioning of Rs into Ra and Rh for a specific site in the absence of measurements and is therefore optimal to use experimental data which closely corresponds to the field where measurements were taken. An experiment was performed during the 2005 growing season at the Oak Park site where 5x2m^2 bare soil patches were left free of plants (and therefore roots) during the growing season, located 0.5m away from conventional tillage plots, meaning they recorded more heterotrophic respiration than measurements taken where roots were present (Kumar Jogi, 2007). Measurements were taking during the growing season, recommended as best practice for croplands (Hoffmann *et al.*, 2017), and found an average Rh contribution of 47% across the growing season (Kumar Jogi, 2007). Application of this multiplier to the chamber data allows for comparison to model outputs and Rh partitioned from ecosystem respiration, and to ECOSSE model output (Figure 4.8).

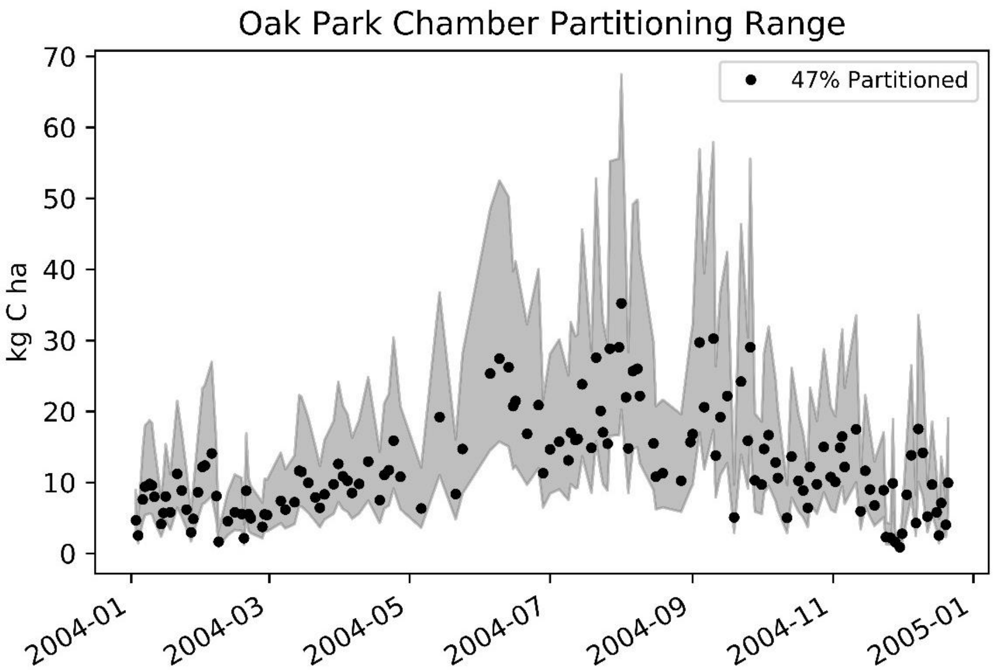


Figure 4.8: Daily chamber data partitioning ranges (grey areas) from 27% to 90% of initial values (from Subke et al., 2006), black dots show data partitioned at 47% (Kumar Jogi, 2007).

4.3.5 *Common Units*

In order for comparison of data to be as accurate as possible, it was first necessary to convert all of the data into comparable units, as NEE is typically presented in units of g C m^{-2} yr^{-1} (units of elemental carbon (Kiely *et al.*, 2018)), and the ECOSSE model outputs in units of CO_2-C, Reco, Rh and chamber data were all converted to the same units in order for them to be comparable. The difference between CO_2 and CO_2_C is significant as the molar weight of C is 12.01 g/mol while the molar weight of CO_2 is 44.01 g/mol, which would have a significant impact on the results. All the observed data are converted to kg C ha^{-1} to match the model output units.

4.3.6 *Soil Water*

In the absence of direct field measurements of soil water tension, field capacity, water content at wilting point and water available at saturation are typically estimated using pedotransfer functions (after Saxton and Rawls, 2006); to determine soil water characteristics based on soil parameters at varying tensions. US based literature widely denotes -33 kPa as the tension at field capacity and -1500 kPa the tension at wilting point; AW is then the difference between the two. However, soil tension at field capacity estimates can range from ~-10 kPa for sandy soils to -33 kPa for loam and clay loam soils (Paul, 2006) with Irish soils being 'commonly near -5 kPa' (Keane and Collins, 2004, pp. 85), further increasing the upper range of available water estimates. Using pedotransfer functions at 33 kPa a sandy loam soil has ~12% available water, at -10 kPa the same soil has 29% available water. This gives a potential range of available water from 30 to 72.5 mm/25cm depending on kPa chosen for field capacity; available water to 25 cm is required as an input parameter to the model. Table 4.4 shows the results of pedotransfer equations for the sandy loam soil at Oak Park based on Saxton and Rawls (2006). These values differ from those reported by Abdalla *et al*. (2009b) who report water filled pore space (WFPS) at field capacity and wilting point, and from Khalil *et al*. (2013) who report AW at field capacity as 55.13mm for 0-25cm depth.

Table 4.4: Moisture characteristics from pedotransfer functions showing the percentage moisture and the moisture quantity to 250mm depth

Sandy Loam	**% moisture**	**250mm**
Saturation (0 kPa)	44.6	111.5
Field Capacity (10 kPa)	38.2	95.5
Wilting Point (1500 kPa)	10.4	26
Available Water (FC – WP)	27.8	69.5

4.3.7 *Radiation*

The flux tower also measured daily radiation in MJ m^2, this radiation data is used to provide context for the relationship between temperature, radiation, ecosystem respiration and leaf area index, to investigate whether the offset shown between model output and observations can be explained by natural environmental factors.

4.3.8 *Leaf Area Index*

Leaf Area Index (LAI) was measured at the field site (plot 13, Figure 4.3) but only during the year 2006 on 19 dates across the year, this data is used to investigate the relationship between temperature, radiation and plant growth, to identify the dominant drivers of growth and whether natural factors account for the offset between measured and modelled data.

4.4 Results and Discussion

The ECOSSE model was initialized using the meteorological, soil and management data outlined above, the results were analysed, and discrepancies investigated.

4.4.1 *Model Evaluation*

Model output and partitioned Rh 2004-2006 are shown with chamber data from 2004 in Figure 4.9. A clear discrepancy exists between model output and Rh over the 3 years. Modelled fluxes peak later than partitioned Rh, and peaks are smaller in magnitude and duration in all years. Chamber data peaks are higher than both modelled output and Rh, and the temporal signal of the chamber data is not matched by the model output, which appears to be suppressed in the earlier part of 2004, throughout all of 2005, and during 2006 also. Dondini *et al.* (2017) suggest that since ECOSSE simulates GHG fluxes from the soil layers defined by the user, whereas the flux data represents fluxes from the entire soil profile, model output will therefore fall below the estimated Rh.

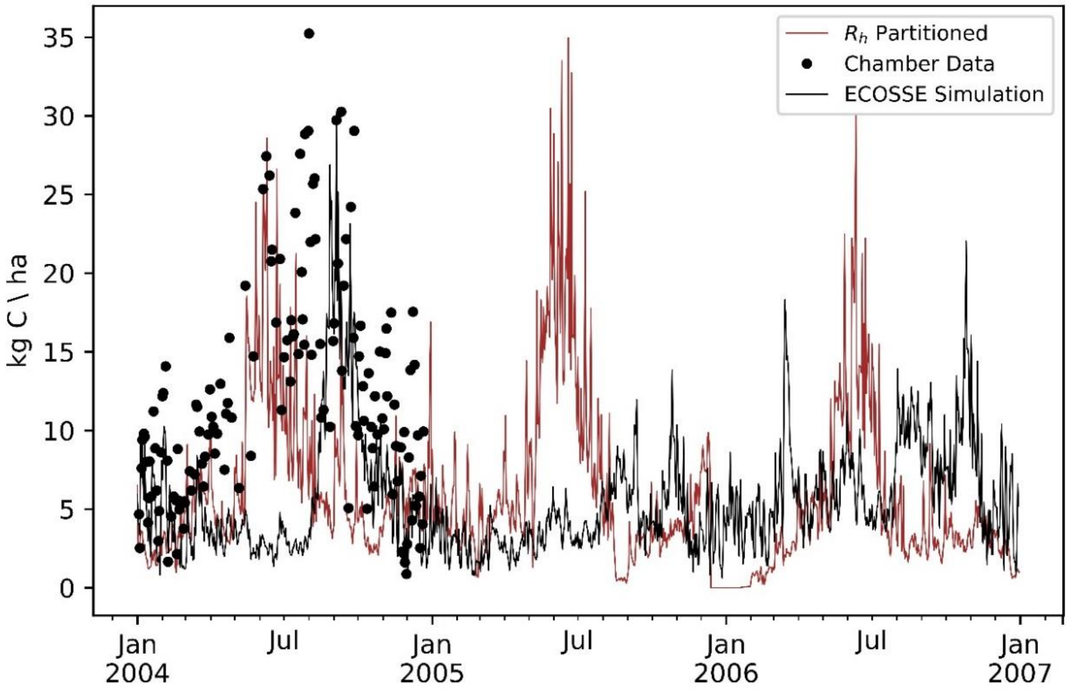


Figure 4.9: ECOSSE model simulated CO_2 output, Flux tower partitioned Rh and chamber data partitioned at 47%

4.4.2 *Cumulative Fluxes*

As the model fails to replicate the seasonal pattern of observations, it is difficult to discern its ability to estimate fluxes. Therefore Figure 4.10 shows annual accumulations of partitioned Rh and ECOSSE simulated Rh, where the model closely replicates fluxes in 2004, underestimates in 2005, and overestimates in 2006. r^2 value for cumulative fluxes compared to cumulative observations is 0.58. Summing the fluxes over three years gives a total of 6495 kg C / ha for partitioned Rh, and 6069 kg / ha for ECOSSE simulated Rh, sums of the output are therefore very similar, though this is due to underestimations in one year being compensated for by overestimations in another. Underestimating of cumulative fluxes has also been observed by Abdalla *et al.* (2011) where the DNDC model is observed to underestimate annual emissions by 13%, while the ECOSSE model underestimates emissions by 6.78% over 3 years. Savage and Davidson (2003) also find trade-offs in temporal resolution where underestimates during some periods of CO_2 flux are compensated for by overestimates in others.

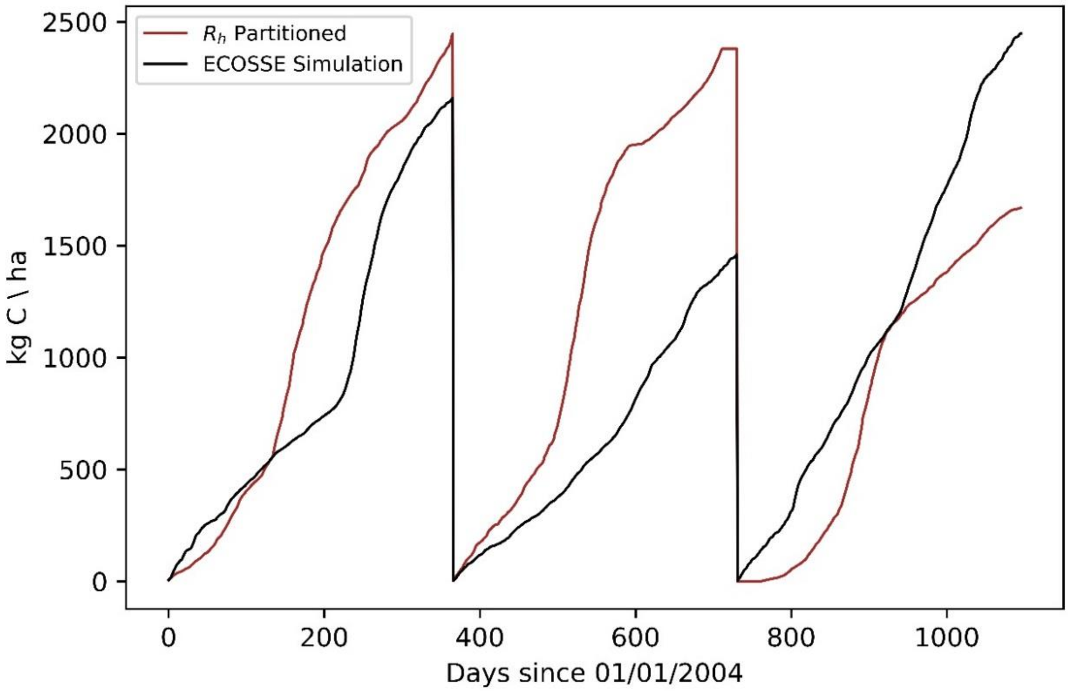


Figure 4.10: Cumulative Flux tower partitioned Rh and model simulated respiration, summed on an annual basis

When examining only chamber data against model output in 2004 (Figure 4.9), a suppression of the fluxes in the earlier part of the year is evident, as the model does not replicate the observations. To investigate the potential causes of discrepancy between the modelled and measured Rh, the sensitivity of the model parameters which influence the C flux were tested to investigate their influence on the results.

4.4.3 *Parameter Analysis*

4.4.3.1 *Soil Parameters*

Changes to the bulk density parameter in the typical range of 1.35-1.65 did not result in any change in the outputted CO_2 flux, even when unrealistic values such as 0.5 or 2 were used. Changes to soil pH also had no effect, even using unrealistic values from 2-10. Changes to the soil structure by adjusting sand and clay contents up to 50% in the input file also had no effect.

4.4.3.2 *Crop Parameters*

To investigate the impact of different crop types on soil respiration and simulated soil water, multiple different crops were specified in the ECOSSE input files, as well as a test-case where the model simulated respiration when no crops were present. Both water and respiration were investigated due to the impact of the water modifier, which limits respiration when soils are too dry or too wet. Running the model with no crop cover impacts the CO_2 output, there is a much lower C flux as the soil is assumed to be bare, meaning there are no plant inputs to the soil providing substrate and stimulus for the microbial activity belowground, meaning the breakdown and release of carbon is not being stimulated (Figure 4.11).

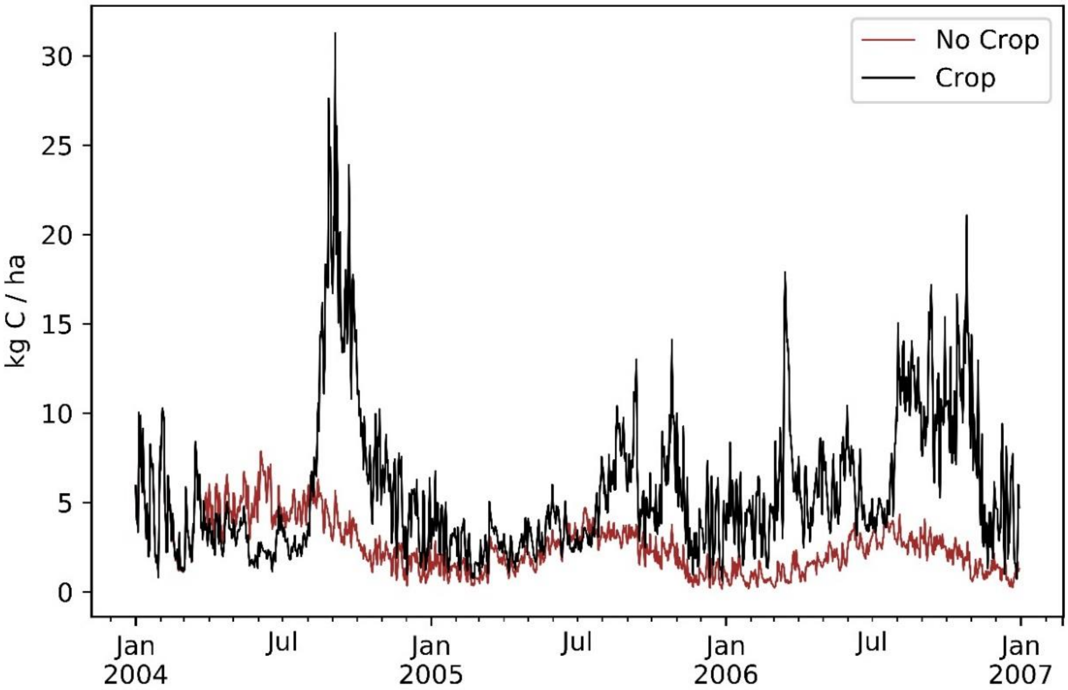


Figure 4.11: ECOSSE model simulated respiration when crops are present (Crop) and absent (No Crop)

To assess the influence of crop cover, various crop types were selected to determine their influence on the simulated fluxes. The crop types selected were Winter Wheat, Potatoes and Spring Cabbage, chosen for their different demands on water and varying inputs to the soil. Changing from Spring Barley to other crop types impacted the magnitude of the CO_2 flux (Figure 4.12) but does not affect the timing of the peaks.

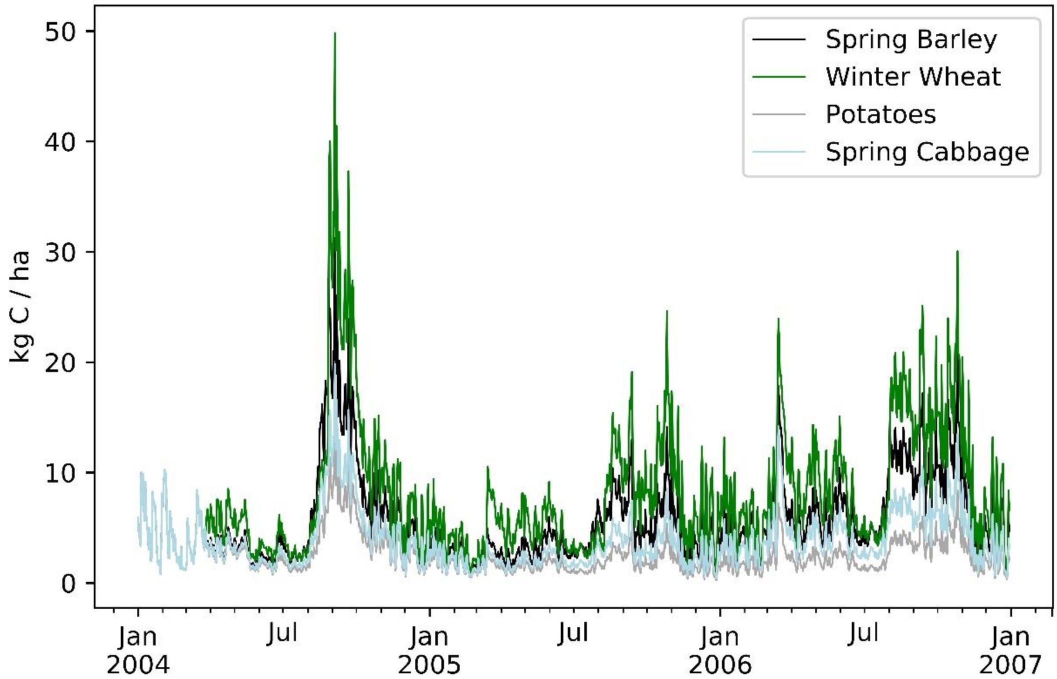


Figure 4.12: ECOSSE model simulated respiration for various crops

Investigating the impact of crop cover on model simulated water to 25cm showed values remaining relatively static and close to the value initially inputted over the period (~50 mm / 25cm), yet when crops are included during the growing season the available water declines to 0 in every year, meaning the soil has dried out and respiration has effectively been inhibited (Figure 4.13). Consequently, the water parameters were assessed.

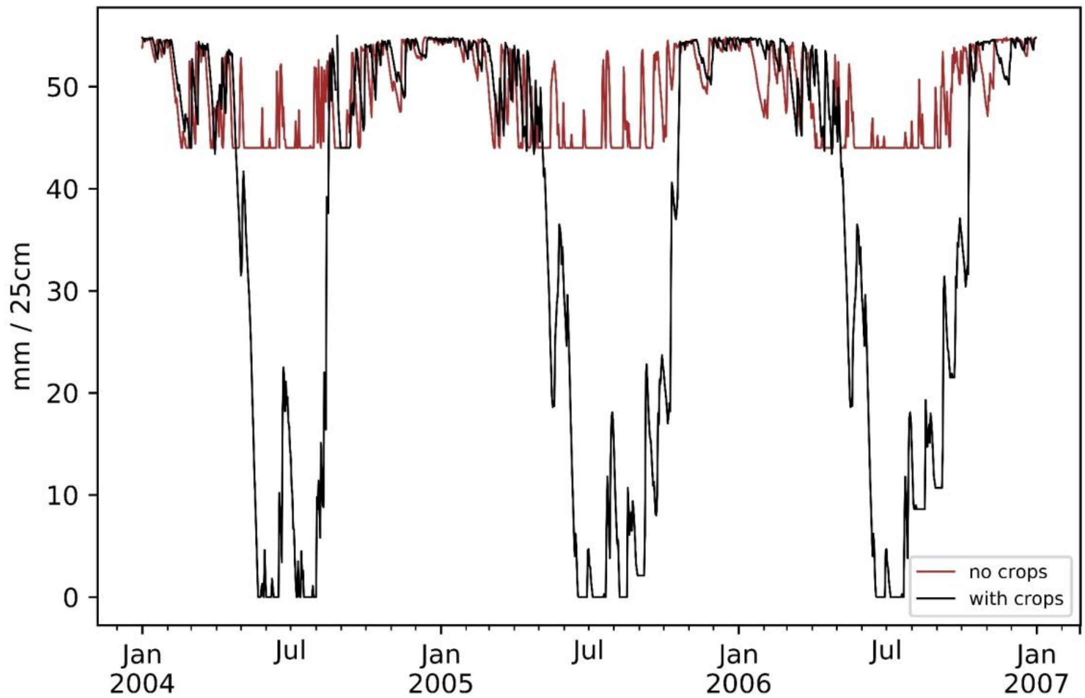


Figure 4.13: ECOSSE model simulated water to 25cm when crops are present (Crop) and absent (No Crop)

4.4.3.3 *Water*

The impact of the water modifier was first investigated by examining the 'Available Water' parameter, which is inputted to the model as 69.5 mm/0-25cm estimated from soil characteristics after Saxton and Rawls (2006). Changes to the available water (AW) input parameter of the model were found to impact the timing, but not the magnitude of CO_2 fluxes, while changes to water available at saturation and water content at wilting point have no apparent impact on simulated CO_2. Figure 4.14 illustrates the ECOSSE model output with the range of ten experimental runs using AW values from 0-110 mm (20-110mm are the wilting point to saturation for this soil – Table 4.4, while values below 20 were used to test the model sensitivity to unrealistic values), the figure also shows the 5 and 95% confidence intervals around these experiments.

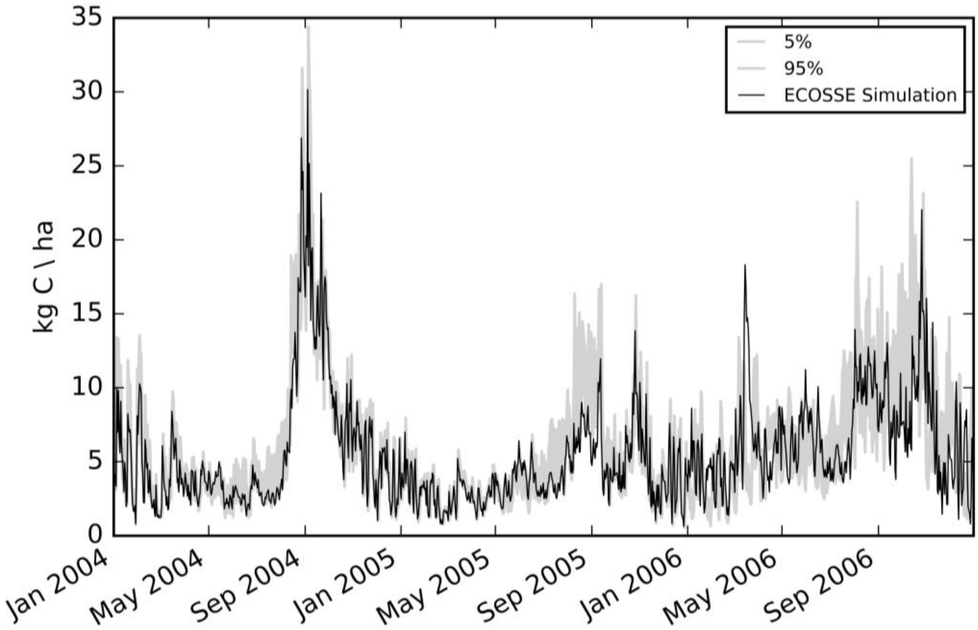


Figure 4.14: ECOSSE model sensitivity to available water (AW) with mean values displayed as a solid black line and grey shading indicating the 5 and 95% confidence intervals.

The values underlying Figure 4.14 show the same CO_2 output is obtained from using AW values of 0, 10, 20mm, while there is variation when using AW values between 30 and 100. To further investigate the processes occurring in the model the outputted available water in each 5cm layer was summed to the 25cm layer (Figure 4.15) which shows that no matter what available water is inputted, drainage within the model reduces available water to zero each year, likely having an inhibiting effect on the CO_2 output as the soil moves into a drought state. Increasing the initial available water value does have the effect of changing the timing of when the soil moves into a drought state, but not the occurrence of the drought, though it does impact the resulting CO_2 fluxes.

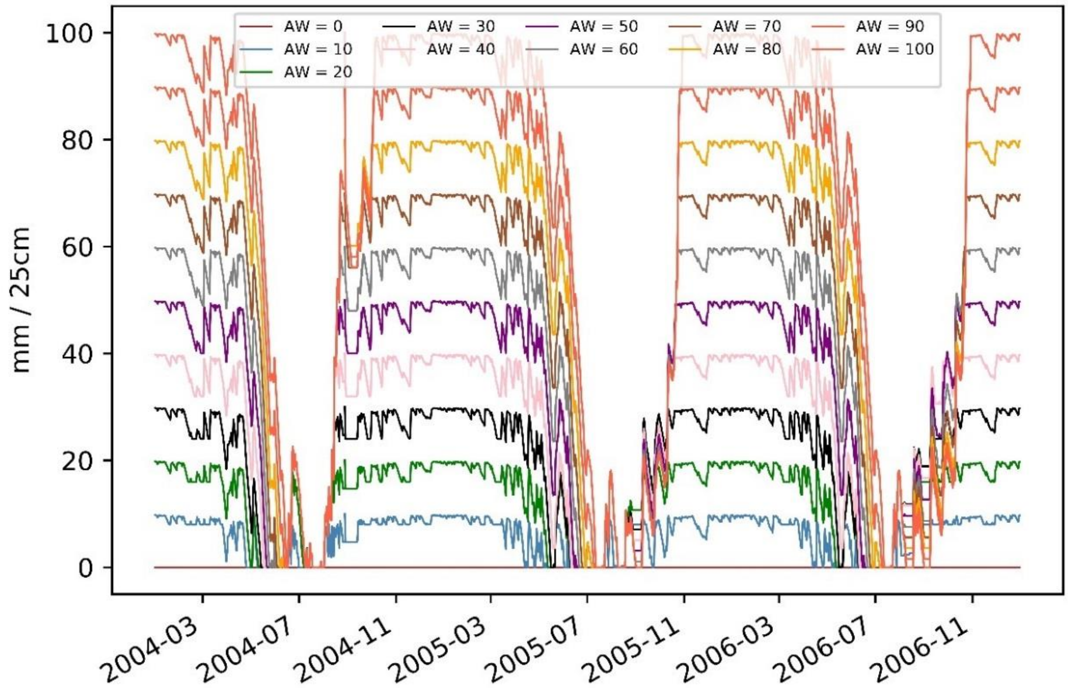


Figure 4.15: Sensitivity of available water (mm/ 25cm) outputted by the model

Adjustments to the water parameters 'water table depth at start', 'water content at saturation' and 'water content at wilting point' were performed to investigate their influence on the fluxes, and ranges from 0-150 for water table depth, 10-100 for saturation and 10-100 for wilting point provided little to no change in the resulting CO_2 flux. When specified in the site details input file water table depth changes had no effect, when altered in the management file there was a slight change in the CO_2 output for values between 10-70cm, after which values above 50 yielded the same results (Figure 4.16). Similarly, some change is evident when adjusting water available at saturation, but the change is minimal (Figure 4.17).

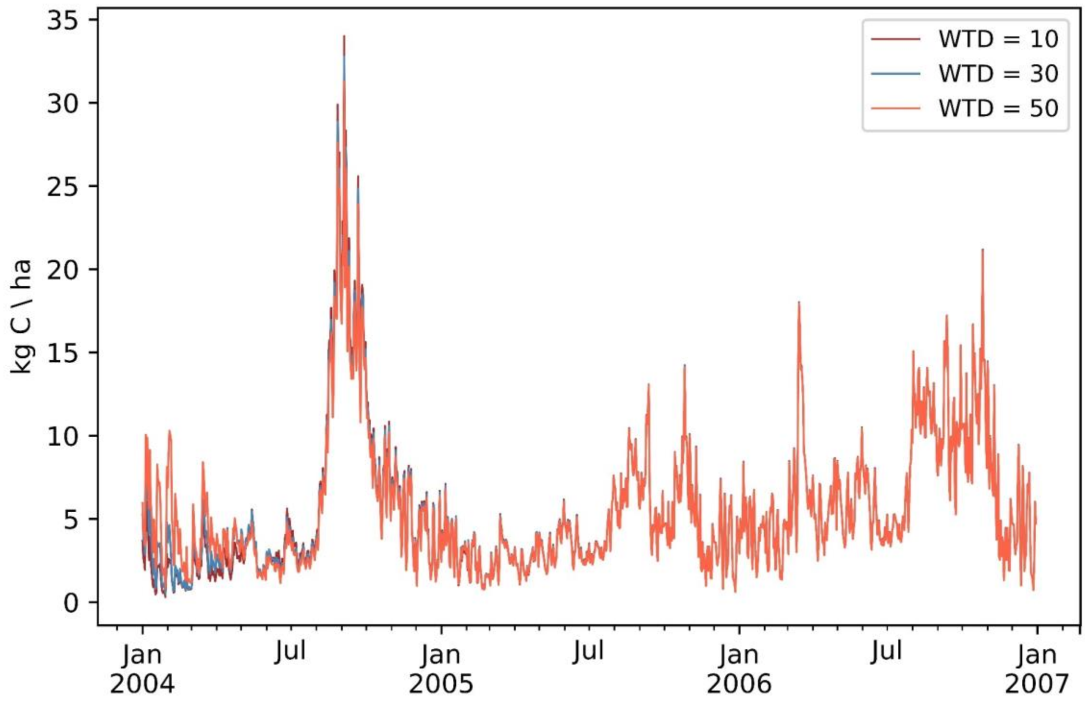


Figure 4.16: Simulated respiration from a range of Water Table Depth (WTD) values inputted into the model

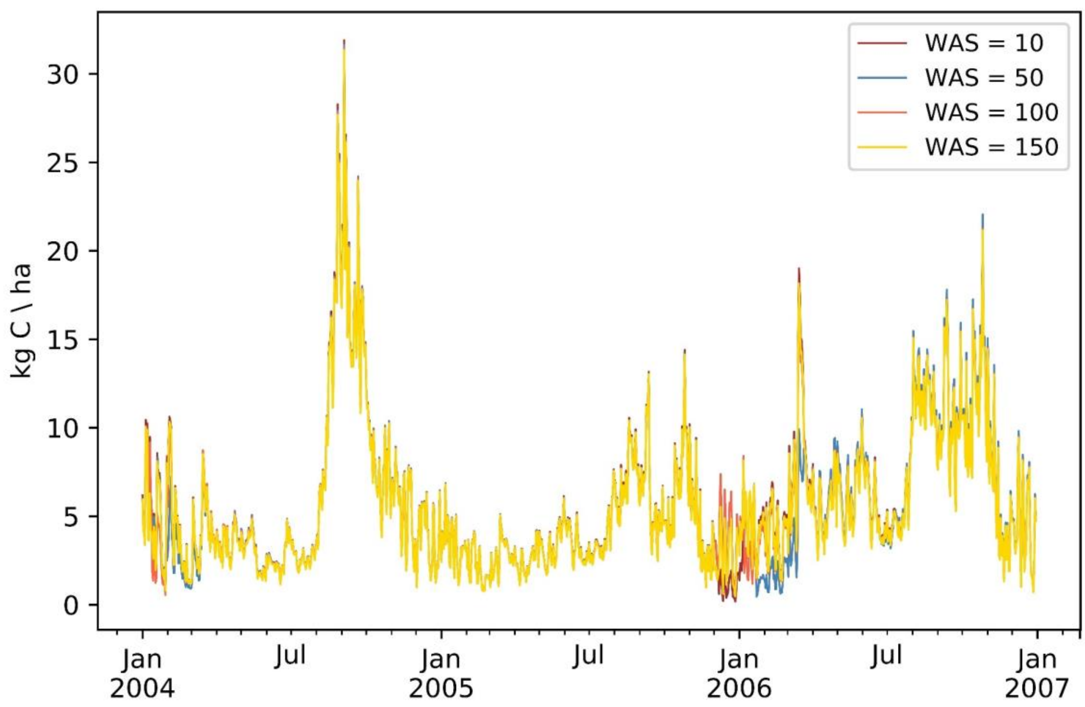


Figure 4.17: Simulated respiration from a range of Water Available at Saturation (WAS) values inputted into the model

As modifying the available water parameter in the model was found to have no influence on the resultant CO_2 fluxes, adjustments to clay content were performed to investigate the effects of soil structure on drainage. Sensitivity testing of both clay and sand content in the soil yielded no change in the excessive drainage or CO_2 output of the model, changes to the 'drainage class' of the soil also showed no change. As this parameter assessment did not account for the discrepancy, potential natural drivers of the apparent offset were examined.

4.4.3.4 *Radiation and Leaf Area Index*

Liu *et al*. (2006) previously found a strong correlation between soil CO_2 efflux and the daily variation of photosynthetically active radiation (PAR). Figure 4.9 shows a clear offset between chamber, Rh and ECOSSE modelled data, to investigate this, potential natural drivers of this offset were investigated to determine whether temperature and therefore the temperature modifier are suitable indicators for plant growth and consequently Rs. The seasonality of Reco is dominated by above ground plant respiration (Barr *et al*. 2004; Matteucci *et al*. 2015), in turn reflecting the seasonal growth of plants. Hence, any partitioning of Reco to derive Rh will ultimately reflect this seasonality. As Rh variability in ECOSSE is primarily influenced / modified by temperature, an offset in model simulated Rh will result. The offset in timing between radiation and temperature at the site is not enough to account for the difference between the model simulated and measured values of Rh seen in Figure 4.9 (Section 4.4.1). Radiation and leaf area index (LAI) data were included in this analysis to investigate the drivers of ecosystem processes and any potential insights this may provide. Figure 4.18 illustrates these variables along with temperature and ecosystem respiration where radiation and Reco correspond closely to one another, as does leaf area index, to be expected as the main driver of plant growth is solar radiation (specifically the region between 0.4 and 0.7 μm). There is a slight offset evident between radiation and temperature, as radiation peaks earlier each year than temperature does. On investigation, a temporal offset is evident between the timing of peak radiation and temperature at Oak Park, with leaf area index, here used as a proxy for plant growth, more closely corresponding with radiation (Figure 4.18). However, this offset is not enough to account for the significant discrepancy between the observed data and model simulated Rs.

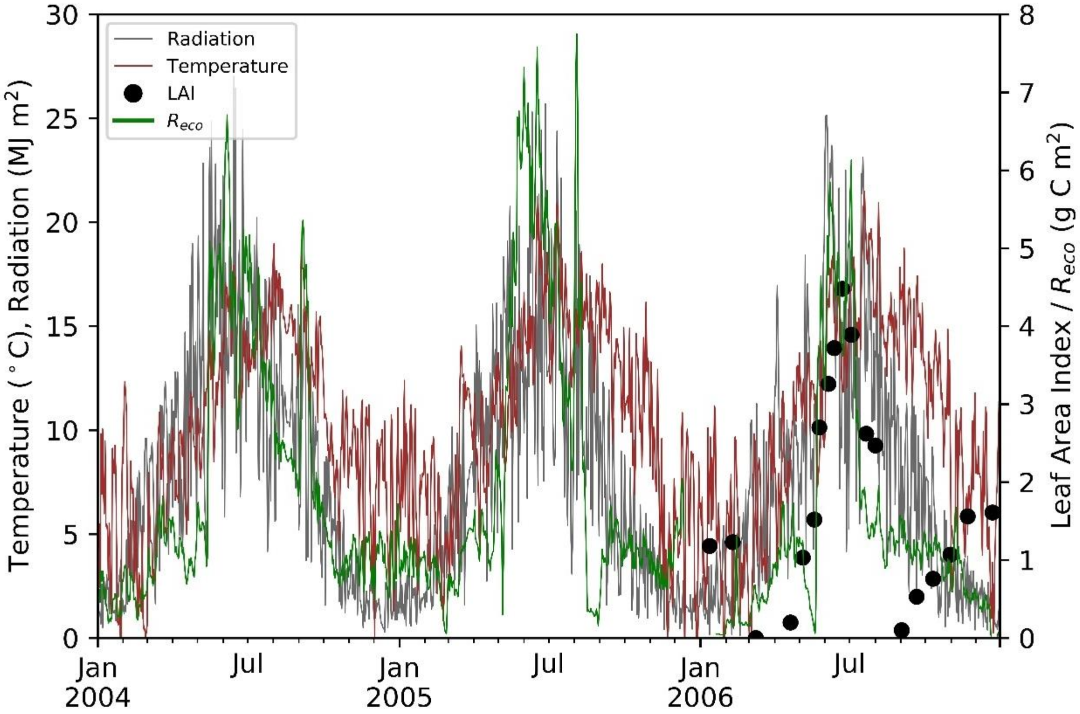


Figure 4.18: Radiation, Reco, temperature (2004-2006) and leaf area index (LAI) (2006) measured at the site.

4.5 Conclusion

Changes to the input parameters of the ECOSSE model including soil structure (sand, silt and clay content) and changes to bulk density did not impact CO_2 fluxes, indicating the model is not sensitive to changes in these parameters. The impact of crop cover on available water is clear from Figure 4.13 where running the model with no crop cover meant the soil did not dry out nearly as much as when a crop was present. The CO_2 flux was inhibited when no crops were present also, presumably due to the lack of priming and belowground activity associated with plant and root growth. Modelled respiration is clearly responsive to changes in the cropping regime, indicating that the crop modifier is functioning as it should. Changing crop types had a significant impact on the magnitude of CO_2 fluxes, but not the timing, again indicating that alterations in the crop file do not account for the seemingly suppressed fluxes when compared to chamber measurements in 2004 (Figure 4.12). Natural factors do create an offset between plant growth and temperature, as plant growth is primarily driven by radiation, but this offset does not account for the larger discrepancy.

From examining the model output against the observed data, the model is not able to replicate the CO_2 flux from either the flux tower or chamber data. Changes to the available water inputs over different ranges did produce some changes in the modelled CO_2 output, but these changes do not provide a significant enough change to explain the discrepancy between measured and modelled data. Interestingly, when the AW values are between 0-30 the resulting CO_2 output is the same, one would assume values this low would inhibit the model's CO_2 simulation, but this does not appear to be the case. When examined alongside the water depth the simulations show identical responses throughout the year with different magnitudes depending on AW specified at initialization, in all cases the water available to the crop declines to zero each year, inhibiting the C flux (Figure 4.15). As Richards *et al.* (2016) highlight, the ECOSSE model uses water table depth and available water at saturation data to calculate the restriction to drainage, and adjustments to these parameters yielded different results (Figures 4.16 & 4.17) with no significant change in output. Investigating radiation and temperature (Figure 4.18) showed natural drivers do cause a slight offset, but not enough to account for that observed in 2004.

In summary, ECOSSE has been previously employed in Ireland and has successfully simulated soil respiration when compared to partitioned ecosystem respiration (Khalil *et al.*, 2013). Attempting to run the model for the same site using similar parameters to drive the model resulted in outputs which did not replicate the previous study. Investigating and testing the parameters which influence the modelled soil carbon flux showed some change in outputs, but nothing which rectified the discrepancy between modelled and measured values. Though the temporal simulation of respiration is incorrect, the cumulative fluxes show that underestimations in some periods can counteract overestimations in others (similar to Savage and Davidson (2003)), indicating that total sums of outputs from the model may be reasonable over longer time periods. As changing the model inputs and parameters which are the dominant influences on the CO_2 flux do not correct the discrepancy between simulations and observations, further investigation of the model and its handling of decomposition processes is warranted.

5 Simulating Soil Carbon Fluxes at an Irish Arable Site: Modifier Assessment

The results of the previous chapter motivated further investigation of the ECOSSE model, to identify potential sources of the discrepancy between measured and simulated soil respiration values. As changing the model parameters did not account for the discrepancy between simulated and observed respiration (Chapter 4), this chapter will investigate the modifiers underlying the model. The chapter presents a background on the importance of conducting this investigation on the ECOSSE model, along with results from testing the modifiers, and recommendations for going forward. A version of this work has been published at the following reference:

Flattery, P., Fealy, R., Fealy, R.M., Lanigan, G., Green, S. (2018) Simulation of soil carbon efflux from an arable soil using the ECOSSE model: Need for an improved model evaluation framework? *Science of The Total Environment*. 622–623, 1241–1249.

5.1 Introduction

Further investigation of the ECOSSE model is warranted due to the outcomes from chapter 4, where the ECOSSE model was initialized using available measurements, parameters and variables derived from observed values and evaluated against Rh, derived as a proportion of Reco. However, due to concerns over the methods used to estimate Reco, additional sources of data were required to investigate the modelled fluxes. In this chapter the model was also evaluated against data obtained from a separate soil chamber experiment at a nearby field, results from which overlapped in time with the model simulations. Following the evaluation of model parameters in the previous chapter, the influence of the individual temperature, moisture, crop cover and soil pH modifiers will be investigated in this chapter. This research seeks to contribute to the existing, growing, literature on the evaluation of ECOSSE, but highlights a potential area for model improvement.

5.2 Data and Methods

5.2.1 *Site Description*

The experimental site used in this study is an arable field located at the Teagasc Oak Park Research Centre, Co. Carlow, Ireland, for further details see Section 4.3.1. The model was initialized using the same input data as the previous chapter. To investigate the influence of the various modifiers, additional evaluation data was required and is outlined below.

5.2.1.1 *Soil Moisture*

Volumetric soil water content (SWC) (%) measurements at the flux tower were available for the period 2004-2006, taken at the same location as the flux tower was positioned, making them highly representative of the site. The SWC data obtained from a previous study (Davis *et al.*, 2010) was measured using a CS616 Water Content Reflectometer (Campbell Scientific) to a depth of 20 cm. The measured Soil Water Content (SWC) in the field ranged from 3.92% to 27.14% with a mean of 16.95% over the period of measurement. As the SWC was measured at a 20cm depth, for comparison with the ECOSSE model which requires water content to be specified to 25cm, the SWC volume percentage was estimated to a depth of 25 cm and converted to mm. Field experiments indicate that volumetric water content at relatively shallow depths does not vary greatly (Qiu *et al*., 2001; Quesada *et al*., 2004; Tromp-van Meerveld and McDonnell, 2006; Martin *et al*., 2012), indicating that this method is appropriate. The derived SWC ranged in values from 9.8 to 67.85 mm, with an average of 42.25 and median of 45.2 mm over the period of measurement.

The ECOSSE water modifier (Equation 4.2) was applied to the model simulated available water (AW), outputted by the model for each 5 cm soil layer. For the purposes of this evaluation, the water modifier was applied to the simulated available water, accumulated over each 5 cm layer to a depth of 25 cm. While the soil depth in the ECOSSE model simulation was set to a depth of 45 cm, the dominant soil efflux typically arises from the uppermost layers - SUNDIAL allocates 80% of SOM to the 0-25cm layers (Bradbury *et al.*, 1993), and for simplification, only the AW accumulation to 25 cm was used. Also, the selection of this depth allowed for a direct comparison with soil water content derived from measurements.

The Oak Park site is on a well-drained sandy soil, Figure 5.1 shows the indicative soil drainage map of Ireland illustrating the different drainage capacities of all Irish soils. Details of categories and their methods of calculation are outlined in Creamer *et al.* (2016).

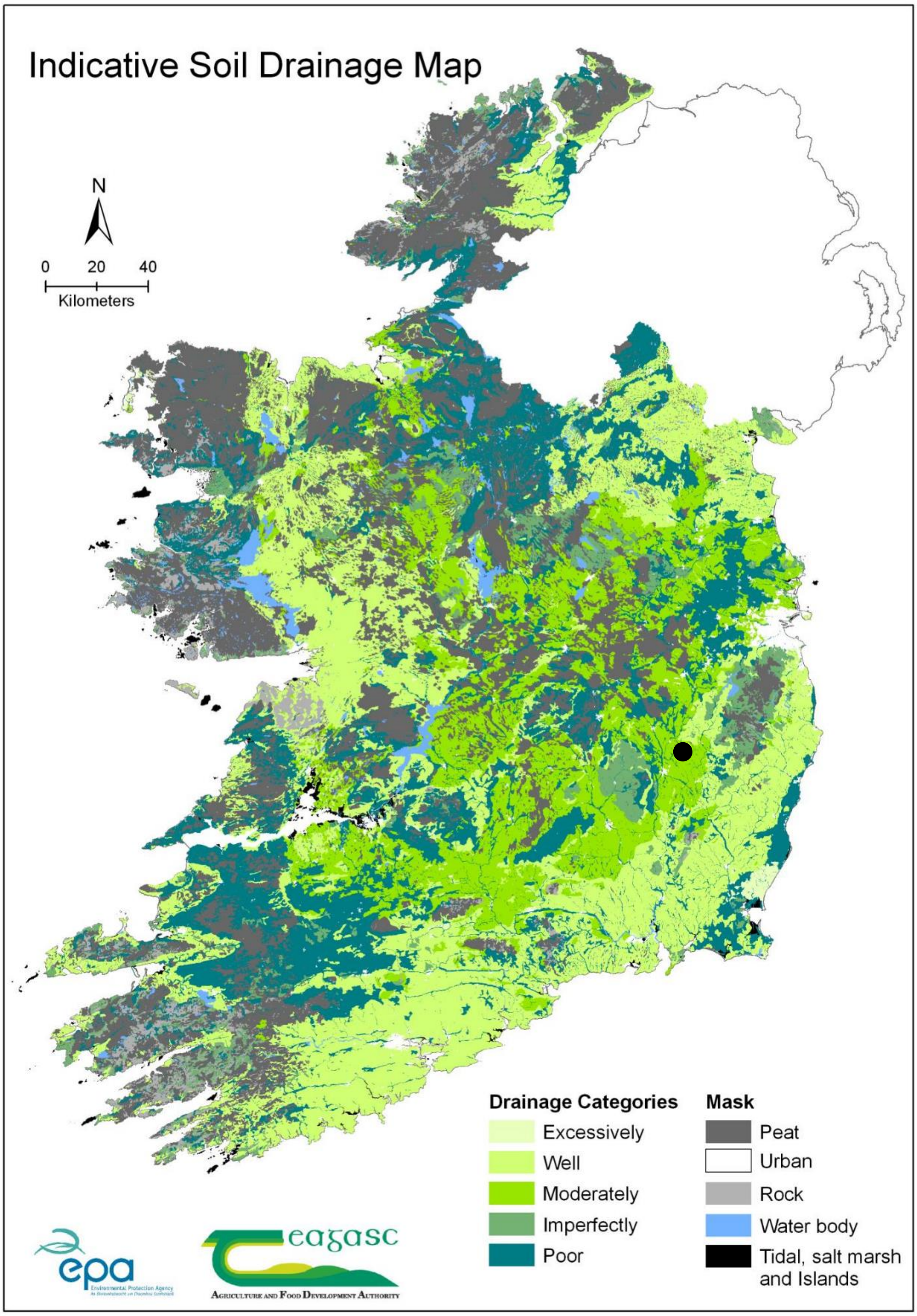


Figure 5.1: Indicative Soil Drainage Map of Ireland showing drainage capacities of different Irish soils (Creamer et al., 2006) with the approximate location of the Oak Park site illustrated as a black circle.

5.2.1.2 *ESA Soil Moisture*

In addition to soil moisture measured at the flux tower, soil moisture data from the European Space Agency Climate Change Initiative (ESA CCI) was used as another test of soil moisture. This data comes from satellites which use active and passive microwave sensors and covers the period from 1980 to the present day and is available at a spatial resolution of 0.25 degrees. Potential errors in ESA soil moisture data can arise from sensors having different wavelengths and having different sensitivities to vegetation and soil penetration depths, from orbital issues which can impact backscatter strength, from topography giving erroneous readings, and from land-surface issues such as building cover and snow cover which obstruct soil moisture information (ESA, 2017). The data was downloaded from the ESA website and a grid box co-located to the Oak Park site was extracted.

5.2.2 *Soil Respiration Simulation*

The ECOSSE model and input requirements have been extensively described elsewhere (Smith *et al*., 2010a; Dondini *et al*., 2016b; Dondini *et al*., 2017; and the previous chapter of this thesis). Although ECOSSE was originally developed for organic soils, it has been widely applied and evaluated on mineral soils (Bell *et al.* 2011; Khalil *et al.* 2013; Dondini *et al.* 2016a; Dondini *et al.*, 2016b; Dondini *et al*., 2017; Zimmermann *et al.*, 2018) to varying degrees of success. In common with several similar models, ECOSSE describes the decomposition process using first order rate equations based on temperature, moisture, crop cover and soil pH (Dondini *et al*., 2017). These ECOSSE modifiers are outlined in the previous chapter, additional empirical formulations which relate the relevant variables to soil respiration are outlined below as they are subsequently employed.

5.2.2.1 *Soil Temperature*

In the absence of soil moisture limitations, the relationship between soil respiration and temperature is generally considered to be positive, with colder soils inhibiting microbial activity and CO_2 generation (Raich and Schlesinger, 1992; Lloyd and Taylor, 1994). However, the determination of the exact relationship remains challenging (Lloyd and Taylor, 1994). Consequently, numerous empirically based formulations relating soil respiration to either soil or air temperature have been proposed. In this study several selected temperature modifiers (outlined below and in Section 3.3.2) were applied to the observed data to compare against the ECOSSE modifier.

Based on analysis of data from a range of different ecosystems and soil temperatures, Lloyd and Tylor (1994) derived a simplified expression (Arrhenius type expression) for soil respiration rate based on temperature, at a standardized temperature of 10°C as shown in Equation 5.1:

$$R_S = R_{10}\exp(308.56\left(\frac{1}{56.02} - \frac{1}{T-T_0}\right)) \qquad \text{Equation 5.1}$$

where R_{10} is the respiration rate at 10°C, T is air temperature and T_0 is a temperature between T and 0 K. Lloyd and Tylor (1994) suggest a value for T_0 of 227.13 K, which provided an optimized fit to the observational data employed in their analysis. Jacobs *et al*. (2007) provide an alternative formulation, originally developed for grasslands, again derived from a simple Arrhenius type expression and includes a correction to modify soil respiration for conditions of soil water stress, as shown in Equation 5.2:

$$R_S = R_{10}\left(1 - f(w)\right)\exp\left[\left(\frac{E_0}{283.15R^*}\right)\left(1 - \frac{283.15}{T_{soil}+273.15}\right)\right] \qquad \text{Equation 5.2}$$

$$\text{Where, } f(w) = C\,\frac{w_{max}}{w_{soil}+w_{min}}$$

where E_0 is the activation energy (kJ $kmol^{-1}$), R^* (kJ $kmol^{-1}$ K^{-1}) is the universal gas constant and T_{soil} is temperature in the first soil layer, and f(w) is a function to modify soil respiration under conditions of soil water stress, w_{max} and w_{min} are reference soil water content values of 0.55 and 0.005, respectively.

The ECOSSE temperature modifier (inherited from RothC) is outlined in Section 4.2.1.1 of this thesis.

5.2.2.2 *Soil Moisture*

There is a complex relationship between soil moisture and microbial respiration within soil (Reichstein and Beer, 2008); major factors affecting the rate of respiration include soil water content, substrate availability and time (Cook and Orchard, 2008) all of which vary with soil water content. Models typically simplify these interactions by using rate modifying factors. For example, the RothC model (Coleman and Jenkinson, 1996) which ECOSSE inherits some characteristics from, employs a modifying factor (b) for soil respiration due to soil moisture based on estimated soil moisture deficits (SMD), derived from rainfall and potential evapotranspiration (PE) data (Coleman and Jenkinson, 2014) as shown in Equation 5.3:

If accumulated (acc) SMD < 0.444 max SMD,

b =1.

Otherwise,

$$b = 0.2 + (1.0 - 0.2) * \frac{\max SMD - acc\ SMD}{maxSMD - 0.444 \max SMD} \qquad \text{Equation 5.3}$$

Once a soil dries beyond a soil moisture deficit threshold, respiration becomes increasingly inhibited until wilting point, after which the modifier is set to 0.2. The ECOSSE water modifier has its origins in the SUNDIAL model and is outlined in Section 4.2.1.2.

5.2.2.3 *Vegetation Cover & pH*

The effect of vegetation cover and pH in the ECOSSE model is outlined in Sections 4.2.1.3 and 4.2.1.4.

5.3 Results & Discussion

Soil chamber measurements for 2004 were used to compare to the ECOSSE model simulated Rh, as chamber measurements are considered more reliable than ecosystem respiration derived estimates (Dondini *et al.*, 2017) (Figure 5.2). It was previously shown that the model simulated values did not compare to the Rh partitioned data across the simulated years 2004-2006. However, from Figure 5.2, the model simulated Rh values appear much closer to the CO_2 soil chamber measurements prior to April and after August, indicating that the model is capturing a component of the measured soil respiration. The model simulated output does not replicate the measured soil chamber values during the plant growing season, from April to August (crop sowing date: 25 March; crop harvest date: 25 August).

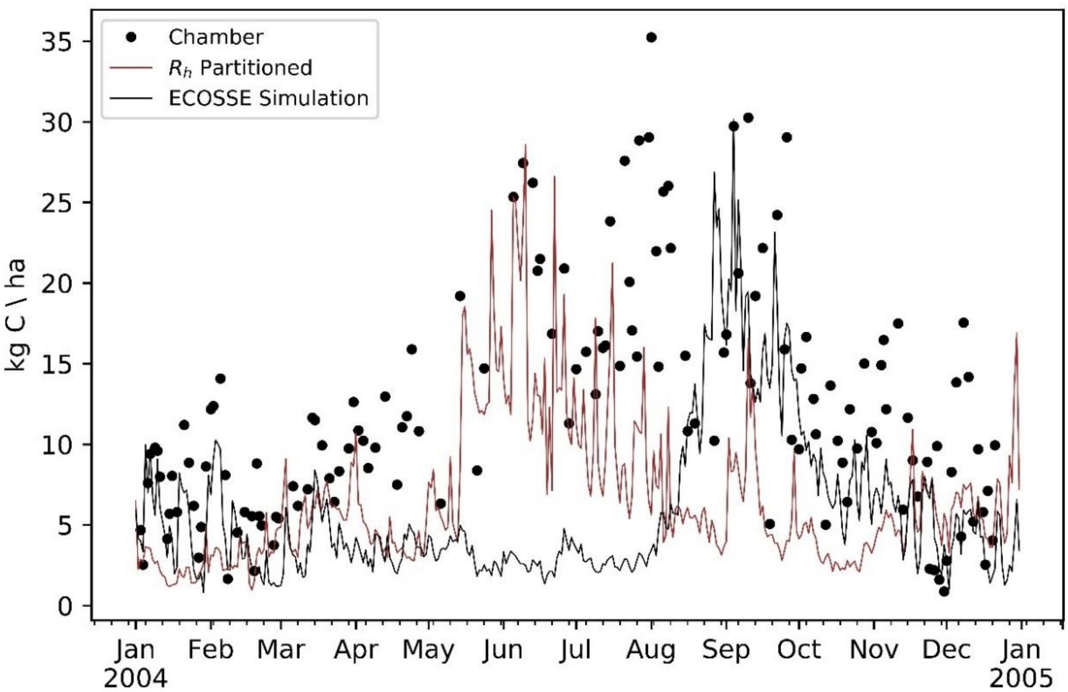


Figure 5.2: Comparison between model simulated Rh, Rh partitioned using DNDC and measured soil respiration from the soil chamber experiment for 2004, partitioned at 47%.

To investigate this, the modifier equations outlined in Section 4.2.1 were applied to the meteorological data at the site to investigate potential sources of error in the timing and magnitude of the ECOSSE simulated values.

5.3.1 *Temperature Modifier*

For comparison, the comparable component expressions from Equation 5.1 (Lloyd and Taylor, 1994) and Equation 5.2 (Jacobs *et al*., 2007) were employed along with the ECOSSE temperature modifier (Equation 4.1) (Smith *et al.*, 2010a) to simulate soil respiration at the site. Figure 5.3 shows the simulated soil respiration response to temperature based on each of these methods, which all produce results positively correlated with the measured soil chamber data (Spearman's Rho of 0.848 for each, significant at the 0.01 level). Despite the Jacobs *et al*. (2007) equation being derived for grasslands, the outcome is consistent with both the ECOSSE and Lloyd and Taylor expressions.

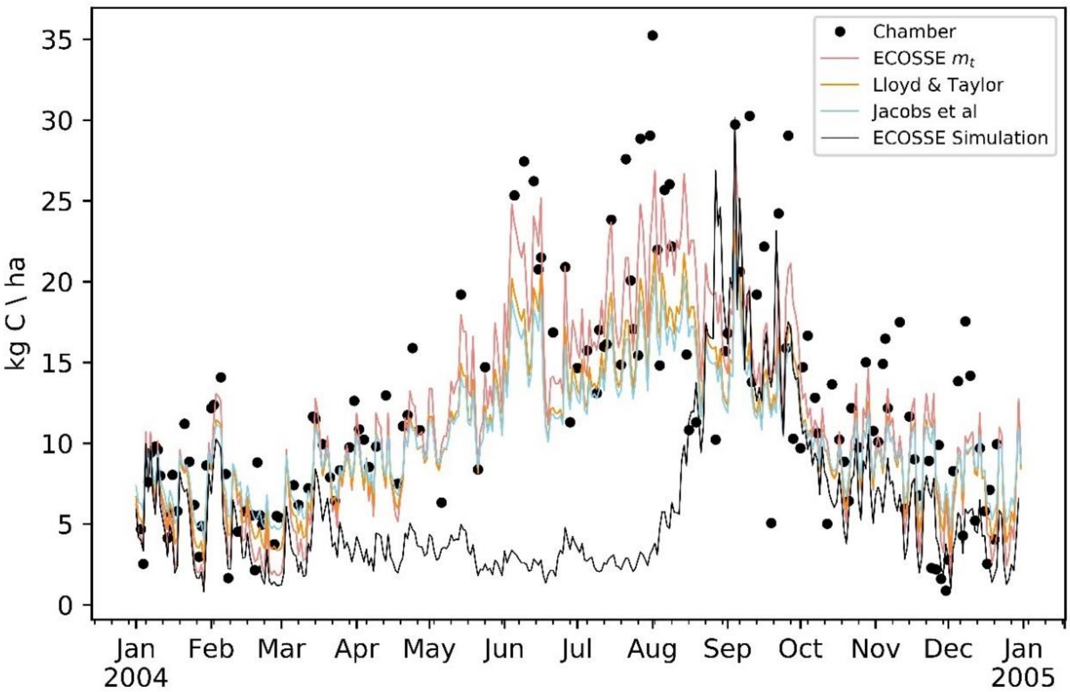


Figure 5.3: Temperature modifiers (coloured lines), chamber data (dots) and model output (solid black line) for 2004.

5.3.2 *Water Modifier*

The model simulated AW and consequently, the water modifier (m_w) has a significant impact on the simulated CO_2 fluxes (Figure 5.4); results from applying both the temperature and water modifier closely replicate the ECOSSE model simulated values (r^2 = 0.78), indicating the importance of model simulated soil water content, and the effect of the water modifier.

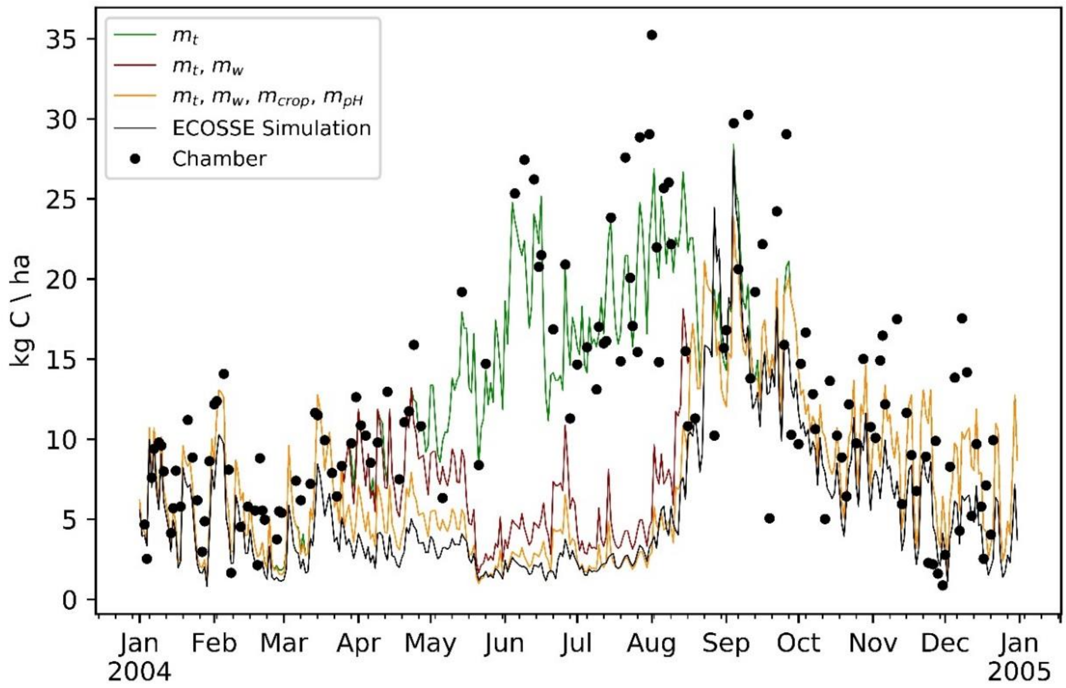


Figure 5.4: ECOSSE modifiers applied as follows, temperature (m_t), temperature & water (m_t, m_w), temperature, water, crop and pH (m_t, m_w, m_{crop}, m_{pH}), and ECOSSE model simulated soil respiration.

5.3.3 *Crop and pH Modifiers*

Finally, the crop (m_{crop}) and pH (m_{pH}) modifiers were applied. The crop modifier follows Jenkinson, (1977) and applies a rate of 0.6 when the crop is growing, and 1 when the crop is absent. This acts to further reduce the CO_2 efflux during the growing season; but, in spite of the threshold value applied (i.e. 0.6) its effect is proportionately small due to the previous effect of the water modifier. The addition of the crop modifier improves the correlation between actual model output and the reconstructed model output presented here, with r^2 = 0.88. The modifier of 0.6 is arguably an arbitrary one, future work could examine the potential for amplified respiration resulting from increased root growth and microbial activity as plants grow.

As soil pH is near neutral (pH ~7.3) at the site, the modifier is assumed to be 1 for well managed arable soils, similar to RothC and SUNDIAL (Coleman and Jenkinson, 1996; Bradbury *et al*. 1993), and thus had no impact on the calculated soil efflux.

5.3.4 *Comparison with Measured SWC*

As a combination of the ECOSSE simulated AW and water modifier were found to have the largest impact on the simulated soil efflux, the model simulated AW was initially compared to the measured soil water content (volumetric % converted to mm over 25cm depth) (Figure 5.5). While the ECOSSE model appears to capture the timing and duration of soil drying, the model overestimates the magnitude. This is particularly evident in 2004, where the measured SWCs remain high (no water stress), but the model simulated AW indicates complete drying of the soil layers to 25 cm (water stress). During 2005 and 2006, the measured SWCs indicate drying of the soil layers, but the model simulated AW again overestimates the magnitude, with complete drying of the model soil layers for ~10 weeks in 2005 and ~3 weeks in 2006. Drying which is not evident in the SWC observations.

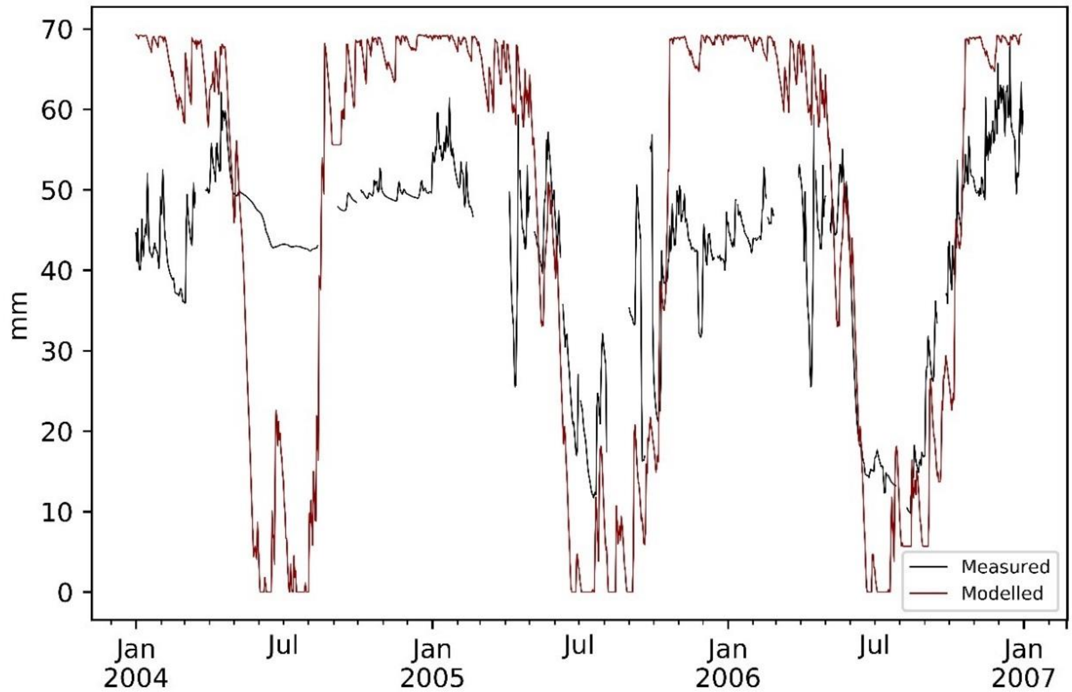


Figure 5.5: Soil Water Content derived for a depth to 25cm, estimated based on measured volumetric soil water content and ECOSSE modelled available water based on an accumulation of each 5 cm layer to a depth of 25 cm.

As measured SWC values were available from the flux tower site, the ECOSSE water modifier was applied to the measured volumetric SWC extrapolated to 25 cm ($m_w(SWC)$), rather than the model simulated AW. The results from this indicate a much lower suppression of soil respiration, relative to the ECOSSE model simulated values (Figure 5.6), particularly during the plant growing season. This is evidenced by lower Root Mean Square Error (RMSE) and Mean Absolute Error (MAE) values for the empirical model using $m_w(SWC)$ compared to the actual ECOSSE model output; similarly, higher correlations are evident between the empirical model using $m_w(SWC)$ and the chamber measurements (Table 5.1). Similarly, using the areal values of soil moisture from ESA CCI, obtained for a location proximate to Oak Park, produced results consistent with observed SWC.

Figure 5.6 illustrates the chamber data with the partitioning ranges from 27-90%, along with the various modifiers and data sources. The model output using observed SWC values is sometimes below the lowest range of chamber measurements during the growing season, and is within the uncertainty bounds for the rest of the year.

Table 5.1: Correlation (gray) MAE and RMSE (white) for ECOSSE modelled water (m_t, m_w, m_{crop}, m_{pH}), water derived from observed SWC (m_t, m_w(SWC), m_{crop}, m_{pH}) and ECOSSE model simulated Rh (Model).

	m_t, m_w, m_{crop}, m_{pH}	m_t, m_w(SWC), m_{crop}, m_{pH}	Model
Chamber	.154	.775*	.238*
Model	.961*	.515*	1
MAE[a]	4.97	2.81	5.25
RMSE[a]	7.21	3.78	7.38

*Correlation is significant at the 0.01 level.
[a]MAE and RMSE compare the chamber data to Rh derived from the ECOSSE modifiers, modifiers using SWC, and model simulated Rh.

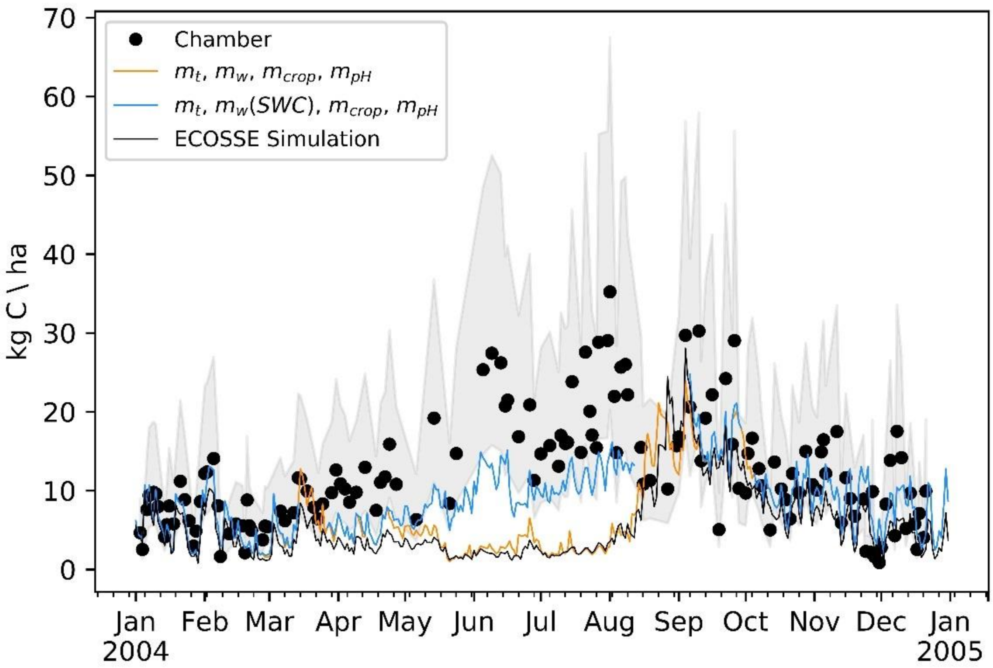


Figure 5.6: ECOSSE modifiers (mt, mw, mcrop, mpH) applied to both model simulated available water (yellow line) and using measured SWC (blue line). Soil chamber measurements partitioned at 47% are also plotted (black dots), along with the ECOSSE model simulated values (solid black line). Grey shaded areas show potential chamber partitioning ranges from 27-90%.

5.3.5 *Weather*

As the water component of the model is shown to be deficient, it was necessary to investigate the factors which influence this. As changes to the soil and water model parameters did not significantly alter model outputs (Sections 4.4.3 and 4.4.4), adjustments to the input data which affect the water modifier (rainfall and evaporation) were performed to investigate their influence on the simulated fluxes. To keep these weather measurements realistic, adjustments were made based on precipitation figures from nearby stations (discussed in Section 4.3.2), where gaps in initial Oak Park meteorology (original) were infilled with nearest neighbours (Carlow NN rain), from the flux tower (flux rain), using data from nearby Kilkenny as rainfall and PE inputs (Kilkenny PE and rain), using only Kilkenny PE and original rain from Oak Park (Kilkenny PE) and using actual evaporation calculated from the latent heat flux measured at the flux tower and converted to mm (Flux Tower ET_a). Results are similar for all methods except for the flux tower ET_a, which is significantly lower than values calculated by the model as the flux tower measurement gives actual evapotranspiration rather than potential evapotranspiration (Figure 5.7).

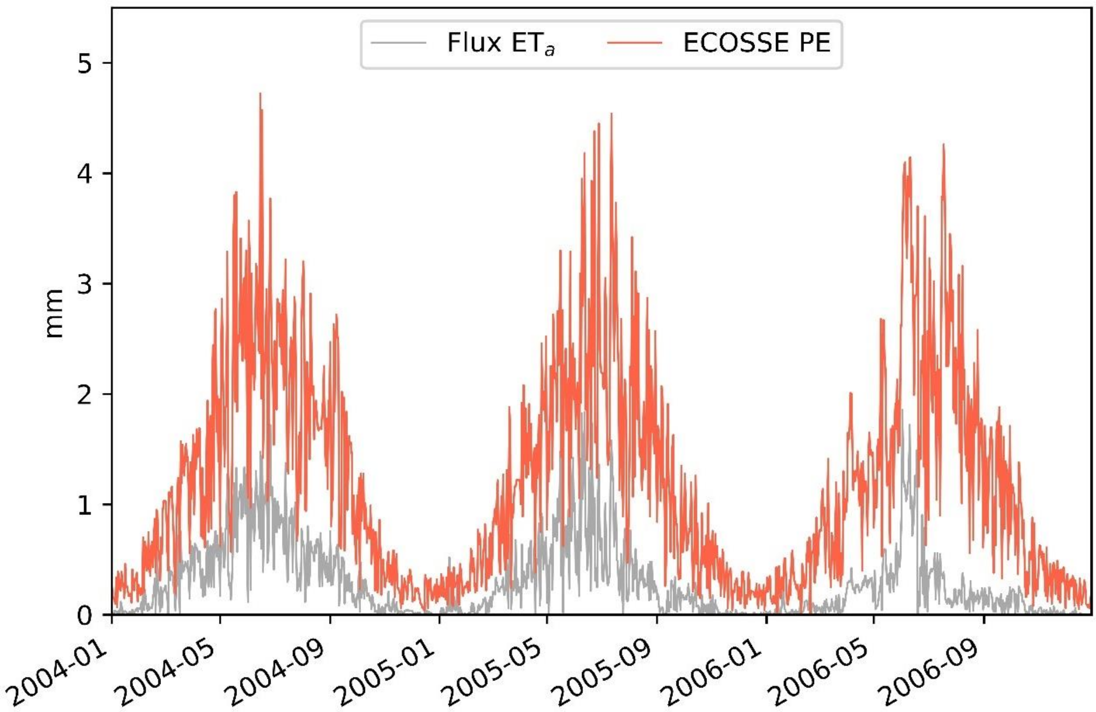


Figure 5.7: Potential Evapotranspiration (PE) calculated using the Penman-Monteith method compared to actual evaporation recorded at the flux tower showing the significant difference between actual and potential evaporation

Using actual evaporation derived from the flux tower measurements of latent heat (ET_a) the fluxes are very similar to Rh partitioned, albeit with peaks later in each year (Figure 5.8). Lower evaporation allows for the soil to stay moist and respiration is therefore uninhibited throughout the growing season, giving fluxes of a similar magnitude to Rh sums. All other weather adjustments altered the model outputs, but not significantly, indicating that adjustments to the evapotranspiration inputs to the model can improve model simulations, and that the larger difference between potential and actual evapotranspiration, particularly on well-drained soils such as this, may be introducing errors to the model.

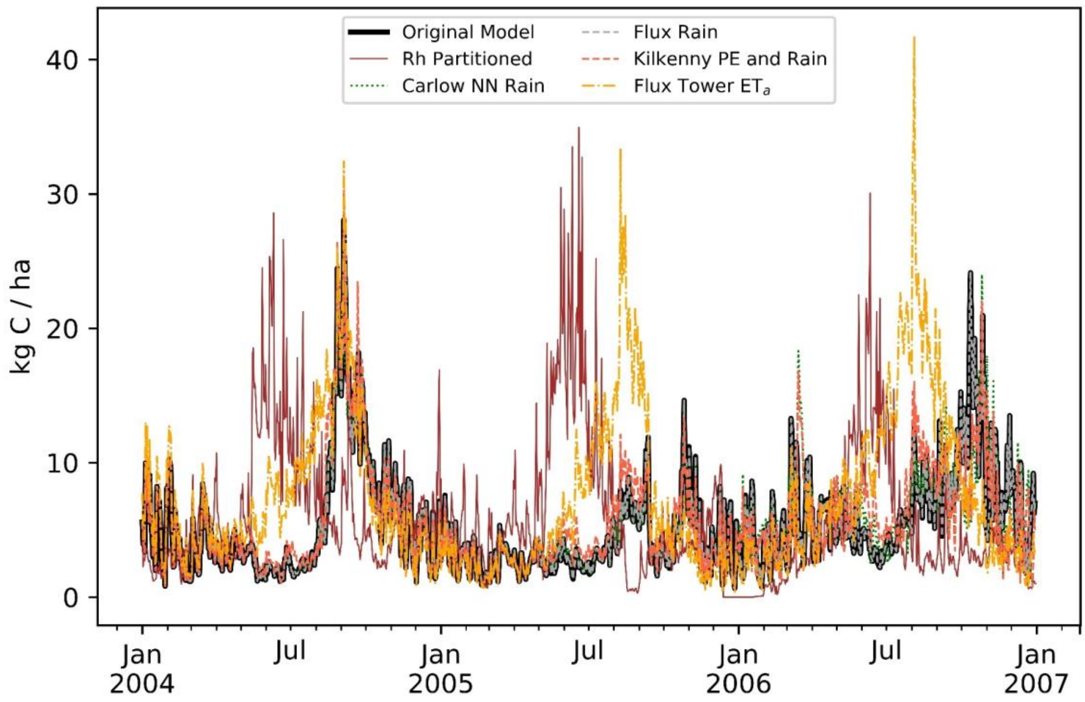


Figure 5.8: CO_2 model output using various instances of evaporation and rainfall data, including evaporation recorded at the flux tower

Comparison of the unchanged model run, the model run using observed SWC, and the model run using flux tower PE is shown in Figure 5.9, indicating that using actual evapotranspiration (recorded at the flux tower) has a similar effect on the CO_2 output of the model as using observed SWC, though the fluxes using evaporation are slightly lower. The use of potential evapotranspiration (particularly the FAO standard Penman-Monteith formulation) may be unsuitable for running the ECOSSE model on similar well-drained sites. The effect of using flux tower derived ET_a produces results consistent with using SWC observed at the flux tower, with a reduced suppression of fluxes during the growing season. This indicates that there are issues with the model simulation of water as respiration is unnecessarily inhibited compared to observations, and the water inputs to the model as PE causes excessive evaporation compared to ET_a. When examined cumulatively, the fluxes using ET_a from the flux tower are above the cumulative fluxes of partitioned Rh during 2004 and 2006, and are below in 2005 (Figure 5.10).

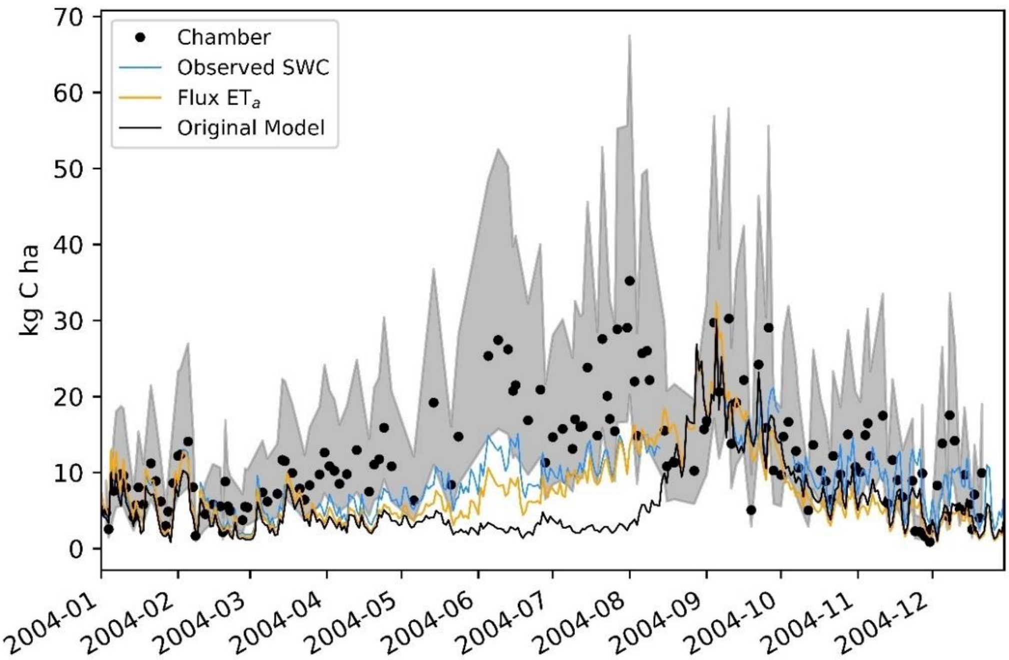


Figure 5.9: Comparison of model runs using default ECOSSE parameters (black line), observed SWC (blue line), flux tower evapotranspiration (yellow line) shown with chamber data partitioned at 47% and ranges from 27-90% for context.

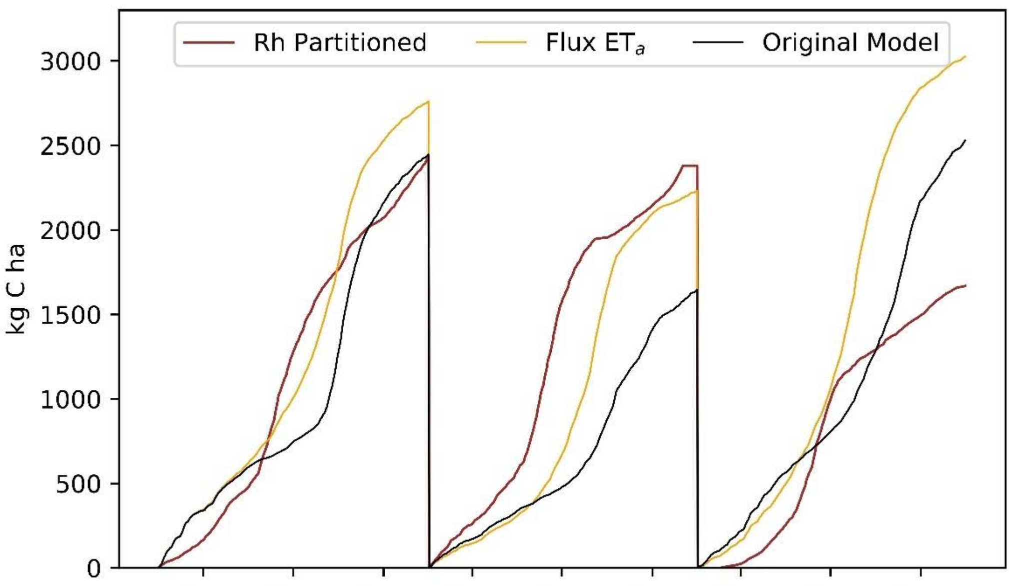


Figure 5.10: Comparison of cumulative fluxes using potential evapotranspiration (Original Model) and actual evapotranspiration (Flux ET$_a$) and derived measurements (Rh Partitioned)

These results show that the simulation of water by the ECOSSE model is not accurately representing soil moisture as evidenced by using observed soil water content instead of model simulated water. Further issues with how the ECOSSE model treats moisture are highlighted by the subsequent investigation of the PE model input, which shows that the use of actual rather than potential evapotranspiration significantly alters the respiration output of the model, having a similar effect to using observed soil water content in the model (Figure 5.9).

5.4 Conclusion

The development and application of models has a key role to play in improving our understanding of soil carbon science but also in informing and supporting future decisions on appropriate LULCC management options. However, prior to their use in decision making, models need to be thoroughly evaluated. The ECOSSE model has previously been widely applied on mineral soils, principally for grassland systems. The current study evaluated the model under an arable system on a free draining soil and found it was deficient in simulating available water. Investigating the modifiers applied by the model to input data indicates that the simulation of soil water in site-specific mode provides an inaccurate representation of SWC when compared to estimates of SWC derived from measurements, and in turn significantly impacts the simulation of soil respiration relative to soil chamber measurements. This may be because tillage systems (particularly on free-drained sandy soils) are highly dynamic.

The use of observed SWC data as input to the water modifier equation clearly illustrates that excessive drainage of water in the model is suppressing CO_2 fluxes from the soil, a trend not replicated in the observations. Model performance is significantly improved when using observed SWC data in the water modifier equation, showing a much higher correlation with chamber measurements than the ECOSSE modelled respiration (r^2 of 0.775 vs 0.154). This shows that the modifier is functioning correctly, and that the issue stems from the simulation of water through the soil layers, as soils dry out more than in reality. This excessive drainage cannot be counteracted by adjusting relevant model parameters indicating a revision of the ECOSSE water component is needed for this model to perform optimally for arable systems on mineral soils. While using ECOSSE for the estimation of soil organic carbon sequestration from cropping systems may prove to be robust as this is often observed on a decadal scale based on cumulative annual fluxes, these findings have implications for the simulation of greenhouse gas emissions (particularly CO_2 respiration and N_2O emissions) for mineral soil-based crop systems.

Similarly, Figure 5.9 shows the changes in simulated Rh resulting from changes in weather parameters, the most notable change occurs when actual evaporation is used rather than PE, it appears the soil stays wetter and allows for respiration to proceed uninhibited by drought. Even when using actual evaporation, an apparent offset between modelled and measured data persists, and chamber measurements are still out of sync with ECOSSE modelled Rh, though magnitudes of fluxes in each year are similar.

Zimmerman *et al.* (2018) assess the usefulness of the ECOSSE and other models at simulating N_2O fluxes from Irish grassland and arable sites, and not only do they find the model to be less useful than previously thought, the authors were also unable to replicate results from previous studies (Khalil *et al.*, 2013; Khalil *et al.*, 2016), a similar finding to the present research. A potential source of uncertainty outlined by Zimmermann *et al.* (2018) is the simulation of variables such as soil water content, a finding echoed by Bell *et al.* (2011) and the present research. Unfortunately, as parameters are often estimated using pedotransfer functions developed in different climate and land systems than the one being modelled, the functions may introduce uncertainty into results that cannot be assessed due to lack of in-situ hydrological measurements. In the case of this study SWC values were recorded on site and the model's ability to simulate SWC for this soil type was found to be deficient. The ECOSSE model is observed by Zimmermann *et al.* (2018) to perform well on grasslands but strongly overestimated N fluxes on arable sites, while this study shows the model underrepresents C fluxes at the site evaluated. Overestimation on arable sites could be attributed to the timing of management events and their interactions with temperature and moisture, though this could not be directly attributed by Zimmerman *et al.* (2018) due to the complexity of model simulation processes.

To generalize the results; 2004 represented a year in which the observed and modelled soil water displayed the greatest divergence, hence the effects on soil respiration are also likely to be greatest. While 2004 may represent an 'anomalous' model year in terms of simulated water, such events provide an opportunity to investigate model response more fully. To what degree are the findings specific to the year and the case study location? At least two other studies have highlighted a similar model deficiency in soil water content (Bell *et al.*, 2011; Zimmermann *et al.*, 2018). If these models are to provide useful guidance to inform mitigation strategies of future soil emissions, then they need to demonstrate a robust response to a broad range of meteorological conditions that could arise from changes in the climate system. A comprehensive framework for model evaluations is ultimately required; identifying a global network of sites with the requisite model input and evaluation data facilitating a more comprehensive inter-comparison of models. The identification of outlier events, such as 2004, for use in evaluations would also provide a focus to where greater research effort could be directed. The ultimate aim of which is to demonstrate the utility of these models and provide confidence in their use for informing policy.

Luo *et al.* (2016b) outline a standard of best practice to reduce biases in soil C modelling such that: 1. Model structures reflect real-world processes, 2. Parameters should be calibrated to match model outputs with observations from both pool and flux-based datasets and 3. External forcing conditions should accurately prescribe the environmental conditions that soils experience. In addition to calling for improvement of the underlying microbial processes that affect soil C decomposition, the use of observations to parameterise models is also highlighted as a key step to reduce biases in projections. Similarly, Tian *et al* (2015) recommend 1. Improvements to estimation and partitioning of NPP, 2. Incorporation of nutrient limitation, 3. Improve representation of litter composition, decay and N mineralisation by comparing model outputs to observations, 4. Inclusion of wetlands/peatlands and their traits, 5. Inclusion of lateral and vertical heterogeneities of SOC when extrapolating from small to large scale, 6. Inclusion of soil thickness so models can represent deep soil C dynamics at high latitudes, 7. Modelled SOC outputs should be compared to raw data instead of interpolated fields which are also modelled estimates. Experiments which combine temperature and precipitation interactions are recommended in order to investigate the importance of their combined interaction on soil C under future climate change (Wu *et al.*, 2011), similarly Suseela *et al.* (2012) find complex responses between temperature and precipitation. Lugato *et al.* (2014) suggest that the most promising solution to the drawbacks of modelling are tier 3 approaches using sub-national data to calibrate and validate SOC models, ideally process based models which can be perturbed to assess alternative scenarios such as extremes or changes in land management. Jackson *et al*. (2017) foresee decades of research ahead in experiments, synthesis and modelling of SOM.

While ECOSSE was found to underestimate emissions at the selected site, the model has previouslybeen evaluated on a range of soils and crop types, indicating that the model underestimation may be limited to well drained soils (shown in Figure 5.1) resulting from a larger difference between actual evapotranspiration and estimated potential evapotranspiration, though further studies comparing model outputs to observations are required to fully understand this. Zimmerman *et al.* (2018) find that ECOSSE outperforms other models at certain sites, suggesting that the model may provide useful estimates in regions where the simulated soil moisture is not limited. The model may therefore perform better on other sites, and as errors can be smoothed from moving from regional to global scale (Xu and Shang, 2016), similar error reduction may occur when moving from site to regional scale. Chapter 6 will therefore investigate the ability of a pre-release version of the

GlobalECCOSE model, a process-based model which functions spatially, to simulate carbon stocks and emissions of GHGs from Irish soils.

6 Estimating GHG Emissions from Irish Soils: Moving from Site-Specific to GlobalECOSSE

This chapter introduces the GlobalECOSSE model, which is in development with the aim of providing regional/spatial simulations of soil carbon stocks and GHG emissions. The data used to drive the model are outlined, along with the daily and monthly observations, with details on how gaps in data were accounted for and corrected. Results of the model runs are initially presented for daily and monthly site data, and regional simulations of GHG emissions are presented for the island of Ireland, with a focus on the cropland and grassland regions of the country. These modelled emissions are then discussed in the context of other national emissions estimates and research.

6.1 Introduction

Xu and Shang (2016) argue that errors in model simulations can be reduced when moving from regional to global scales due to reductions in noise and time-lag effects, suggesting that similar upscaling from site-specific to regional scale may smooth errors produced from attempting to replicate the intricacies at site scale. Zhou *et al.* (2018) recommended that future SOC assessments take place at grid/regional rather than global scales, to incorporate more region-specific factors and uncertainties. de Vries *et al.* (1998) investigate the influence of scale on soil acidification models and find that model simplification is an adequate step in upscaling results from local to regional scale. Peters *et al*. (2010) recommend a combination of top-down and bottom up methods which complement one another to get a fuller picture of soil carbon processes. It has been suggested that the most promising solutions to the drawbacks of GHG modelling are tier 3 approaches which use sub-national data to calibrate and validate SOC models, ideally process based models which can be perturbed to assess alternative scenarios such as climate extremes or changes in land management (Lugato *et al.*, 2014). For these reasons as well as the recommendation by Smith *et al.* (2015) that research should focus on the current state of knowledge and use this knowledge to make decisions, instead of focusing on what we do not know, this chapter will assess the ability of the ECOSSE model to scale from site to regional level to produce national spatial and temporal model outputs of soil GHG emissions, something which has never been attempted for Ireland before. This work is undertaken while recognising the findings of the previous chapter which highlighted issues with the simulation of water by the ECOSSE model. The results from modelling studies are useful even if the model itself may not reflect the full complexities of the soil system (Smith *et al.*, 2015), for this reason the uncertainties associated with measurement and modelling are outlined explicitly in this thesis, and the shortcomings of the results are highlighted, so that this study can at the very least provide a basis on which to build better models or to better parameterise models to improve results in future. It is also intended to provide a basis to examine where the application of such models may be useful.

6.1.1 *Context*

Agriculture is responsible for ~33% of Ireland's total national GHG emissions, significantly higher than the EU average of 9% (Kiely *et al.*, 2017). This is due to Ireland's large agriculture sector which employs 167,500 people, with Irish food and drink exports valued at €12.7 bn in 2017 (Teagasc, 2017). The implementation of an agricultural expansion strategy called 'Food Harvest 2020' has resulted in estimates of Ireland's projected agricultural emissions to be revised upwards by 4% by 2020 and 7% by 2030, if existing measures are left unchanged, meaning Ireland will overshoot our 2030 climate change targets by in excess of 50 Mt CO_2eq, and face significant fines (EPA, 2018b). Emissions reporting for agricultural land in Ireland is split into different categories, with N_2O emissions from agricultural soils listed under agriculture, and other GHG emissions from cropland, grassland and wetlands listed under land-use, land-use change and forestry (LULUCF) (Duffy *et al.*, 2018). Emissions from Irish agricultural soils were estimated using the IPCC accounting methods as 5598.85 kt CO_2eq in 2016, an increase of 1.4% from the previous year (EPA, 2018a).

The latest report on emissions from agricultural soils in Ireland (Duffy *et al.*, 2018) splits the sector into cropland and grassland and uses the Land Parcel Information System (LPIS) data to designate each area. The ratio between Irish agricultural land and the total area of land in the country is the highest in the EU-27 at 71.5% of the entire territory (Eurostat, 2018). Grassland is the dominant land-use category in Ireland, with the area of natural grassland currently around four million hectares (Teagasc, 2018). The area of cropland in Ireland has been in steady decline since the 1850s, with temporary increases during the world wars in the 20th century. Cropland area has fallen from 1,400,000 ha at its peak in the 1850s to under 400,000 ha in 2016. The definition of cropland has broadened since previous reports and is now defined as 'those lands which have been cultivated in the reporting year, and those lands which are under temporary grassland, but have been recorded as having been also used to cultivate a crop at some time since 2000', with no distinction given to crop types as it is assumed that the main factor in influencing changes in soil C stocks is the period under grassland, and conventional tillage practices (Duffy *et al.*, 2018, pp. 241).

Soil carbon emissions in Ireland are currently calculated in a top-down manner based on SOC stock, with the SOC content in Irish soils determined from the soil type, and the default reference carbon stocks for cold, temperate moist regions from the IPCC good practice guidance on LULUCF, Table 2.3, Chapter 5, Volume 4 (IPCC, 2006). The basic data source for soil type information is the Indicative Soils Map of Ireland (Fealy and Green, 2009), with plans to incorporate the Irish Soil Information System in future. Mineral soils are allocated to the categories of High Activity Clay (HAC), Low Activity Clay (LAC), sandy and humic classes, and peat soils allocated to IPCC wetlands class based on assessment of soil C stocks in Ireland by Tomlinson (2005). Around 98% of cropland soils are associated with LAC soils, with under 2% for HAC and <1% for peat soils (likely temporary grassland). For agricultural land on organic soils, default emission factors of 0.25 t C ha^{-1} yr^{-1} for managed grassland soils and 1 t C ha^{-1} yr^{-1} for cropland are used for cold temperate climatic regions, however it is assumed that no cultivation occurs on Irish organic soils (Duffy *et al.*, 2018). Table 6.1 outlines the proportions of soils in each category and their associated SOC contents calculated using the IPCC tier 1 approach to reporting GHG emissions.

Table 6.1: Soil Class Coverage and SOC content for Irish soil types (adapted from Duffy et al. 2018).

GSM Soil Association	IPCC Soil Class					Proportion of soil association area in Ireland
	HAC	LAC	Sandy	Peaty/Humic	Wetlands	
Basin Peat					0.34	0.06
Brown Earth		0.19				0.13
Brown Podzolic		0.21				0.15
Gley		0.30			0.02	0.22
Gley Brown Podzolic		0.30				0.21
Lithosol			1.00	0.22		0.04
Lowland Blanket Peat					0.31	0.05
Podzol				0.78		0.08
Renzinas	1.00					0.01
Upland Blanket Peat					0.33	0.06
Proportion of IPCC Soil class in Area of Ireland	0.01	0.71	0.01	0.10	0.17	
SOC_{ref} (t C/ha)	95	85	71	115	NA	

Irish emissions are calculated based on activity data and country specific emission factors, under the Tier-1 methodology cropland remaining cropland and grassland remaining grassland are assumed to have zero net emissions where land-management practices are well established (Duffy *et al.*, 2018). In 2016 (latest available year) Irish cropland is therefore estimated to be a sink of -131.93 kt CO_2eq with an uncertainty of ± 72.15 kt CO_2eq, highlighting the significant issues with tier 1 simulations. Uncertainties in estimating cropland emissions are highlighted by Duffy *et al.* (2018) who recalculate emissions based on refining the LPIS data and find a reduction in emissions of 77% from 1990 to 2015, cropland is a source of emissions during some years, and a sink in others. This fluctuation occurs as carbon uptake is higher when croplands are designated as temporary grasslands, and lower when under tillage.

Grassland is the dominant land-use category in Ireland, and though the IPCC (2006) guidelines assume that grassland remaining grassland has zero change in biomass C stocks, the soil C stocks use the same designations as Table 6.1 above, where C quantity is established using default reference SOC stocks. Essentially grassland remaining grassland is assumed to be a carbon sink, or at least "not a source" of emissions (Duffy *et al.*, 2018). The main change to grasslands which results in a decrease in soil carbon and the release of GHGs are C and CH_4 losses resulting from draining organic soils, and the conversion of grassland not in use to rough grazing. Grassland as a whole is estimated to be a source of 6889.15 kt CO_2eq in 2016 with uncertainty of ± 90.83 kt CO_2eq (Duffy *et al.*, 2018), though much of this comes from drainage of organic grassland soils. Natural unmanaged wetlands and peatlands are estimated to be sources of 2061.28 kt CO_2eq with uncertainty of ± 101.45 kt CO_2eq (*ibid*).

6.1.2 *GlobalECOSSE*

Spatial simulations using ECOSSE have been undertaken in the past (Richards *et al.*, 2016; Dondini *et al.*, 2016) using the 'limited data' mode of the ECOSSE model. GlobalECOSSE is a new spatial version of the ECOSSE model which is currently undergoing evaluation and has not been fully released to the modelling community. The model allows for the 'limited data' mode of the ECOSSE model to be employed at multiple locations using input data derived from spatial datasets, and collates the results of model runs producing outputs for regions, countries or continents. The following analysis serves as a further part of the ECOSSE evaluation procedure, parallel to the analysis of the site-specific model. As GlobalECOSSE is a regional model it runs at a different temporal and spatial resolution in contrast to the site-specific version, ingesting monthly spatial data to produce monthly outputs for specified regions (in this case Ireland). GlobalECOSSE also has the advantage that it simulates outputs for multiple GHGs and therefore could facilitate the calculation of total GHG fluxes. The model has not been evaluated elsewhere, this thesis serves as the first test of the model to simulate GHG emissions.

The move from site-specific to national scale requires less, and lower resolution, input data in order to simulate fluxes. In the initial study (previous chapters) the model is parameterised using daily temperature, precipitation and potential evapotranspiration, along with site-specific soil and management data with information on crop type, sow date, fertilizer application etc., whereas the regional model uses gridded temperature and precipitation data to calculate PE using the Thornthwaite method (Thornthwaite, 1948), and utilises soil data from the Harmonised World Soil Database v2.0 (HWSD) to calculate soil C content. Management data are not inputted into the regional model, though it is possible to change the land-use type to assess the potential changes in GHGs to investigate. Land-use masks can also be created, and the model can run selectively at these locations. For instance the limited-data version of the model has been employed spatially in the past, the impact of introducing bioenergy crops (Richards *et al.*, 2016), short rotation forestry (Dondini *et al.*, 2016a; Dondini *et al.*, 2015), or the impact of a reduction in fertilizer use (Abdalla *et al.*, 2016). Xu and Shang (2016) recommend models be built on annual rather than monthly time-steps to reduce noise and time-lag effects, it is reasonable to assume that this reduction of noise would also happen in the move from daily to monthly models also.

It is recognised that process-based models do not satisfactorily simulate the seasonal patterns of greenhouse gas emissions, even in cases where the sum of seasonal emissions compares well to observations, thought to be due to the uneven spatial distribution of input variables as spatial data inputted into models is typically averaged over surfaces, meaning the model simulates an averaged pattern while observations are taken at a much smaller, specific area (Cai *et al.*, 2003). For this reason multiple studies report cumulative emissions when validating models by comparing to cumulative observations (Abdalla *et al.*, 2010; Abdalla *et al.*, 2011; Yamulki *et al.*, 2013). Cumulative fluxes can be calculated by summing the daily output of a model (Cai *et al.,* 2003), by summing the products of weekly mean flux and summing the number of days between samples (Deng *et al.*, 2010), or using interpolation (Hinton *et al.*, 2015) though different methods of interpolation can introduce uncertainty (Gana *et al.*, 2018).

Initially, the ability of the ECOSSE model to move from site to regional scale using different data requirements will be assessed, then emissions of different greenhouse gases and CO_2 equivalents for Ireland will be presented.

6.2 Data & Methods

6.2.1 *Chamber Data*

Two sets of chamber flux data for this area were available, one chamber for the year 2004 which is outlined in Section 4.3.4, and another from a nearby field (Site 2) where measurements were taken from the beginning of 2003 until mid-2005, and the crop type was the same (spring barley). The site is a well-drained sandy loam soil with bulk density between 1.36 and 1.5, pH of 6.8 to 7.3, and organic carbon content 1.6-1.9%, (16-19 g C kg). The data from a nearby site is included here to provide context for the other chamber data, to ensure measurements are on the same scale as one another. Observations were taken sporadically, but at least once a month within the time period for each site. In order to scale the data, the interpolate function from Python's pandas library (pandas.interpolate) was used to fill the gaps between the datapoints, a method which produced results analogous to using an average of the measurements in a month, multiplied by the days between measurements in that month.

As previously discussed, the potential contribution of Rh to Rs ranges from 3% to 99% in the literature across biomes, land-use types and seasons, and the values taken from temperate arable and grassland land-uses range from 27 to 90% (Subke *et al.*, 2006), highlighting the complexity and heterogeneity of the flux partitioning problem. Daily chamber flux partitioning is discussed in Section 4.3.4.1, where the chamber fluxes were partitioned using the average Rh contribution from a nearby study (Kumar Jogi, 2007), giving a fraction of 47%. Figure 6.1 presents the ranges of 27-90% as shaded areas behind the line graphs, and illustrate the 47% partitioning from the nearby field (Kumar Chamber), the ranges indicate a potential Rh of between 350 and 1500 kg C ha^{-1} for the month of July, illustrating the significance of the choice of partitioning option, and the associated uncertainties.

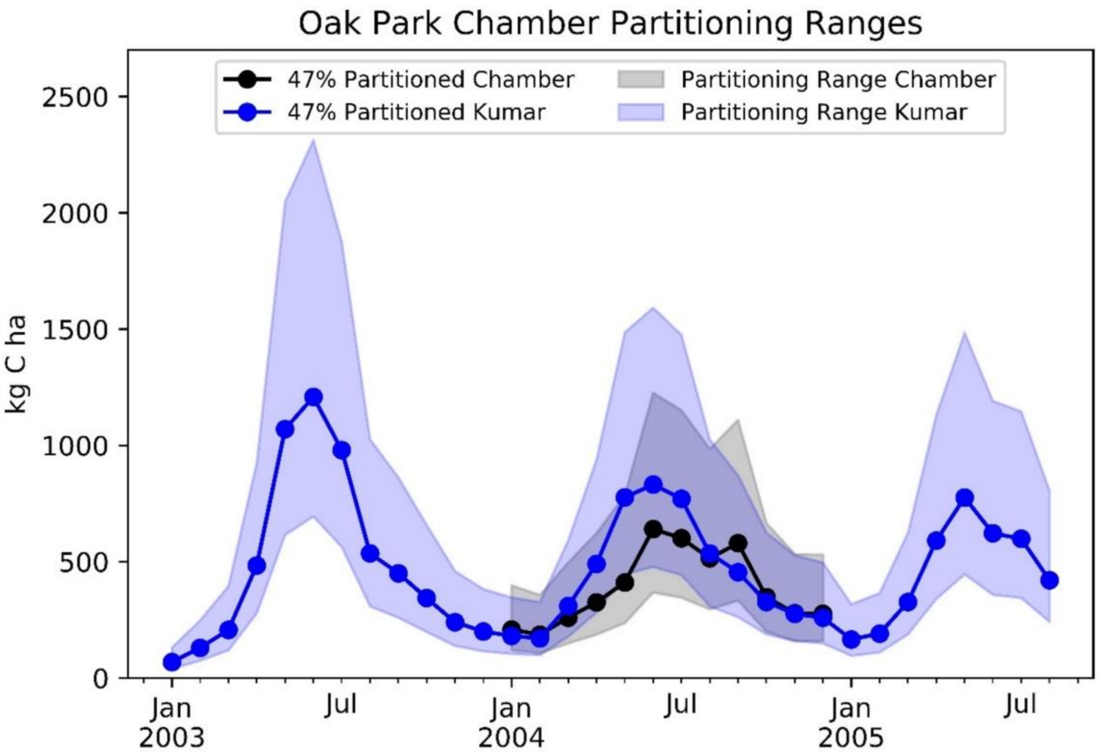


Figure 6.1: Oak Park Chamber (Chamber) and nearby chamber (Kumar Chamber) partitioning ranges from 27-90% (shaded areas) and chambers partitioned at 47% (black and blue lines) based on Kumar Jogi, 2007

6.2.2 *Flux Data*

The flux data partitioning is outlined fully in Section 4.3.3, to summarise; Reco was derived from NEE measured at the flux tower, and partitioned into Rh by running DNDC using the same site parameters and partitioning the data based on the DNDC fraction of heterotrophic respiration.

6.2.3 *Gridded Climate Surfaces*

EObs data was employed for the current analysis, it represents a European land-only daily high-resolution gridded dataset with data for precipitation and temperature from 1950-2006 (Haylock *et al.*, 2008), with the latest version (v17.0) providing updated data to December 2017 on a 0.25° regular grid. Daily data were transformed to monthly averages for temperature and monthly sums for precipitation using Climate Data Operators (CDO) commands in a Linux environment (CDO, 2018).

6.2.4 *HWSD Data*

The Harmonised World Soil Database (HWSD; FAO/IIASA/ISRIC/ISSCAS/JRC, 2012) combines the European Soil Database (ESDB), the 1:1 million soil map of China, regional SOTER studies (SOTWIS Database) and the Soil Map of the World in a global effort to harmonise the disparate collections of soil data that are available. The data are available at 30 arc second resolution (~1km grid scale), giving 21,600 rows and 43,200 columns of data covering 221 million grid cells over the Earth's land. From these grid cells 16,000 soil mapping units (MU_Globals) are all linked to harmonised attribute data in the form of a MS Access database containing information on organic carbon content, pH, water storage capacity, soil depth, cation exchange capacity, clay percentage, exchangeable nutrients, lime and gypsum content, sodium exchange percentage, salinity, textural class and granulometry (FAO/IIASA/ISRIC/ISSCAS/JRC, 2012).

6.2.5 *Land-Use Data*

The CORINE land-cover map was used to determine areas of grassland and cropland by merging the categories of *Non-Irrigated Land* and *Complex Cultivation Patterns* for cropland and *Pastures* and *Natural Grassland* for grassland using ArcGIS and creating raster and point shapefiles for each land-use, then linking these based on latitude and longitude to the MU Globals in the HWSD database (raster shapefiles shown in Figure 6.2). The arable shapefile covered 11.3% of total land area, while grassland made up 72% of total land area. These are then converted to csv files which restrict the model to running at those locations. Though there are issues with the CORINE land-cover dataset, particularly with the classification of sparse vegetation, it is estimated that agricultural classes have a high-level of reliability (EEA, 2006). Though these issues may result in some erroneous classifications, it is chosen here for its accuracy on agricultural land, and broad coverage and applicability to multiple countries.

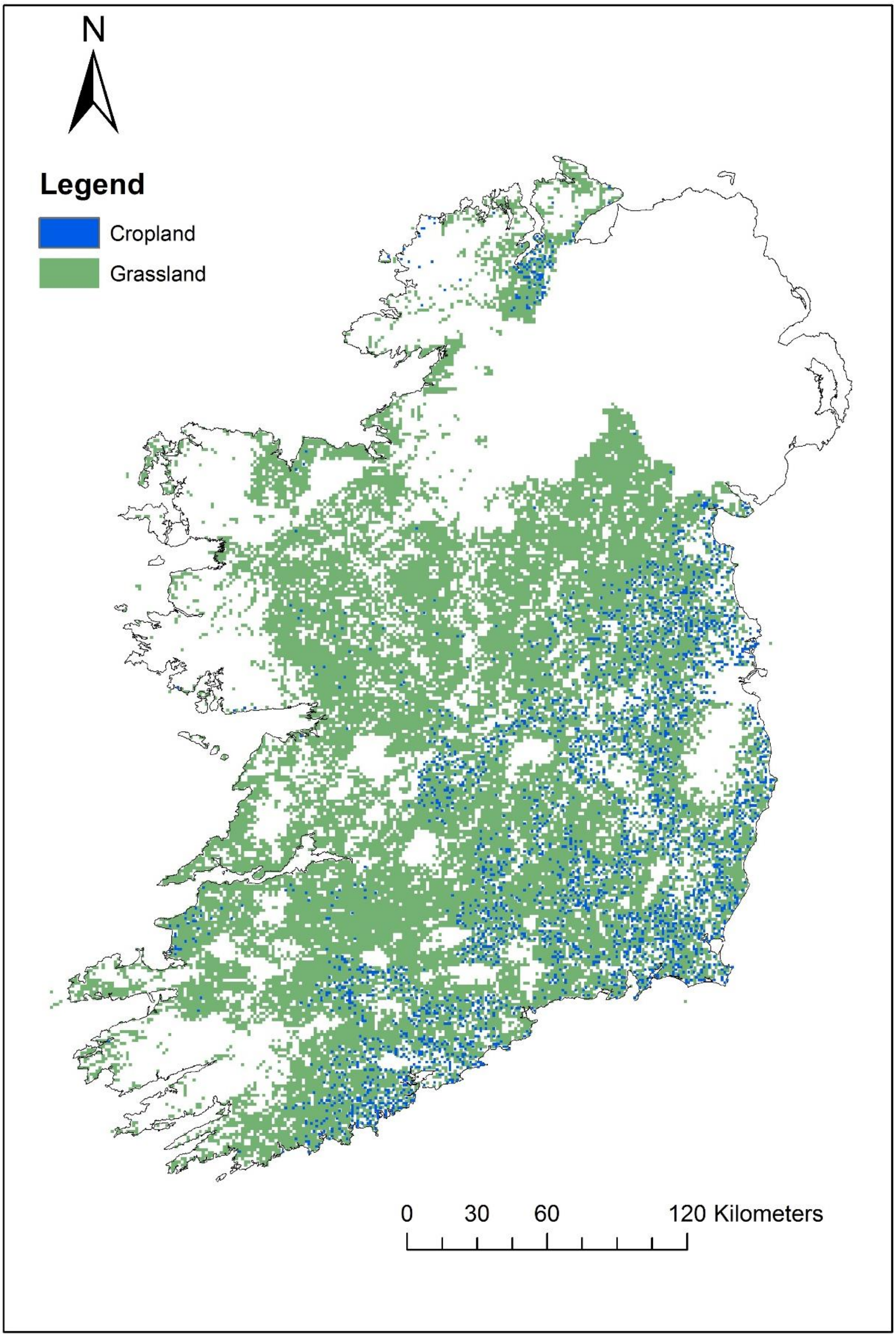


Figure 6.2: Irish Cropland (blue) and Grassland (green) locations from the CORINE land-cover dataset

The model can then determine which soil type is associated with each land-use and produce outputs for that land-use only. Plant inputs are determined from RothC.

6.2.6 *SoilR*

In order to evaluate the daily and monthly versions of the ECOSSE model and to investigate the model's ability to scale-up temporally, the SoilR package (Sierra *et al.*, 2012) developed for the R environment for statistical computing (R Development Core Team, 2011) was employed. The use of SoilR here is an attempt to provide an independent, albeit statistically based, assessment of the output from the ECOSSE model, and to investigate the scalability of results when moving from a daily to a monthly model. SoilR is a much simpler model than ECOSSE and allows for alterations to its modifiers and structure. SoilR includes the modifiers for the RothC model (hereafter SoilR RothC) along with a range of others, and allows for pool sizes and decomposition rates to be changed. SoilR was initialised using the climate and soil data for the Oak Park site, along with data on plant inputs to attempt to replicate ECOSSE. The SoilR RothC model is initialised with empty pools for DPM, RPM, BIO and HUM, with IOM calculated using the Falloon method (Falloon *et al.*, 1998), and run to equilibrium for 500 years until the pool sizes match the observations. This was an iterative process and depended strongly on the amount of plant inputs. Plant inputs were set to 5.0 t ha yr^{-1} for the model spin-up, resulting in pool sizes equivalent to those found using the pedotransfer method, and those measured in the field. These pools sizes are outlined in Table 6.2 and displayed in Figure 6.3 and sum to 42.376 t ha^{-1}, similar to the 42.888 t ha^{-1} measured at the site (Flattery *et al.*, 2018).

The SoilR package contains a function '*RothCModel*' which takes arguments for time, pool sizes, carbon inputs from plants, clay content, with a dataframe containing the temperature and water modifiers for each timestep, then calculates stocks for each pool per timestep, and the CO_2 released from each pool. The RothC decomposition rates employed by SoilR are equivalent to those employed by both ECOSSE and GlobalECOSSE.

Table 6.2: Pool sizes after the 500-year spin-up of the SoilR RothC model using annual inputs of 5 t C ha^{-1}

DPM	RPM	BIO	HUM	IOM
0.032	6.146	0.816	31.972	3.41

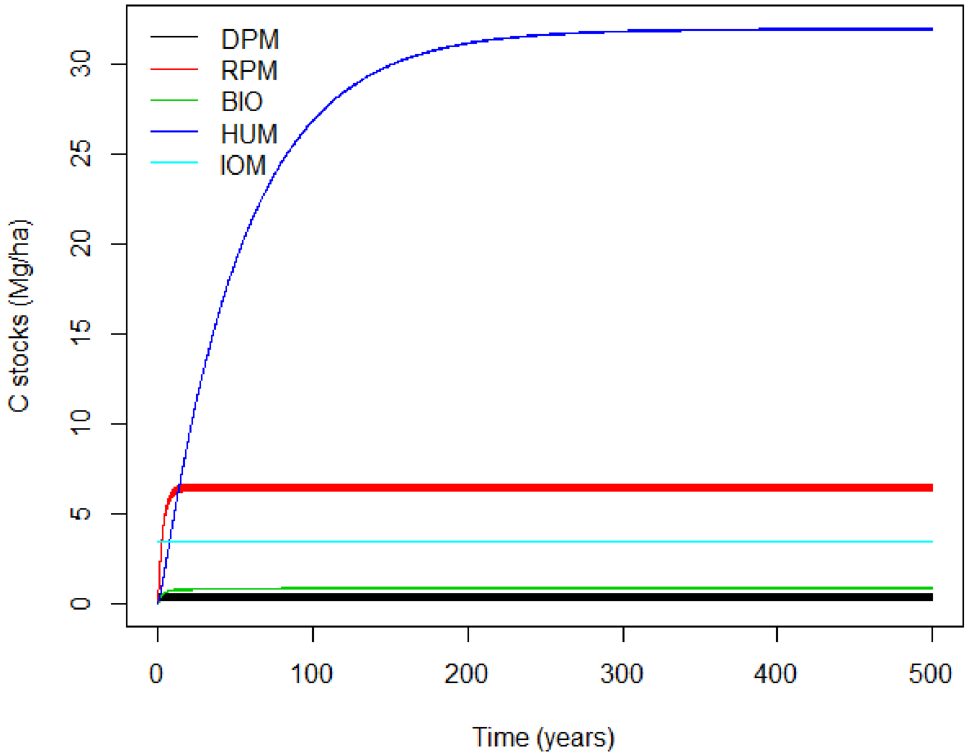


Figure 6.3: SoilR pool sizes over time after running the model for 500 years using annual inputs of 5 t C ha^{-1}

After the 500-year spin-up run the model was then initialised and run on a daily timestep using the RothC temperature modifier (equivalent to the ECOSSE temperature modifier) and the Daycent water modifier (other water modifiers produced significantly different results, as is outlined in Section 3.3.3). Figure 6.4 shows model outputs using different water modifiers, including European Space Agency (ESA) soil moisture, observed SWC, and water calculated using the SoilR RothC model. The Daycent2 water modifier using both ESA soil moisture and observed SWC produced identical output (the modifier does not dry out the soil). The RothC water modifier clearly has a more pronounced effect on the fluxes. Using a water modifier of 1 produces results with almost identical temporal signal to ESA and observed water, but the magnitude is slightly higher. This reinforces the findings of the previous chapter where the model's treatment of water is shown to significantly alter fluxes, and highlights the importance of the water modifier in soil models. For the purposes of this analysis observed water is used for comparison with observations, and the RothC modifier is used in an attempt to replicate the water modifier response in ECOSSE.

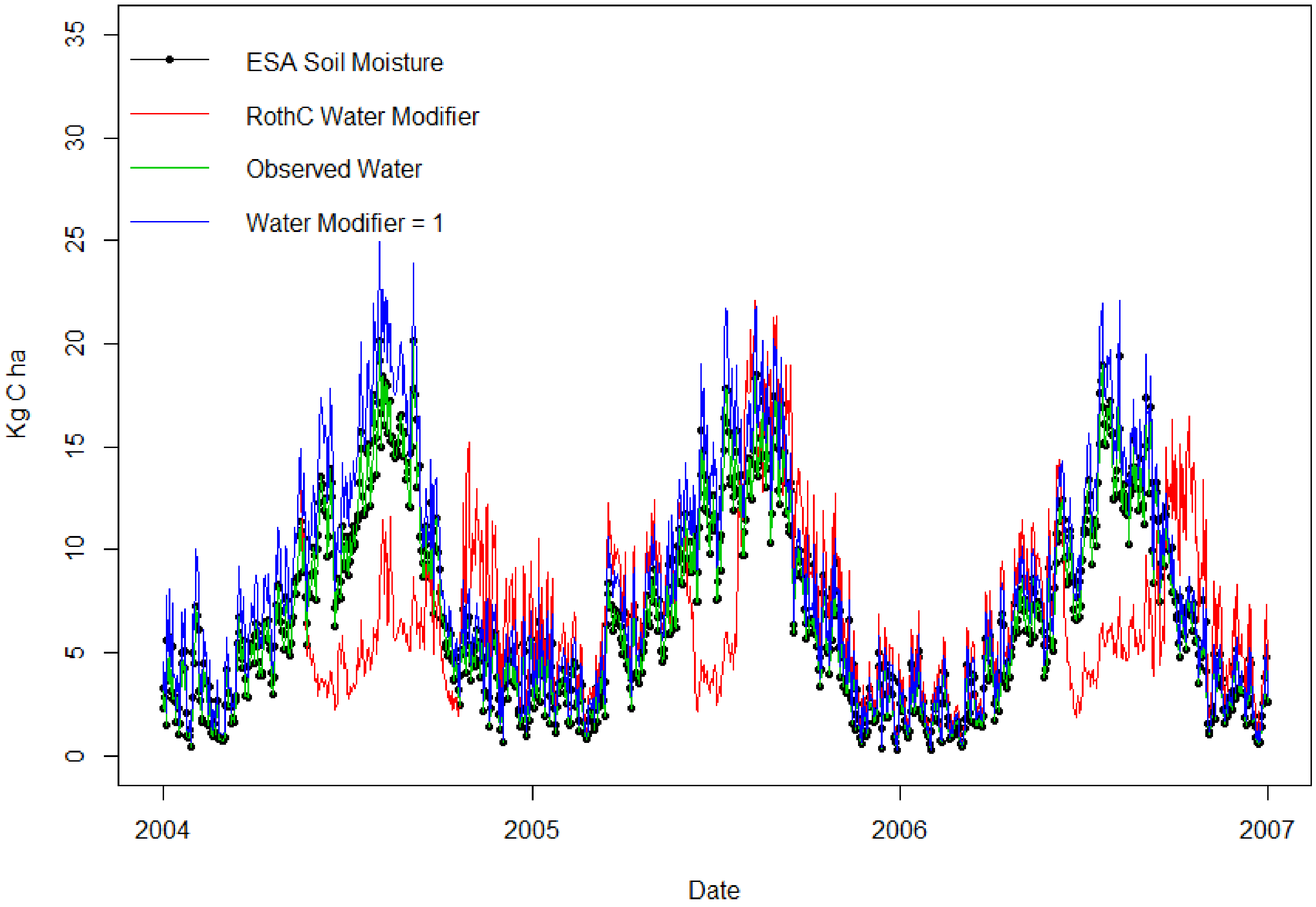


Figure 6.4: SoilR model outputs using ESA Soil Moisture data and the Daycent 2 water modifier (black dots), water simulated from weather data using the RothC modifier (RothC Water Modifier – red line), water observed at the flux tower and the Daycent2 water modifier (green line) and using a water modifier of 1 (blue line)

The model was then rerun, but on a monthly timestep. In order to produce simulations that replicate the ECOSSE model. For comparison, a crop modifier of 0.6 was applied to the SoilR output for the growing season months of March, April, May, June and July.

6.2.7 *Global ECOSSE*

Global ECOSSE facilitates the running of the ECOSSE model's limited data mode on a regional basis using gridded climate and soil data, and is currently in the pre-release stage of production. Climate data comes from the EObs dataset (Haylock *et al*., 2008) while soil characteristics are obtained from the Harmonised World Soil Database (HWSD, Wieder *et al*., 2014). The model allows for a specification of the period to use as the 'average' weather data (in this case 1971-2000), and a period for a 'future' run. It is also possible to create a land-use mask with which to run the model, which was created from the CORNIE dataset. In order to compare the model to observations the years 2001-2010 were chosen as outputs. The model generates simulation files based on the inputted temperature and precipitation data from EObs, and estimates PE based on the Thornthwaite method (Thornthwaite, 1948). The model generates simulation files which take soil data from the HWSD, where top and subsoil organic carbon percentage weight is converted to kg C ha^{-1} using information on bulk density. These simulation files point to files related to climate data (EObs in this case) where data are aggregated for each grid box on a monthly basis for each year, and an average for a specified period (e.g. 1970-2000). Where subsoil data is available, a new layer is created by the model to simulate soil carbon at depth. The model creates a number of input files based on lat/lon grid boxes, then uses these to run the ECOSSE model in limited data mode to obtain outputs for SOC, CO_2, NO_3 and N_2O. These outputs are then aggregated and written to NetCDF files.

To assess the ability of the GlobalECOSSE model to simulate soil C emissions, HWSD and EObs data for an areal/grid location proximate to the Oak Park site were initially used to run two different model executable files (model versions Agile and ELUM) and results were compared to observed Rh and chamber data in order to assess changes in outputs due to different input data. The ELUM model has been previously employed in the UK and has been parameterised for UK conditions, and was ultimately chosen for this analysis.

GlobalECOSSE model parameters are set according to the values listed in Table 6.3, where certain sub-models can be specified or switched on and off. The model creates simulation files for each latitude and longitude location based on the HWSD and EObs characteristics, and the Model_Switches.dat file specifies the particularities of the model run for each of these sites. This file must be set up initially in a master folder, and is then included for each lat/lon location for the multiple model runs, ensuring the model functions in the same way across all regions.

Table 6.3: Setup of the Model_Switches.dat file, this file outlines how the model runs for each lat/lon area specified by the Global ECOSSE model

2	Denitrification model chosen (Bradbury, 1 or NEMIS, 2)
0	Crop model type: 0=SUNDIAL, 1=MAGEC
2	Soil parameter model (from file, 1 or calc, 2)
1	Methane Model 0 = off 1 = on
2	DOC model 1 = off, 2 = on
0	N limitation spin-up used? 0 = No, 1 =Yes
0	Modify plant inputs according to full run using long term average weather data
0	Modify decomposition according to full run using long term average weather data
0	Choice of moisture rate modifier (0=ROTHC or 1=HADLEY)
0	Choice of temperature rate modifier (0=ROTHC or 1=HADLEY)
0	Use full equilibrium run of ECOSSE to initialise or not (0 = off, 1 = on)
2	Initialisation of N by assuming steady state (after Bradbury = 1) or initialisation of N by passing the C:N ratio of DPM and RPM (=2)
1	0 = pH set to neutral or passed from parameter file, 1 = pH is read in from input file and does not change, 2 = pH is calculated using VSD (a very simple dynamic version of the MAGIC model by Ed Rowe & Chris Evans, CEH, Bangor)
0	Output full 0 = false, 1 = true
1	Output summary 0 = false, 1 = true
1	Plant Input from input or estimated from Total Organic Carbon (PI input = 1, PI est from TOC = 2)

6.3 Results

6.3.1 *Evaluation of SoilR and ECOSSE Daily Simulations*

Figure 6.5 presents all observations and model outputs on a daily basis for the years where data exists, with the nearby chamber beginning in 2003 and ending in August 2005. The Oak Park chamber covers the entirety of 2004 with observations taken at a frequency of approximately once per week or higher. Both chambers have been partitioned at 47%. Partitioning fluxes by 47% results in outputs of a similar scale to Rh derived from eddy covariance data, and model outputs. The partitioning of 47% is the average Rh contribution from an experiment in a nearby field with the same crop, and is considered the optimum partitioning method amid significant uncertainty. Also presented is the output from the ECOSSE site-specific model using actual evaporation calculated from the latent heat flux measured at the flux tower (Section 5.3.5), and SoilR daily model output using the Daycent 2 water modifier. Though there is clear temporal variation across all variables, the magnitude of observations and model outputs is similar.

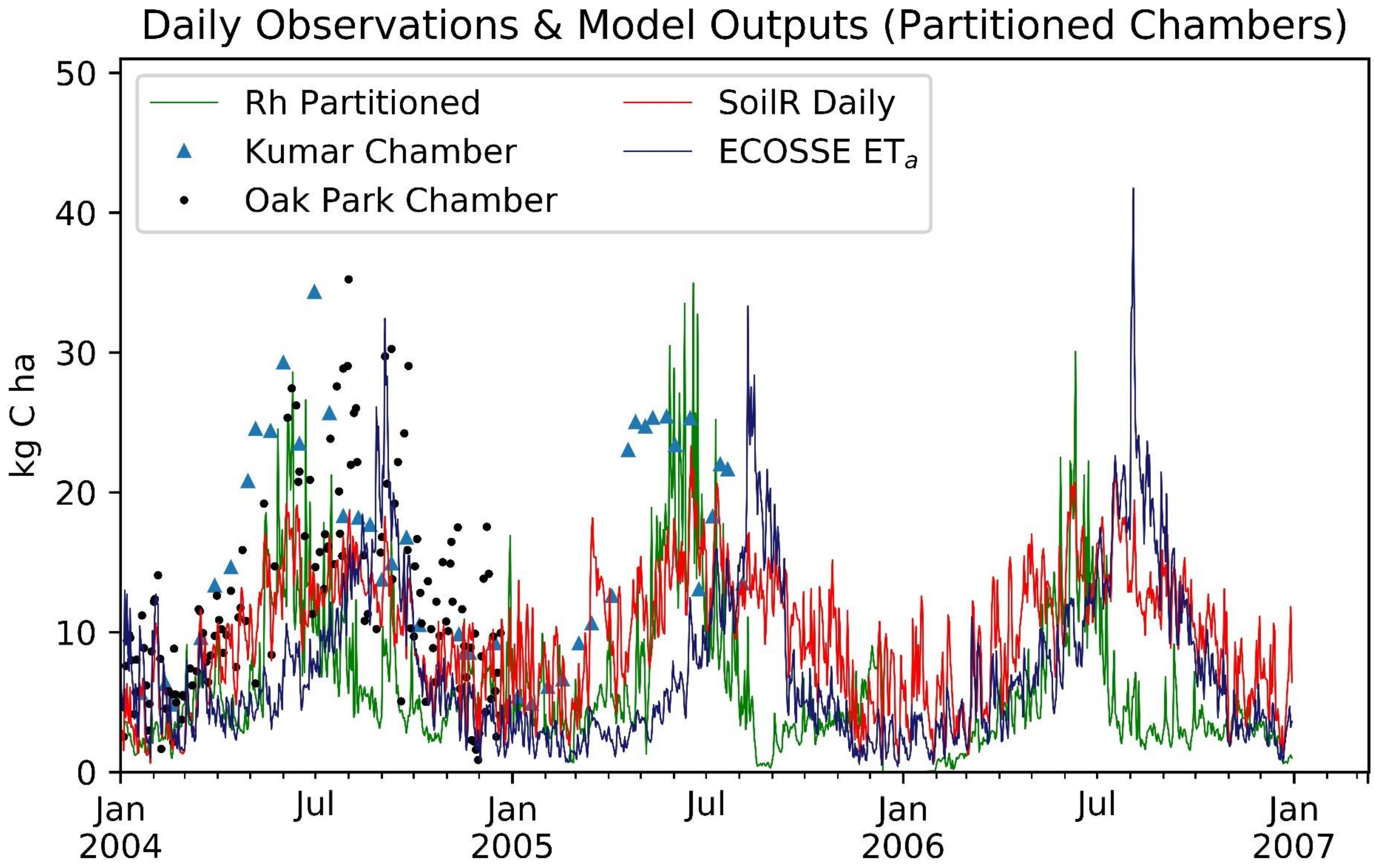


Figure 6.5: Daily observations and model outputs for Oak Park with chambers partitioned at 47%. SoilR uses the Daycent2 water modifier with observed SWC

6.3.2 *Replicating Daily ECOSSE using SoilR*

ECOSSE is a much more complex model than SoilR RothC, nevertheless the daily results are of a similar scale and magnitude to both the ECOSSE output and observations (Figure 6.6). This figure presents similar data to Figure 6.5, though the SoilR flux in this case uses the RothC temperature and water modifiers in an attempt to replicate ECOSSE output.

While both site-specific ECOSSE and SoilR RothC do not accurately replicate the timing of fluxes from the chamber or Rh, the much simpler SoilR RothC model using similar inputs underestimates fluxes compared to ECOSSE in 2004, overestimates in 2005, and is similar during 2006, likely due to less inhibition by the water modifier compared to ECOSSE. The Pearson's r value for ECOSSE and SoilR RothC for the entire period is r = 0.21. Comparing SoilR RothC to observations gives a correlation of r = 0.21 compared to the chamber, and r = 0.004 compared to Rh. Using a different water modifier (e.g. Daycent2) produces results which are less constrained by dry periods, and match more closely to chamber and Rh (Figure 6.7). Correlation values improve significantly using the Daycent2 water modifier, with r = 0.76 when compared to chamber, r = 0.34 compared to Rh, and r = 0.3 compared to ECOSSE. Both figures indicate that SoilR is reproducing ECOSSE model outputs on a similar scale, suggesting the outputs from the ECOSSE model are reasonable.

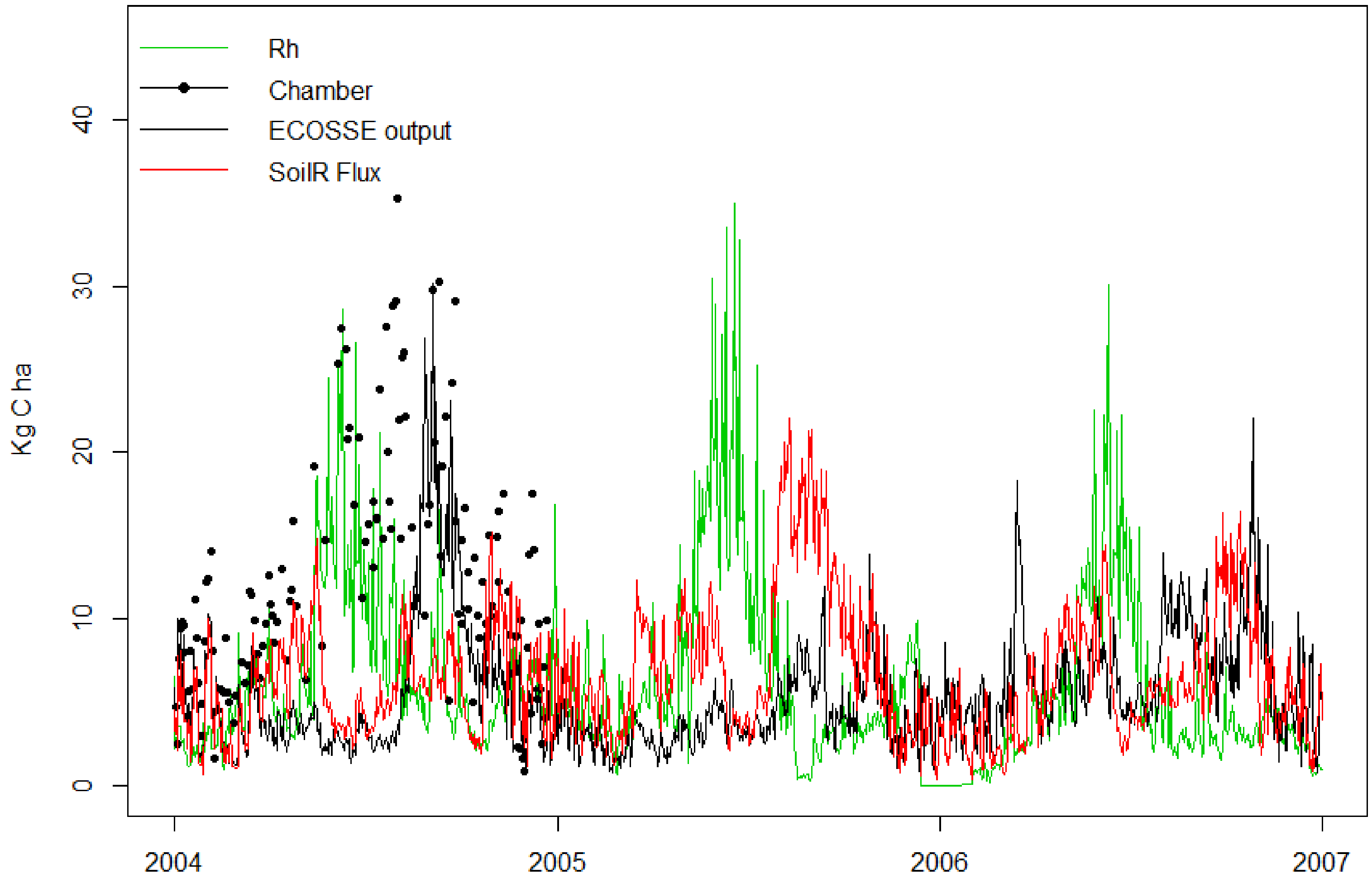


Figure 6.6: ECOSSE and SoilR outputs shown with observations for context –the chamber has been partitioned at 47%, SoilR uses RothC temperature and water modifiers, choice of water modifier can significantly affect the output.

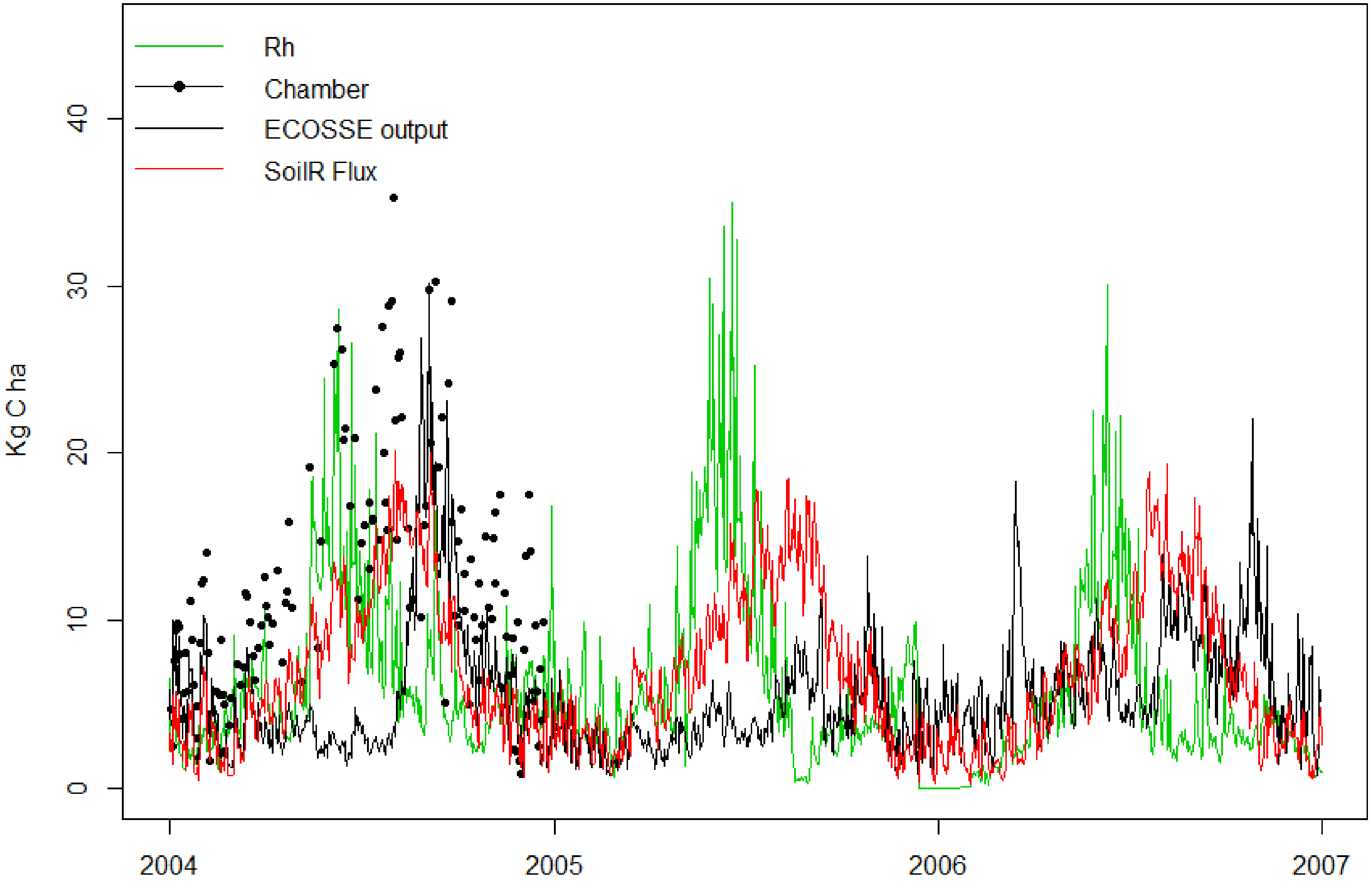


Figure 6.7: ECOSSE and SoilR outputs shown with observations for context –the chamber has been partitioned at 47%, SoilR uses RothC temperature modifier and the Daycent2 water modifier with observed SWC

To assess SoilR's ability to move from daily to monthly timestep the model was run daily, with values then summed monthly and the outputs compared to the monthly timestep run. The results indicated that the model is performing similarly on daily and monthly timesteps, meaning it is suitable for use in comparison to Global ECOSSE which runs on a monthly timestep.

6.3.3 *Evaluation of Global ECOSSE Simulations*

The outcome of running the model for a location proximate to the Oak Park site is presented in Figure 6.8. This figure illustrates the differences between the ELUM models when employed in site (daily) and regional (monthly) modes. Daily sums of the ECOSSE model and ELUM model are illustrated with dashed lines while the model run on a monthly basis is represented by a solid line. Differences are evident across all model runs on daily and monthly timesteps. Based on total sums the limited data model runs using EObs and HWSD data perform better in comparison to Rh than the outputs of the models using site data. Sums of the data show that ELUM sums to 6384 kg C ha^{-1} using EObs and HWSD data, close to the 6495 kg C ha^{-1} Rh sum, though it is clear the model is well below the values for both chambers, though some values are within the chamber range during the 2nd half of 2004.

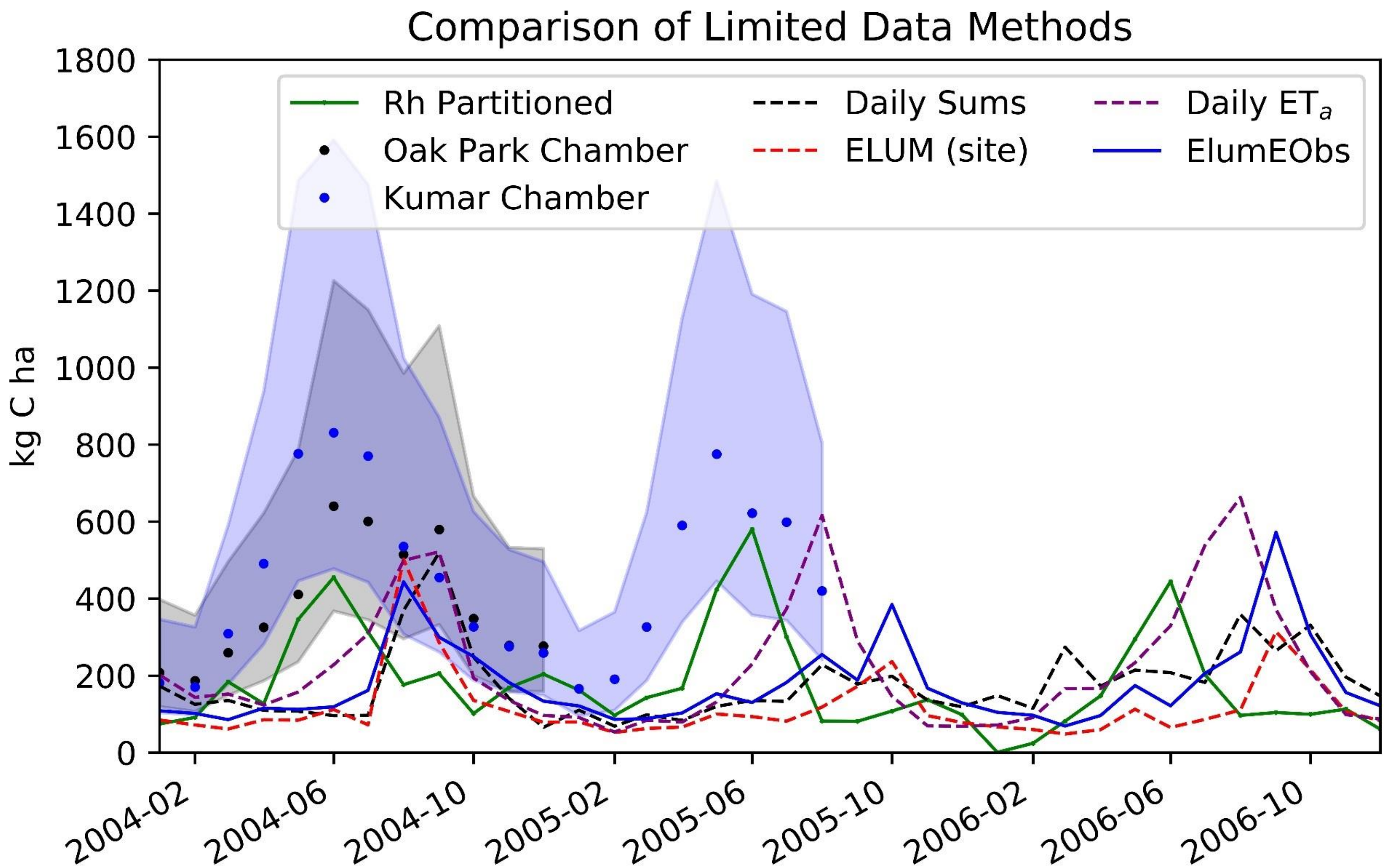


Figure 6.8: Comparison of limited data models using site data (Elum (site)), EObs and HWSD data (ElumEObs), observations (Rh partitioned using DNDC, Chamber partitioned at 47%), and daily ECOSSE site specific model using raw climate data summed monthly (Daily Sums)

6.3.4 *Evaluation of Monthly Simulations*

For all data to be comparable, the SoilR RothC model was parameterised using HWSD data approximate to the Oak Park field, while Global ECOSSE output is obtained by querying the gridded NetCDF file outputted by the model for the lat/lon coordinates of the Oak Park field. Figure 6.9 shows monthly observations (chambers, Reco, Rh) and model outputs (Global ECOSSE and SoilR) where chamber data has been partitioned by 47% and SoilR monthly output has had a multiplier of 0.6 applied for the growing season, in order to best replicate global ECOSSE. The SoilR model peaks higher than Global ECOSSE throughout most of the period, both follow a similar pattern as the water modifiers in RothC and Global ECOSSE are alike. While the models correspond reasonably well to Rh, there remain significant timing and magnitude issues between Global ECOSSE and the chamber data, with models being below the chamber ranges over the four-year period. The discrepancy between partitioned chambers and Rh makes interpretation of the suitability of a model difficult, as the temporal pattern may obscure the total fluxes.

6.3.5 *Cumulative Fluxes*

Figure 6.10 highlights the significant differences across models and observations when examined cumulatively. The figure illustrates annual sums of two SoilR RothC model outputs (one using the RothC water modifier, another using observed SWC, both using the DayCent2 water modifier), Daily ECOSSE output summed annually using actual (ECOSSE ET_a) and potential evaporation (ECOSSE ET_o), GlobalECOSSE output, and observations. Heterotrophic respiration (Rh partitioned) is derived from ecosystem respiration, which is itself derived from NEE, and is mostly below even the lowest partition range of the chambers, with the global ECOSSE model output lower still. In 2004 and 2005, Global ECOSSE is around half the magnitude of Rh, with similar results for Rh and Global ECOSSE in 2006. Daily ECOSSE summed on an annual basis is closer to Rh in both years, and is included here to illustrate the scale of the ECOSSE model in comparison to SoilR. Also included is ECOSSE ran in limited data mode using actual evaporation from the flux tower (Flux ET_a), which shows similar results to daily ECOSSE and Global ECOSSE. Partitioning ranges for chambers illustrate the significant uncertainty associated with the choice of partitioning method, as annual flux values can range from ~3000-12000 kg C ha^{-1}. Both SoilR models correspond more closely to chamber data than Global ECOSSE, yet are significantly higher than Rh.

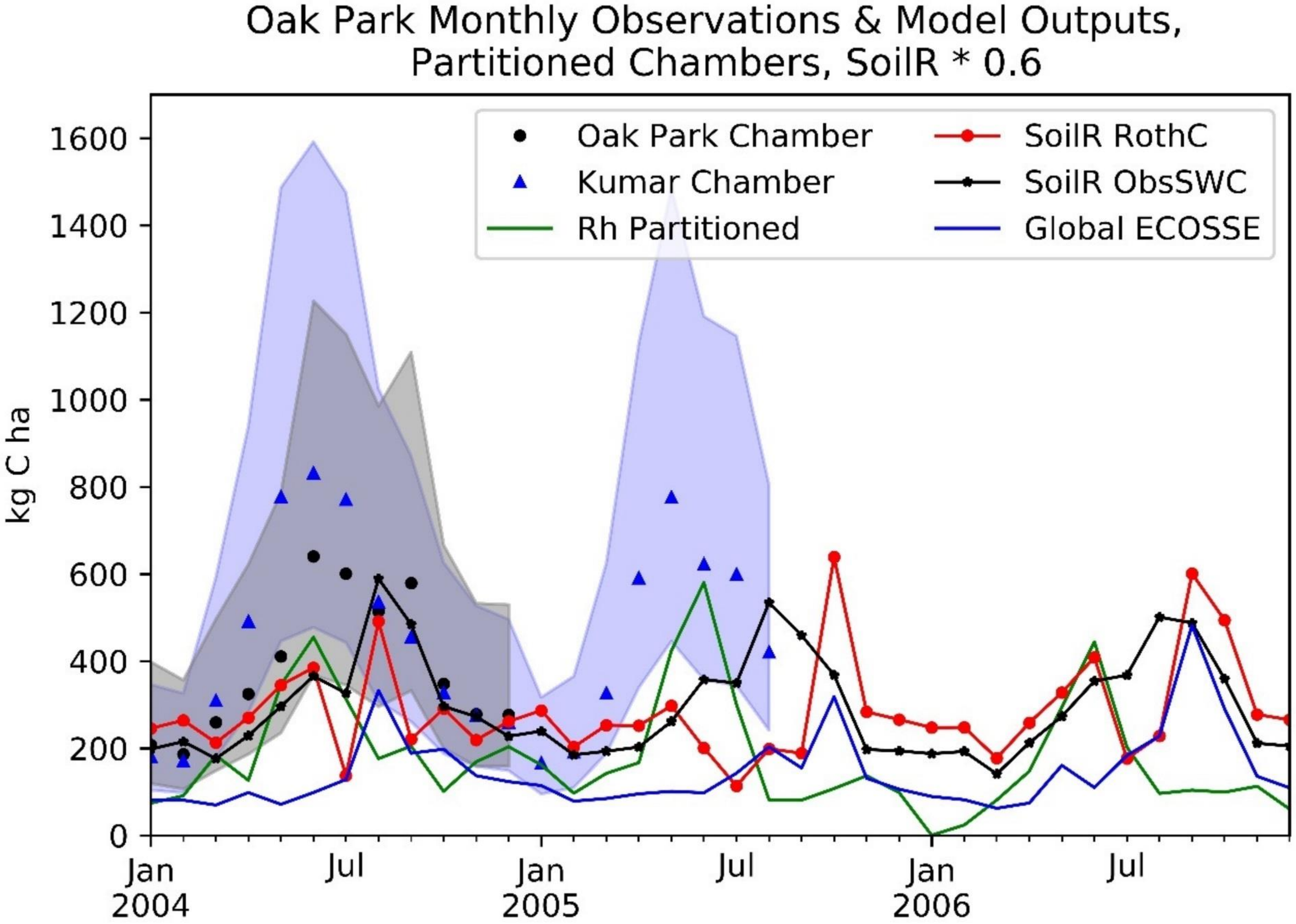


Figure 6.9: Monthly observations and model outputs, shaded areas are the 27-90% Rh partitioning ranges for the nearby and site-based chambers

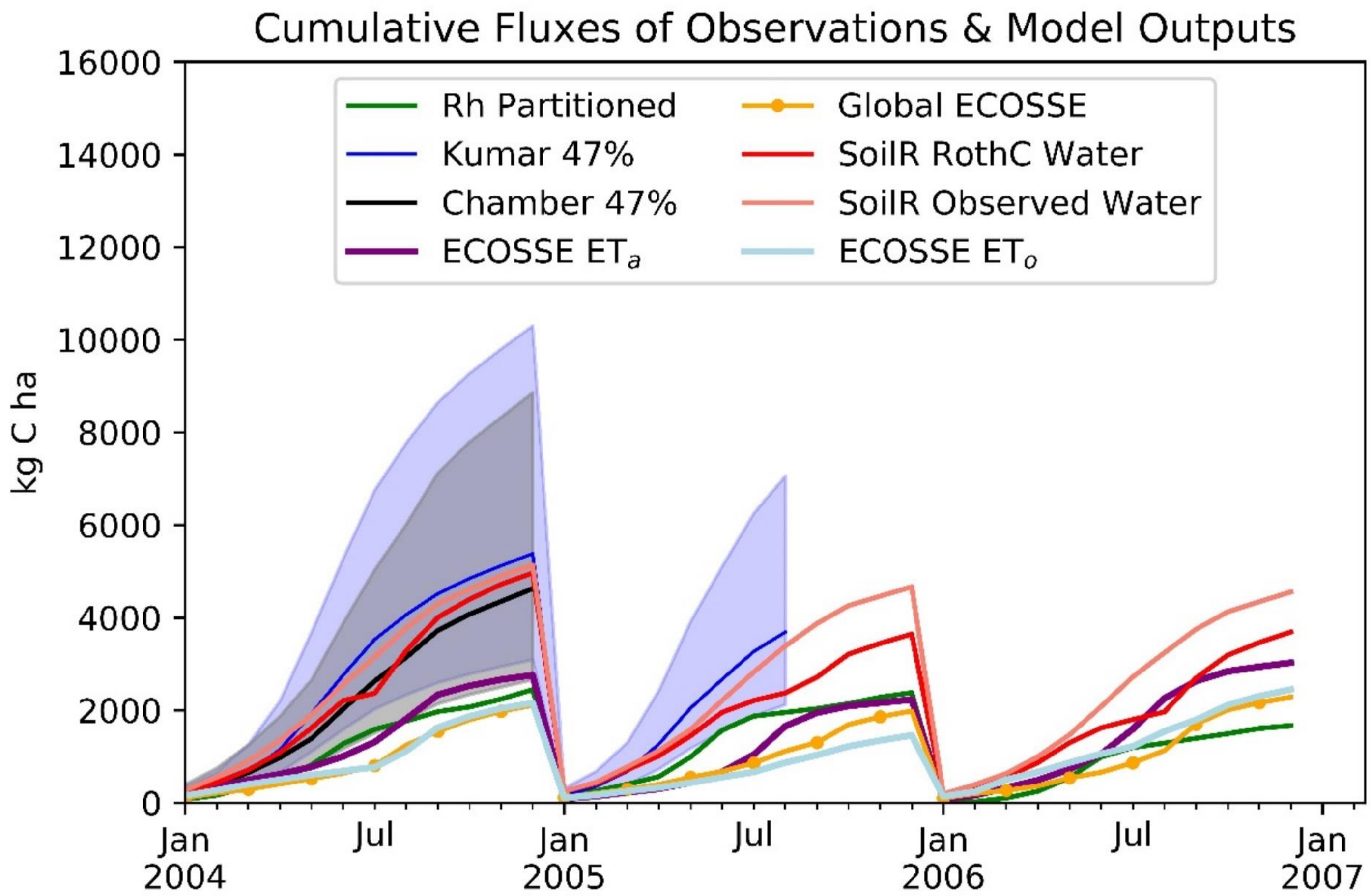


Figure 6.10: Cumulative fluxes for observations and model outputs for the years where data is available. Shaded areas indicate potential partitioning ranges of 27-90% for the Rh contribution to Rs.

6.3.6 *Statistical Analysis of Simulations*

Table 6.4 shows statistics for models compared to observations, ECOSSE ET_a is not included in these simulations as it requires unrealistic alterations to the model inputs, therefore the unaltered GlobalECOSSE Elum model is used. r^2 values indicate that the model which most closely corresponds to all observed data is the SoilR model using observed water and the Daycent2 water modifier (SoilR Obs) with r^2 values between 0.5 and 0.78, followed by SoilR using the RothC water modifier (SoilR RothC) with values from 0.03 to 0.37, then Global ECOSSE with values from 0.03 to 0.24.

However, due to the seasonality of the data, typical correlation and regression techniques such as Pearson's r and r^2 are likely capturing the seasonality in the relationships (Wooldridge, 1991), giving erroneous results. To more accurately compare the modelled and measured data to each other mean absolute error (MAE) and root mean square error (RMSE) (which are unaffected by seasonality) were chosen as evaluation metrics. When examining RMSE and MAE the lowest values across all datasets are for Global ECOSSE compared to Rh, with all models having their lowest scores when compared to Rh ahead of the chambers.

Table 6.4: Statistics for models vs observations, SoilR RothC uses the RothC water modifier, SoilR Obs uses observed water content and the Daycent2 water modifier.

	r^2	RMSE	MAE
Global ECOSSE Vs Chamber	0.24	529.55	415.07
Global ECOSSE Vs Kumar	0.09	622.36	476.67
Global ECOSSE Vs Rh	0.03	164.96	120.57
SoilR RothC Vs Chamber	0.03	387.06	316.86
SoilR RothC Vs Kumar	0.15	439.32	317.42
SoilR RothC Vs Rh	0.37	189.12	163.99
SoilR Obs Vs Chamber	0.66	278.32	235.46
SoilR Obs Vs Kumar	0.78	347.41	241.75
SoilR Obs Vs Rh	0.55	205.23	180.26

Having evaluated the ECOSSE model versions and investigated their ability to scale up using SoilR, the GlobalECOSSE model performs 'best' ahead of SoilR test models when compared to Rh data (based on RMSE and MAE scores), though Table 1.4 shows that the statistical method of assessment and the observed data used for comparison can affect the results. As RMSE and MAE scores are independent of seasonality they are regarded as better measures in this case. These data are also based on results from of a well-drained field in Ireland which has been shown to be problematic when simulating water (Chapter 5), simulated respiration is therefore likely to be lower than observed. Recognising these limitations, the next section presents national outputs of the Global ECOSSE model, which has the advantage of providing outputs for carbon dioxide (CO_2), Nitrous Oxide (N_2O), nitrate (NO_3) and methane (CH_4), allowing for the calculation of CO_2 equivalent emissions of GHGs. Not all Irish soils are well-drained (Figure 5.1), suggesting that the model may perform well on other soils.

6.3.7 *Global ECOSSE National Outputs*

The GlobalECOSSE ELUM model requires a .json file which contains land-use information which it uses to determine plant inputs, optional inputs are as follows: 'Arable', 'Forestry', 'Miscanthus', 'Grassland', 'Semi-natural', 'SRC' (short-rotation coppice), 'Rapeseed', 'Sugar cane', 'SRF' (short-rotation forestry), 'Wheat'. As it is not possible to run the model with different land-uses at the same time, the land-use file used for these national output runs regards all land-use as grassland, as this is the majority land-use in Ireland. This has the effect of altering the monthly plant inputs to match that shown in Table 6.5. Treating all land-uses as receiving the same plant inputs will introduce uncertainties and errors, ideally multiple different land-uses would be specified in the model, though as this is not yet possible the majority land-use was used. Irish cropland and grassland areas with their associated plant inputs will be examined separately in a later section.

Table 6.5: Default pattern of plant carbon and nitrogen inputs to the soil for Arable and Grassland, patterns for other land-uses are not included but are available from Smith et al., 2010a

Month	1	2	3	4	5	6	7	8	9	10	11	12
Arable												
0-30cm	0.00	0.00	0.30	0.30	0.30	0.60	1.87	0.00	0.00	0.00	0.00	0.00
30-100cm	0.00	0.00	0.30	0.30	0.30	0.30	1.17	0.00	0.00	0.00	0.00	0.00
> 100cm	0.00	0.00	0.30	0.30	0.30	0.30	1.17	0.00	0.00	0.00	0.00	0.00
Grassland (Improved grassland)												
0-30cm	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.89	0.25	0.25	0.25	0.25
30-100cm	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21
> 100cm	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.21

6.3.7.1 *SOC*

Average SOC from 2001-2017 outputted by GlobalECOSSE is presented in Figure 6.11, these carbon contents are calculated from organic carbon contents in the HWSD and associated bulk density values. As the HWSD reports organic carbon percentage weight (c), the following process is undertaken to convert to kg C ha^{-1} where total C content TC is:

$$TC = \left(\frac{\left(\frac{c}{100}\right) * 100000000}{1000}\right) * LD * BD$$

This converts c to a proportion, from cm^3 to ha^{-1}, from g to kg, LD is layer depth and BD is bulk density. C content ranges from below 100,000 kg C ha^{-1} to over 500,000 kg C ha^{-1}, highest values are observed in the midlands and western regions of the country, and correspond to peatland areas of the country with high organic C contents.

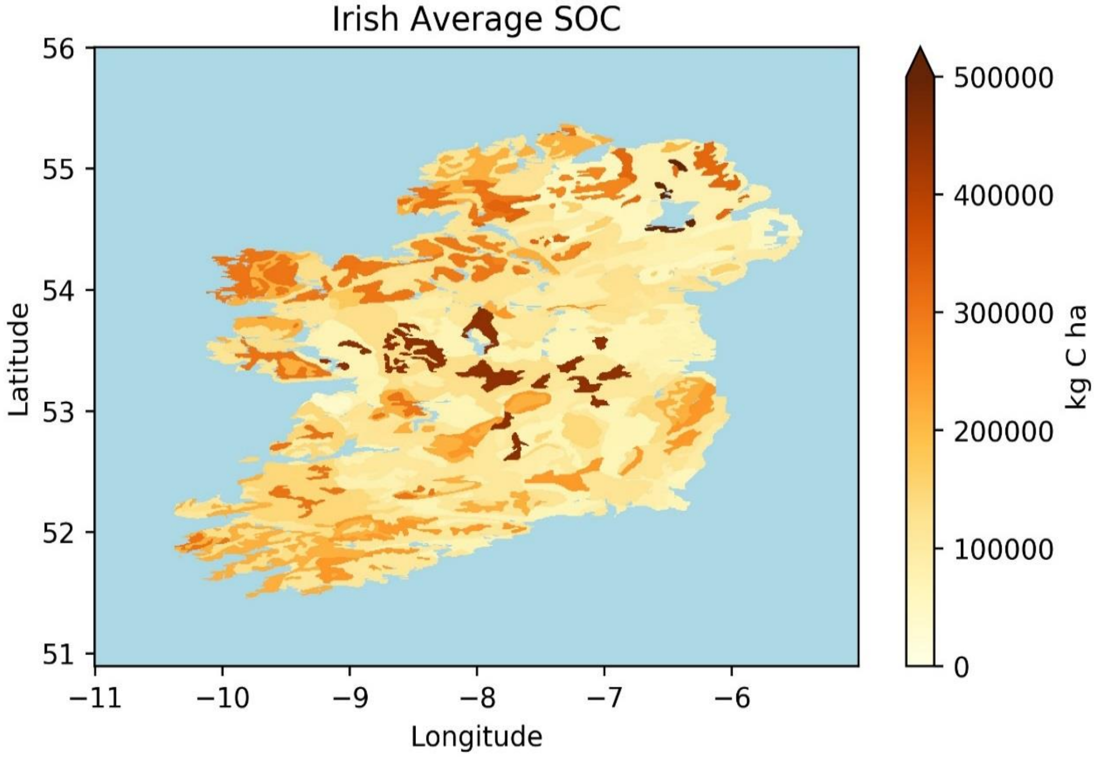


Figure 6.11: Soil Organic Carbon content for Irish soils outputted from the Global ECOSSE model

6.3.7.2 *CO_2*

Annual mean CO_2 emissions from 2001 to 2017 are presented in Figure 6.12, with highest emissions evident in the year 2007. The spatial pattern of emissions shows higher emissions in the south-east of the country in most years, with lower emissions on the east coast and in mountainous uplands. A patch of low emissions is evident in the west of Ireland each year, corresponding to the karst landscape of the Burren, where low emissions are present. Simulated emissions are over 300 kg C ha^{-1} yr^{-1} for certain locations (particularly the south-east of the country) during most years, likely due to the higher sunshine hours (PAR) and temperatures experienced in this part of the country.

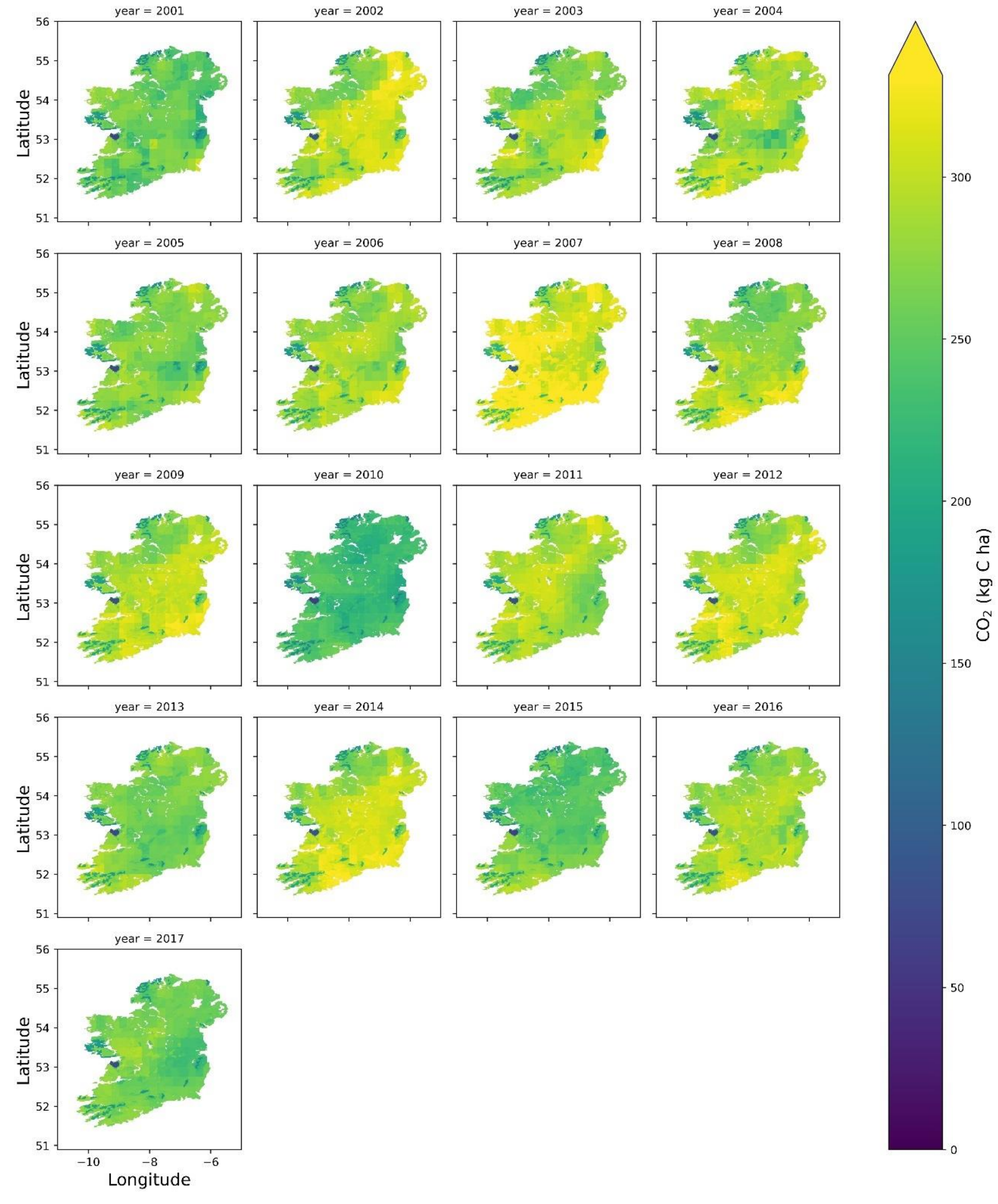


Figure 6.12: Annual average soil CO_2 emissions outputted from the Global ECOSSE model for the years 2001-2017

National outputs for Global ECOSSE are presented for CO_2 on a seasonal basis (Figure 6.13), as averages of data from 2001-2017. Seasonal outputs show summer having the highest emissions, while spring has the lowest. Emissions appear highest in the north-west of the country during the summer months, in the south-east during winter, and are evenly distributed during spring and autumn. While the winter months have got the lowest values (darkest blue colours) in some parts of the country, there remain some high-emission areas in the south and south-east which are not present in spring and autumn.

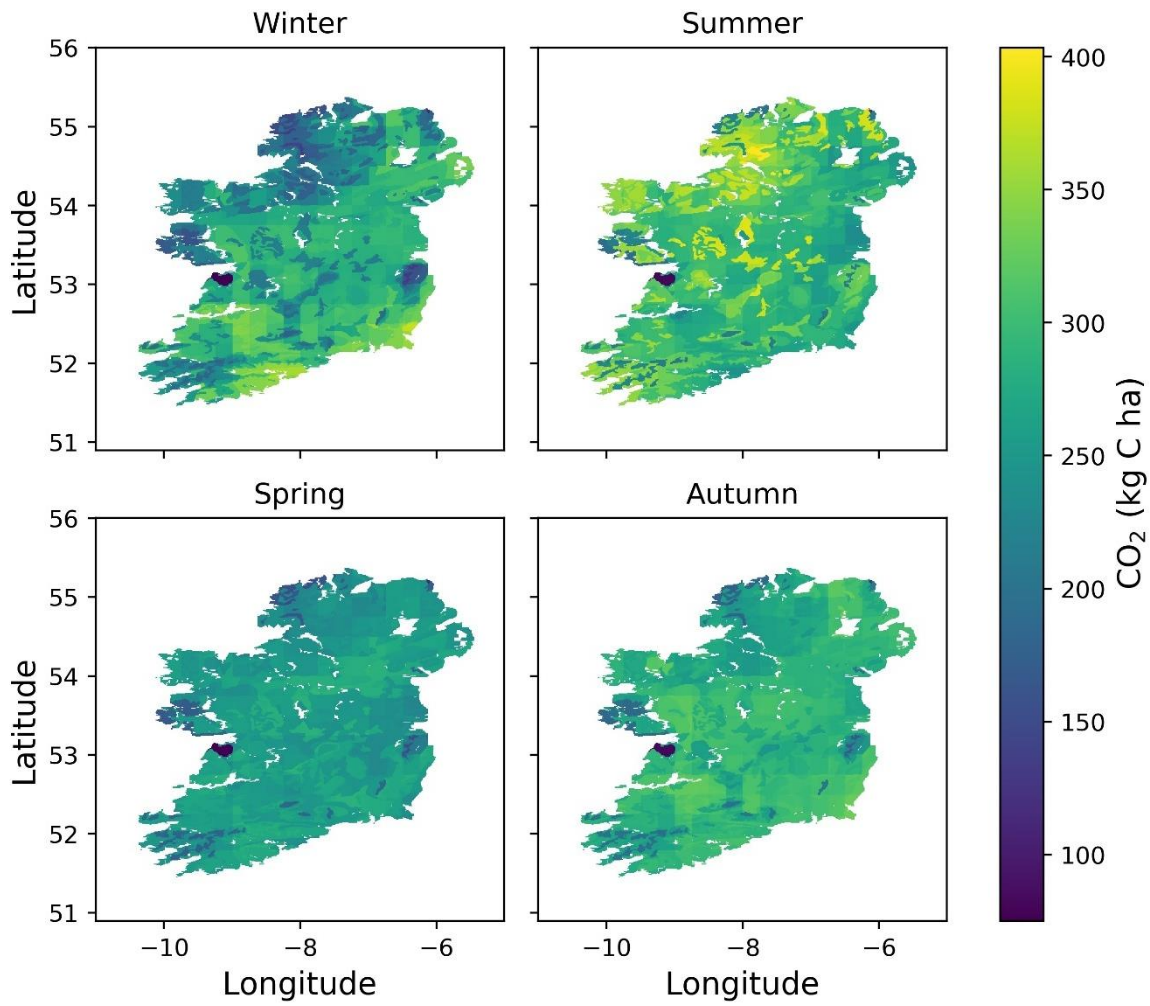


Figure 6.13: Seasonal average soil CO_2 emissions outputted from the Global ECOSSE model from 2001-2017

The average annual CO_2 emission over the entire period is illustrated in Figure 6.14 and shows the spatial distribution of emissions over time, with the lowest emissions observed on the west coast and in mountainous regions of the country, and the highest in the south, south-east and midlands. The orographic influence is clear in the south-west of Ireland as emissions are lower in mountainous regions. Grid-boxes visible on this graph indicate the dominant influence of temperature data and are more pronounced due to averaging the data. The influence of climate in the average CO_2 emission maps is clear as emissions are higher during the warmer months showing the driving effect of temperature data. Plant inputs are also higher during these months (Table 6.5) which provide more substrate for decomposition and therefore higher emissions.

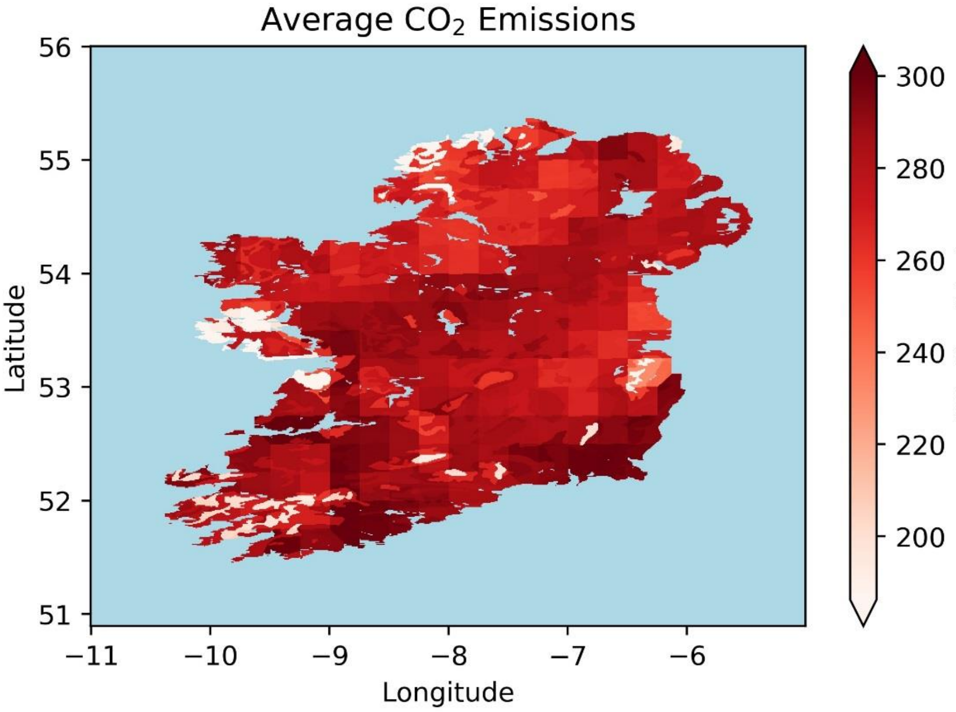


Figure 6.14: Average CO_2 emissions from Irish soils outputted from the Global ECOSSE model for the period 2001-2017

6.3.7.3 *NO_3*

Nitrate is a form of inorganic nitrogen which occurs naturally in soils and arises from decomposing plant material, animal manure, chemical fertilizers, plant exudates, rainfall and lightning. Figure 6.15 shows seasonal average emissions of nitrate which follow a clear spatial pattern, where emissions are highest inland and lowest in coastal and upland areas. Emissions of nitrate are highest in spring and summer but are uniform across all seasons, as all land is being treated as grassland there are no spikes that would be seen at the start of the growing season (spring) if the land were treated as arable. There is a clear influence of the climate data on the seasonal outputs as emissions are lowest in areas with high rainfall (west coast and upland areas) while high emissions are experienced in high-C midland soils.

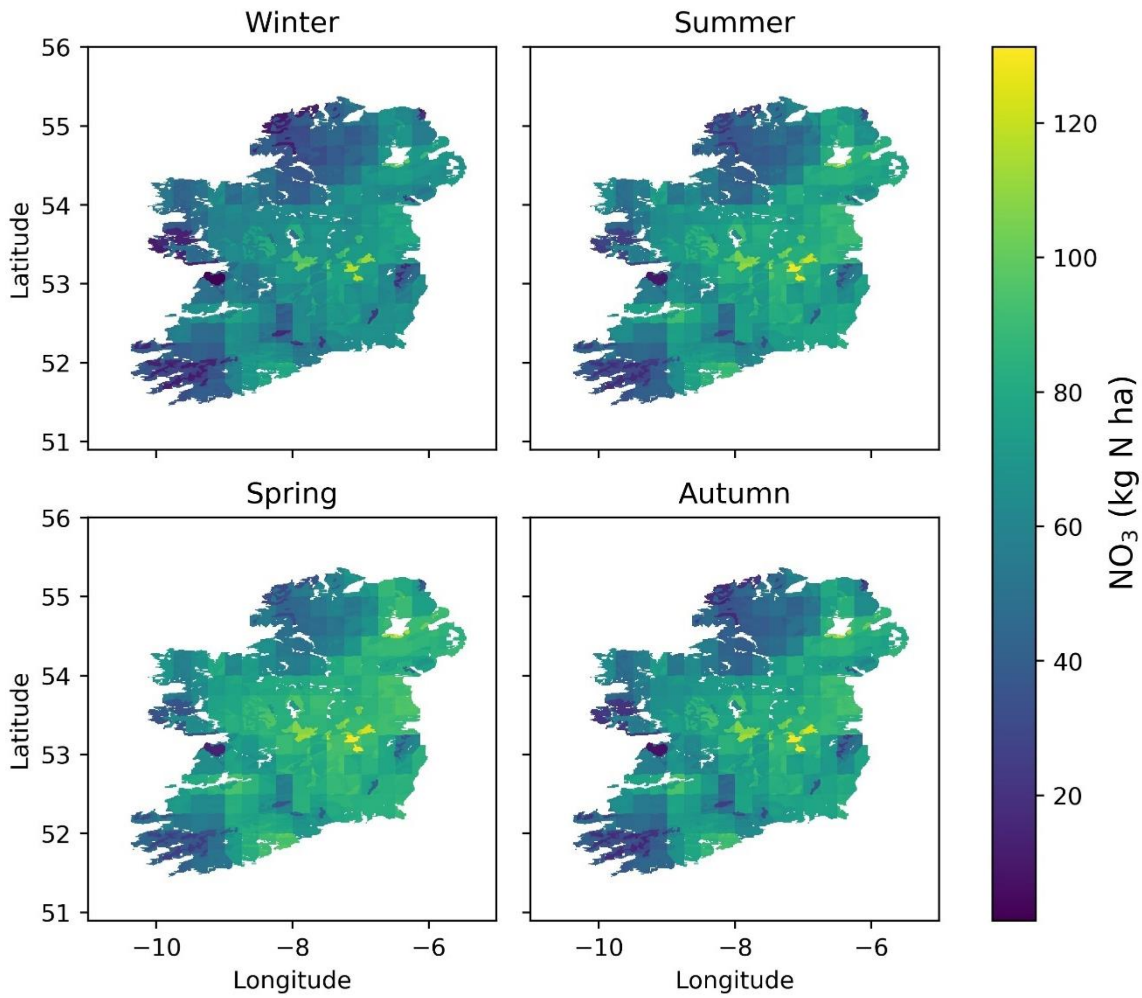


Figure 6.15: Seasonal average nitrate emissions from Irish soils outputted from the Global ECOSSE model in kg N ha^{-1}

Figure 6.16 shows average NO_3 emissions for the period 2001-2017 where a clear spatial pattern is evident with lowest emissions observed in the north-west and south-west of the country, and in upland locations. Highest emissions are evident on the east coast in lowland areas indicating that NO_3 emissions are low in mountainous regions with high rainfall and high in lowland areas in soils which have a high C content. Giles *et al.* (2012) caution against drawing clear conclusions however, as the controls on denitrification and nitrate release are not well understood, though it is recognised that nitrate release is influenced by many factors including community composition, soil type and environmental conditions.

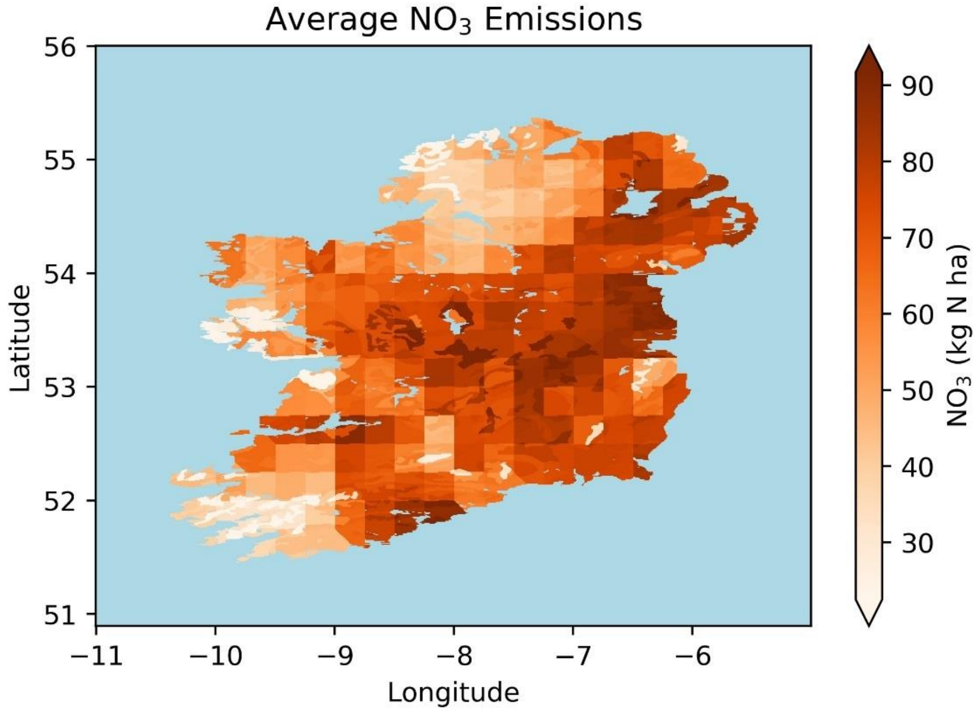


Figure 6.16: Average NO_3 emissions from Irish soils outputted from the Global ECOSSE model for the period 2001-2017

6.3.7.4 *N_2O*

Nitrous Oxide emissions are highest in soils during spring, with emissions low in summer and autumn and very low during winter (Figure 6.17). Emissions are spatially uniform in each season, with all areas having similar emissions during each season. As all land-use is treated as grassland the plant inputs are common across the country, giving a similar spatial response.

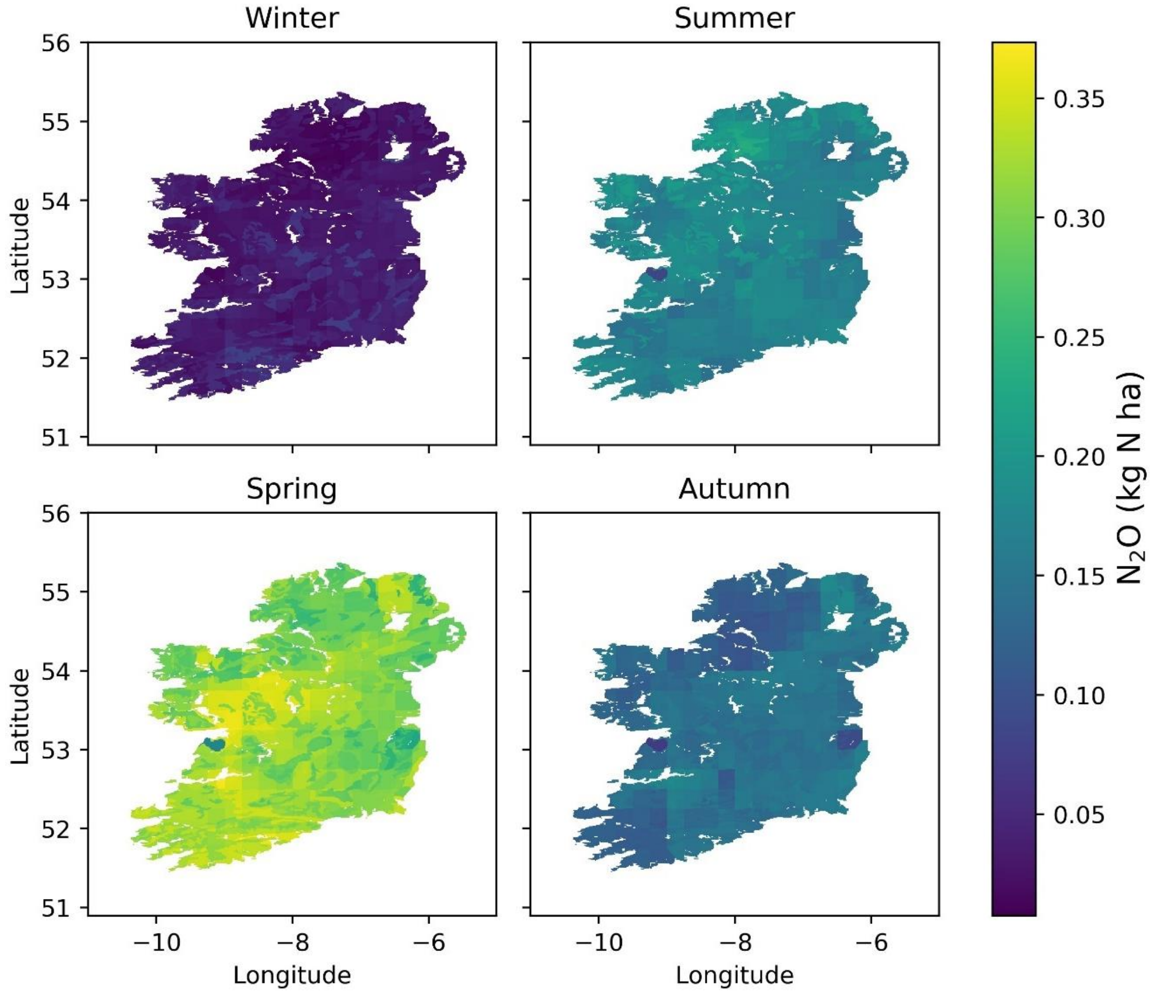


Figure 6.17: Seasonal average N_2O emissions from Irish soils outputted from the Global ECOSSE model for the period 2001-2017

Average N_2O emissions (Figure 6.18) show a more distinct spatial pattern, emissions are lowest in the north-west, south-west coast and east coast, and are high in the north-east and midlands. Emissions range from 0 to 0.18 kg N ha^{-1} yr^{-1}, indicating that emissions are low regardless of spatial differences. Springtime emissions are the dominant source of N_2O while winter emissions are extremely low, with moderate fluxes in summer and autumn.

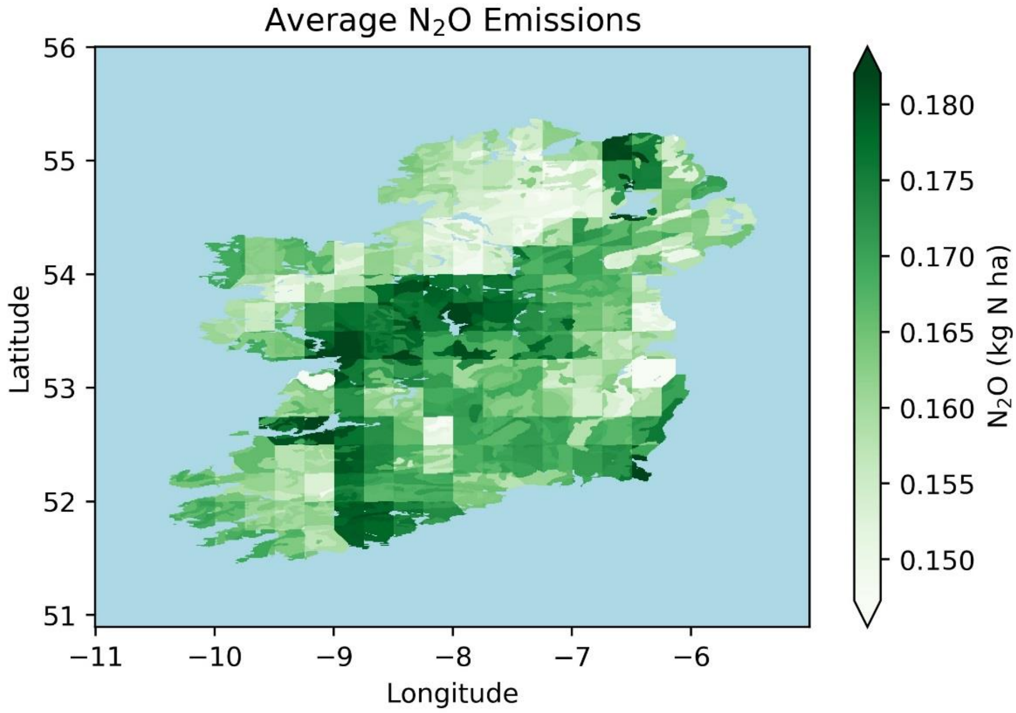


Figure 6.18: Average N_2O emissions from Irish soils outputted from the Global ECOSSE model for the period 2001-2017

6.3.7.5 *CH_4*

Methane is the only variable which shows negative emissions (sequestration), with the most sequestration happening during summer, very little in winter, and a small amount in spring and autumn (Figure 6.19). The negative fluxes are present in the same areas that have the highest C contents in Figure 6.11, suggesting that these high C soils act as C sinks during the warmer months. The influence of climate data on methane fluxes is much lower than with the other modelled variables, as the dominant source of emissions is the carbon content of the soil, with high C soils in the uplands and midlands being the largest CH_4 sinks during the summer months.

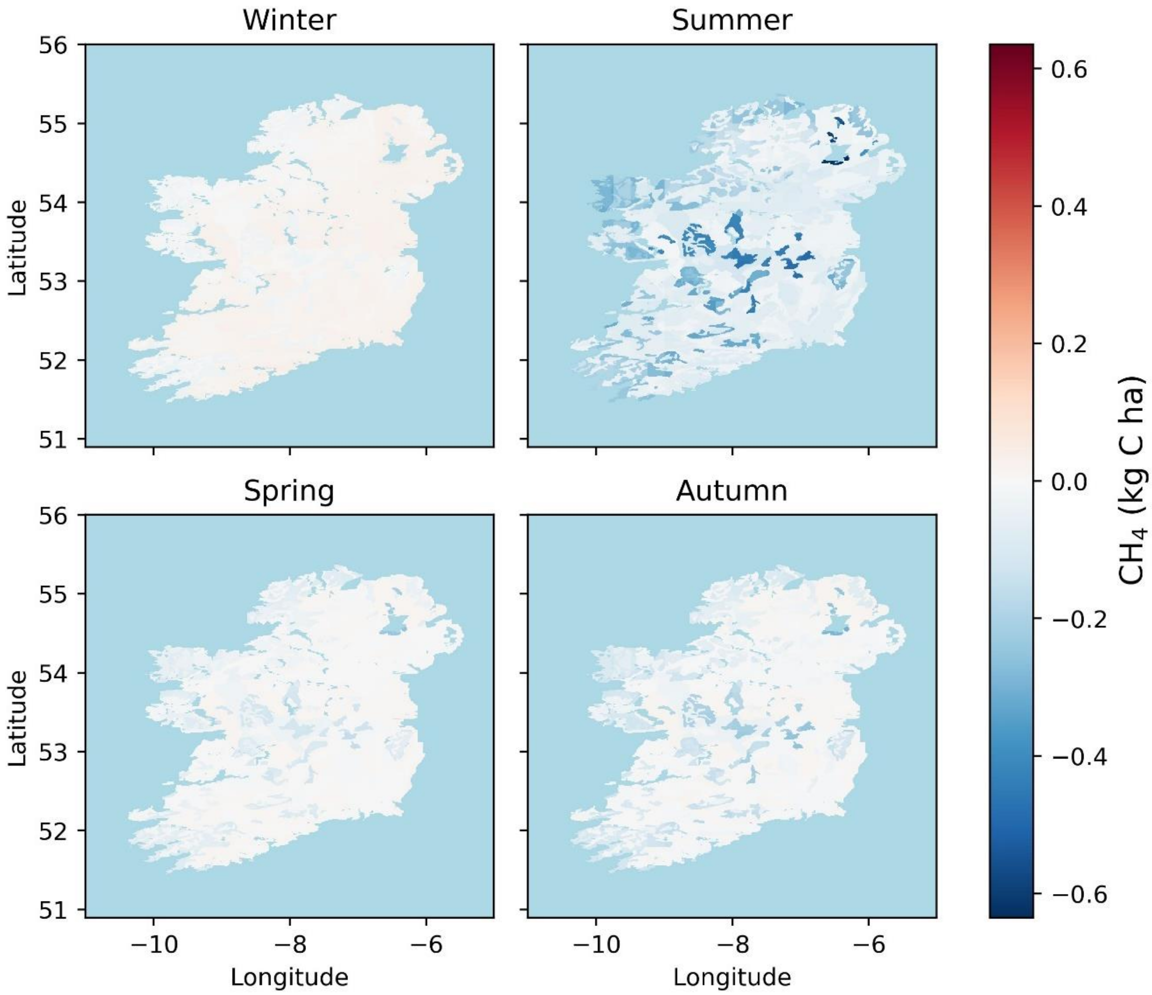


Figure 6.19: Seasonal average CH_4 emissions from Irish soils outputted from the Global ECOSSE model for the period 2001-2017

Average CH_4 fluxes (Figure 6.20) effectively follow the same pattern of summer in Figure 6.19, with smaller values accounting for the inclusion of the lower sequestration values in other seasons. There is no evidence of the influence of climate data on this map indicating that soil type and plant inputs dominate the fluxes. C sequestration is highest in upland and peatland areas of the country, while most other areas have zero or negligible fluxes.

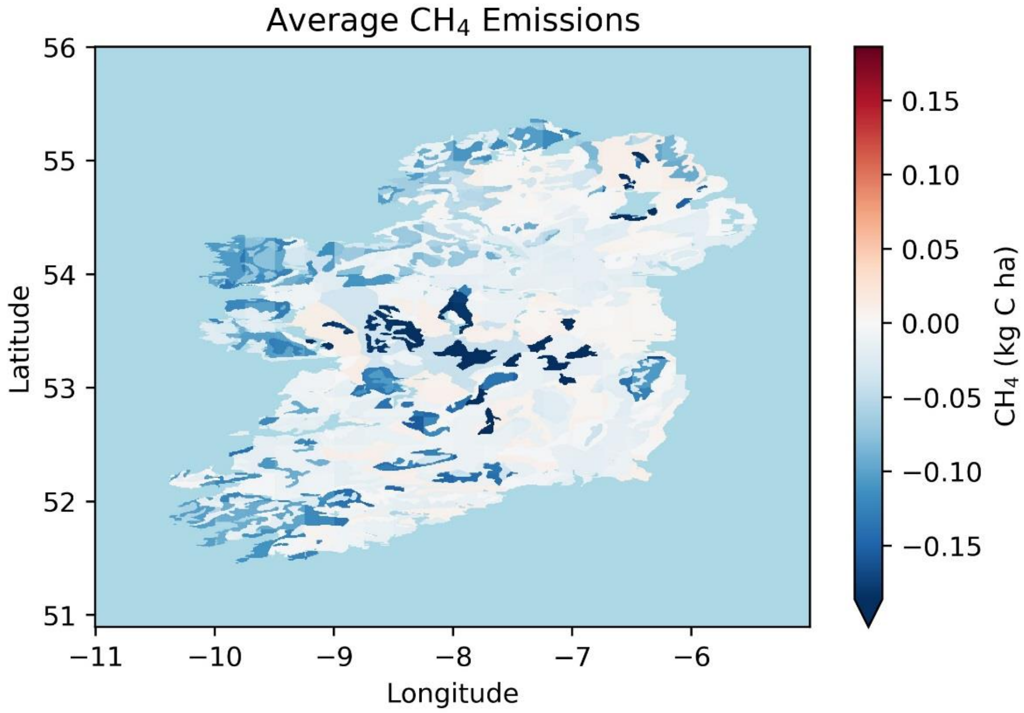


Figure 6.20: Average CH_4 fluxes from Irish soils outputted from the Global ECOSSE model for the period 2001-2017

6.3.8 *Emissions from Agricultural Land-Use Types*

6.3.8.1 *Grassland*

Grassland emissions were obtained by using the grassland areas outlined in Section 6.2.5 and restricting the model to running only at these locations. This analysis only takes into account soils from the Republic of Ireland to facilitate comparison to national emissions inventory stocks (Duffy *et al*., 2018), for this reason Northern Ireland is not included. Average annual grassland emissions are estimated as 281 kg C ha^{-1} over the period 2001-2017 (Figure 6.21), while cumulative emissions for the year 2016 equal 322.80 kt C. Total grassland area covered by the model run is 48,897km^2. Emissions are lowest in upland areas of the country and highest in the midlands, south and east on average.

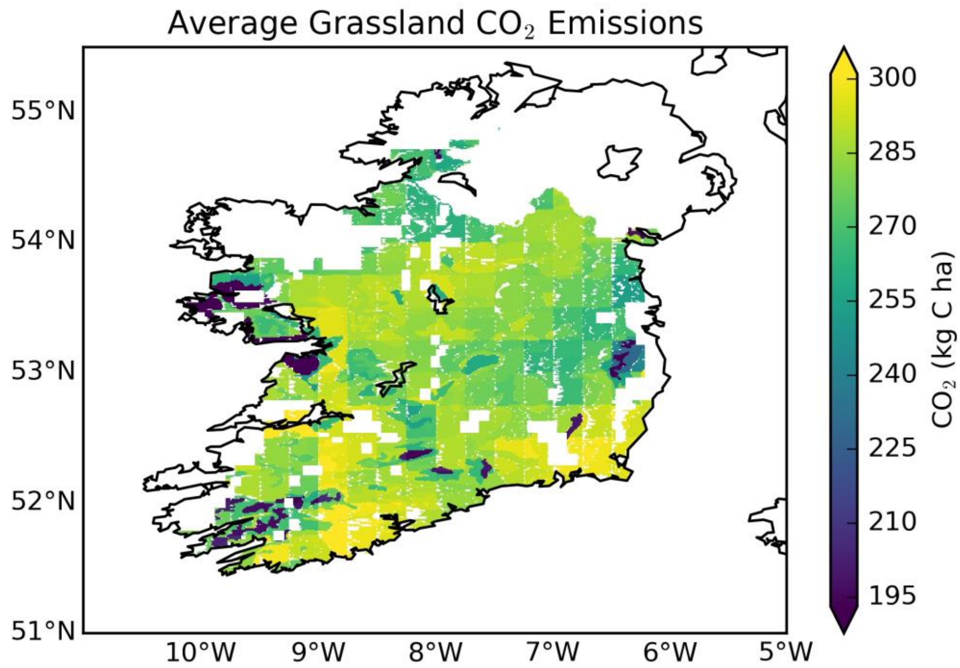


Figure 6.21: Average grassland CO_2 emsisions outputted from the Global ECOSSE model for 2010-2016

As the ECOSSE model only simulates soil respiration and not sequestration, to investigate gains/losses of SOC, the sum of SOC for each month was calculated and aggregated for the entire country (Figure 6.22). This graph shows declining levels of SOC, a loss of 1.41% over the period 2001-2017 (calculated as the mean value in 2001 compared to the mean value in 2017), a loss of 0.08% per year. The decline is higher in the earlier years of the period and appears to level off after 2010 as the soils adapt to a new equilibrium.

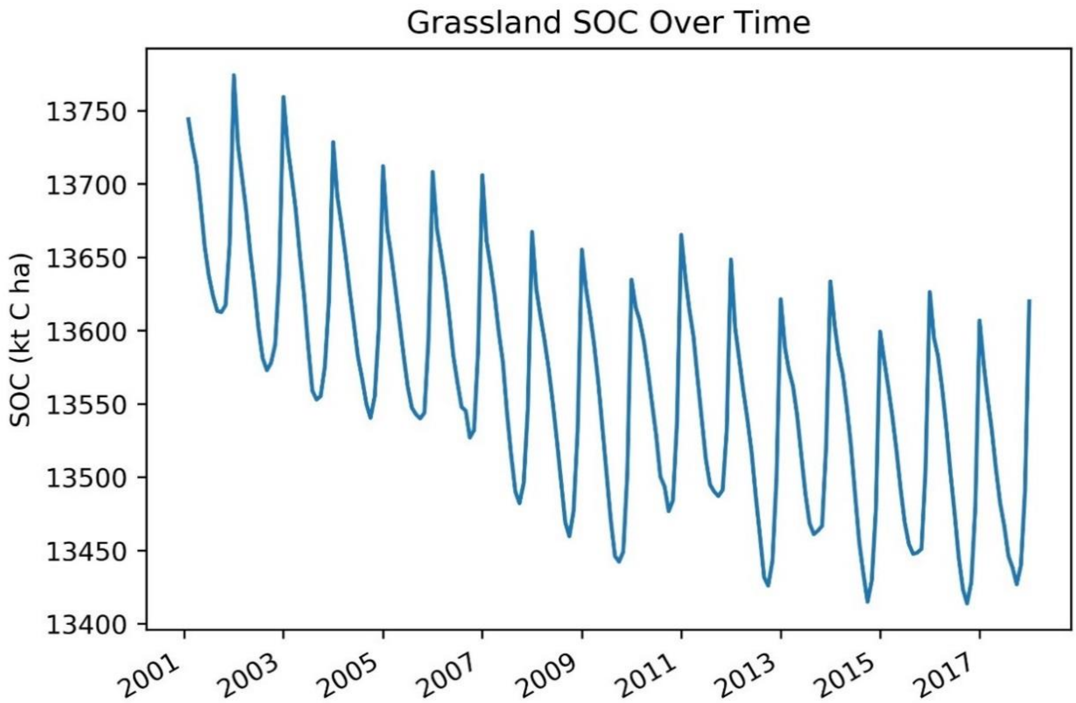


Figure 6.22: Monthly average model simulated Grassland SOC content from 2001-2017

The importance of including gases other than CO_2 in estimates is highlighted by Figure 6.23, where most Irish grasslands are GHG sources rather than sinks. Highest sequestration levels occur in the south and southeast of the country, while highest emissions occur in the midlands and close to the border.

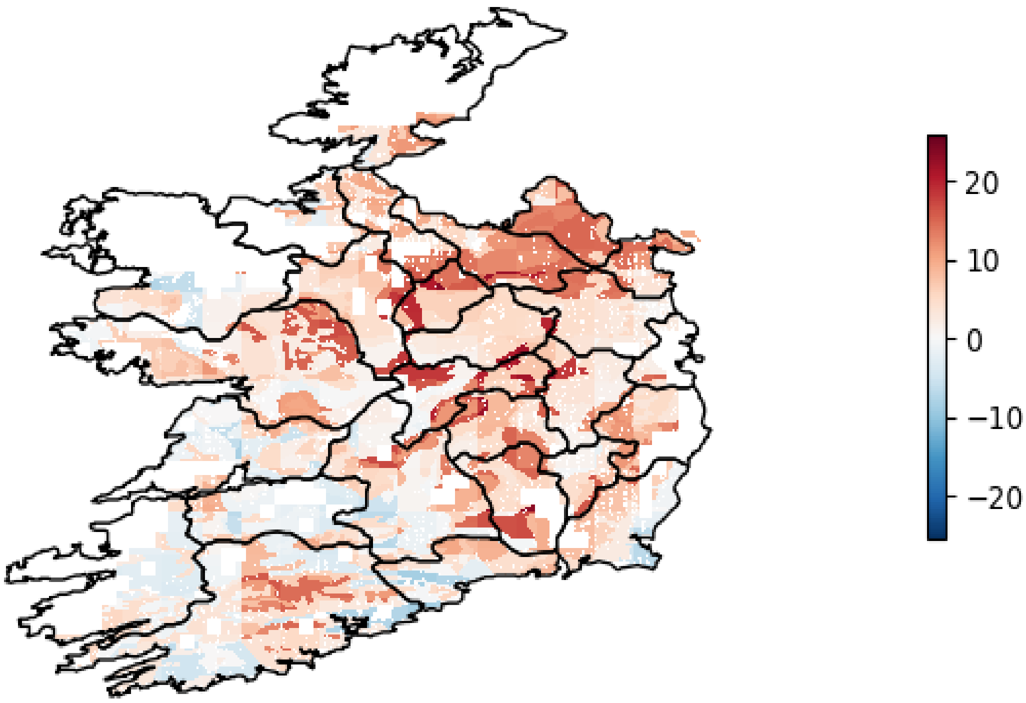


Figure 6.23: Average annual GHG fluxes for Irish grasslands outputted from the Global ECOSSE model, units in kg C ha

6.3.8.2 *Cropland*

Cropland emissions were obtained by using the cropland areas outlined in Section 6.2.5 and restricting the model to running only at these locations. Average cropland emissions over the period 2010-2016 are 111.12 kg C ha, with the annual CO_2 sum for 2016 being 14.50 kt C. The cropland area consists of numerous relatively small areas on the map, making up a total of 3777.75 km^2. Though it is difficult to identify a pattern on this map as the areas are so small, it is clear the highest emissions are in the south, southeast and midlands while lower emissions (blue colours) are evident in the east, southwest, west and northwest (Figure 6.24).

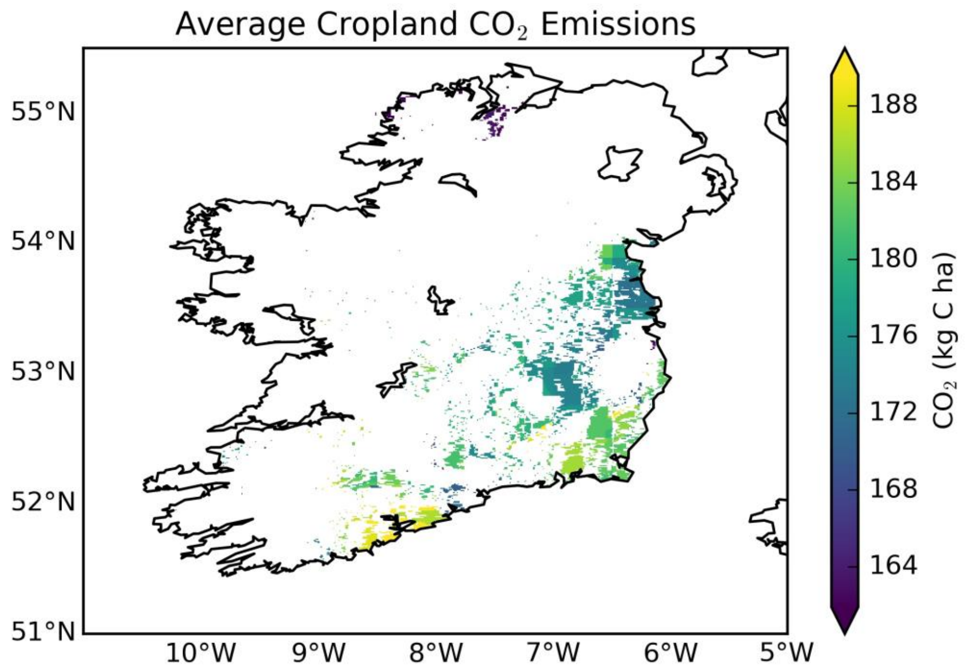


Figure 6.24: Average cropland CO_2 emissions outputted from the Global ECOSSE model for 2011-2017

As the model does not simulate sequestration, to assess C losses or gains the quantity of SOC is examined (Figure 6.25) and shows a decline of 1.44% over the period 2001-2017, a loss of 0.085% per year, a rate slightly higher than grassland decline. The degree of decline appears to level off after 2010, though not to the same degree as grassland.

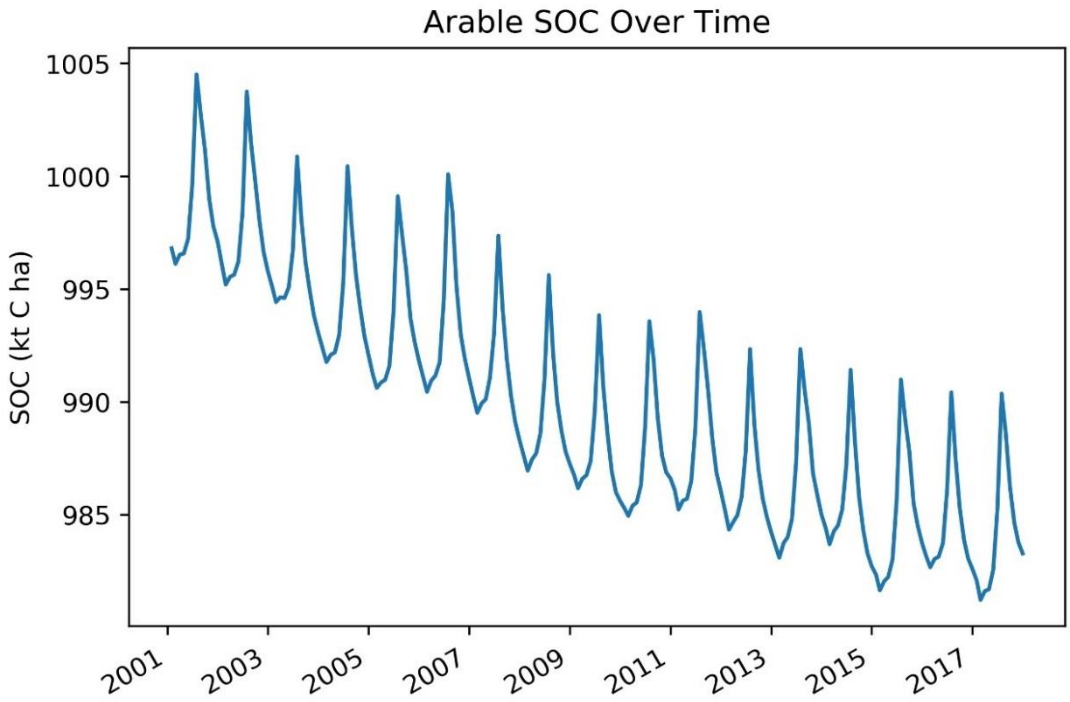


Figure 6.25: Arable average SOC content for Irish soils from 2001-2017

Figure 6.26 shows the GHG fluxes from cropland areas of the country, all fluxes are positive meaning no sequestration is simulated by the model. Highest emissions occur in the southeast and midlands with patches of lower emissions in the midlands and Donegal.

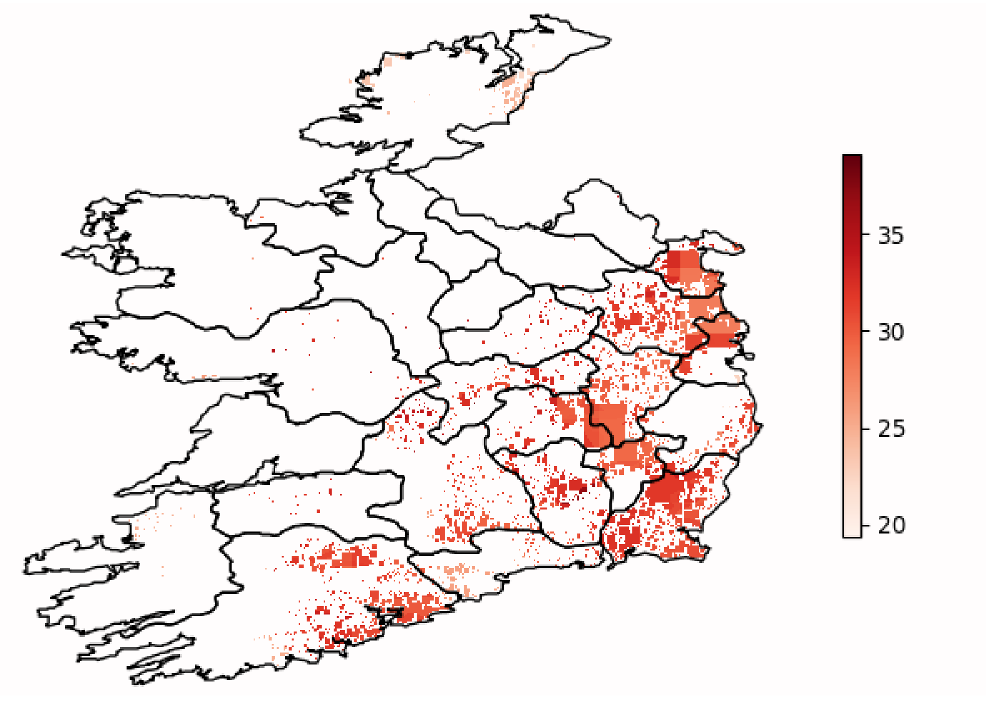


Figure 6.26: Average annual GHG fluxes for arable soils outputted from the Global ECOSSE model for 2011-2017, units in kg C ha

6.4 Discussion & Conclusion

Difficulties arise in soil carbon model evaluation and assessment when observations from eddy covariance towers and chambers can have such a large range of uncertainty associated with them, and models output values without uncertainty bounds. Depending on the observed data chosen to compare the model to, and the metric used to represent model accuracy, different models will emerge as the 'best' (Table 6.4). The choice of model and comparison data clearly affects the results of the study, for example if the SoilR model were to be judged against chamber data partitioned at 47%, it would be assessed as the optimally performing model, as the Global ECOSSE model has higher MAE and RMSE scores compared to chambers than SoilR. However, were the Global ECOSSE model to be compared to Rh, it would be judged the optimally performing model for the same reasons. The large differences between chamber and Rh data and the lack of metadata on both significantly hinder the evaluation process, as no particular set of data can be seen as 'better' than the other; however, more metadata is available for the Rh data, and the partitioning range is more certain, indicating it may be a more useful resource than chambers, depending on network protocols used.

R-values for correlation have been used in previous studies to assess the usefulness of the ECOSSE model (Dondini *et al.*, 2016), yet these values are likely to be capturing the seasonality of the data, giving a stronger correlation than may be present otherwise. For example, were the r^2 values listed in Table 6.4 to be used as the sole metric for model performance, the recommendation would be different than using MAE and RMSE values. The statistics presented here compare the model outputs to chambers partitioned at 47%, the accuracy of which is questionable due to large potential ranges, though a certain level of partitioning must be chosen for evaluation to be possible and for statistics to be derived. Based on the statistics, the SoilR model using observed SWC and the Daycent2 water modifier performs best in comparison to chamber data, SoilR using RothC water performs best in comparison to Rh, as does Global ECOSSE, which has lower values for both MAE and RMSE than the other models in comparison to Rh. SoilR does not have the same capabilities as ECOSSE however, and is limited in its ability to simulate national emissions. As Rh is the variable with the least range of uncertainty associated with it, and the MAE and RMSE scores are better metrics than r^2, the ECOSSE model is deemed appropriate for simulating soil C emissions, though the model is likely to be underestimating the actual respiration due to the discrepancy with chamber data, though this is similar to that observed in other studies (Dondini *et al.,* 2017). Even with significant underestimation of totals, r values from Dondini *et al.* (2017) for the arable site are 0.8, much higher than observed in this study, though these values come from running ECOSSE in site-specific mode using more accurate parameters than Global ECOSSE. r^2 values of ~0.2 have been reported previously for the ECOSSE model in the past (Zimmerman *et al.,* 2018), where the model has been reported as out-performing others. r^2 values of 0.3-0.5 have also been observed (Khalil *et al.,* 2013, Abdalla *et al.,* 2014), indicating that the model can perform well at certain sites, but typically underestimates observations. Uncertainties in observations are not reported by these studies however, the statistics shown in Table 6.4 emphasise the importance of observations and statistical method chosen to evaluate model performance, as the assessment of model performance can change significantly based on the chosen metrics.

Several complexities are unearthed when trying to move from site to regional scale, particularly due to the lack of observations across time and space. It is clear from the cumulative fluxes (Figure 6.10) that the ECOSSE model remains on a similar scale when moving from site-specific to limited-data mode, with differences in outputs likely due to input data discrepancies as site-specific mode allows for more inputs to be specified. The site-specific model is initialised using characteristics measured at the site or nearby (Section 4.3.1), while the regional model uses interpolated fields of precipitation and temperature (EObs data) combined with interpolated soil characteristics (HWSD). HWSD data has been observed to underestimate field stocks of carbon by 80-90% compared to observations (Tifafi *et al.,* 2018), which raises questions on the accuracy of Figure 6.11.

Querying GlobalECOSSE then introduces further uncertainty, as the output is also an interpolated surface which can be queried for a specific point location, but will select a point which represents an area, perhaps accounting for the lower values seen in the regional model when compared to site-specific ECOSSE. From examination of the cumulative fluxes it is likely that Global ECOSSE is underestimating the actual fluxes as it is lower than both chamber and Rh, though it is difficult to be confident in the degree of underestimation due to the significant uncertainty surrounding observations. The model outputs being significantly lower than observations from both eddy covariance and chamber derived fluxes are consistent with at least one other study on arable land as Dondini *et al.* (2016) show. Though the model is underestimating the fluxes Dondini *et al.* (2016, pp. 937) say the model ‘adequately simulates soil processes under different land-use systems’.

6.4.1 *CO_2*

National emission estimates of the variables simulated by Global ECOSSE follow a pattern which is to be expected based on understanding of how the model functions, with emissions responding strongly to temperature as the highest emissions correspond to significantly warm Irish years (Met Éireann, 2018b), and low emissions from soil types which contain very little carbon e.g. the negligible emissions in the Burren, Co. Clare (Figure 6.14). Seasonal analysis of the data shows highest emissions during the summer months with the lowest emissions of CO_2 (darkest blue colours) evident in winter and spring, meaning soil respiration is responding to temperature as expected, and the model is performing as it should (Figure 6.13). Figure 6.14 outlines the average emissions over the period where the spatial pattern shows the importance of soil type along with temperature, as lowest emissions come from peatland and mountainous areas along the west coast. A drawback of these modelled emissions is that management practices such as fertilizer applications, sowing and tillage are not simulated, as these practices would affect decomposition and respiration. Figure 6.9 shows Global ECOSSE underestimates CO_2 output in comparison to observations, this is similar to findings on arable sites in other studies (Dondini *et al.,* 2016; Zimmerman *et al.,* 2018) though the model has also been shown to overestimate fluxes at some locations (Abdalla *et al.,* 2014). Possible explanations for the underestimation are discussed by Dondini *et al.* (2017) who hypothesize that the soil may not have been in a steady state at the start of the simulation, causing excessive SOM to be lost and an underestimation of decomposition, though there are not enough observations for this theory to be validated, leading the authors to recommend increased observations of Rh across a wider spatial area.

6.4.2 *Other Gases*

Nitrate emissions are relatively constant throughout the year (Figure 6.16), likely due to consistent plant inputs as all land-use is treated as grassland (Table 6.5), though it is unusual that there is little response to seasonal temperature changes, as it has been shown that NO_3 emissions have a positive relationship with temperature (Malhi *et al.*, 1990). Emissions of nitrous oxide are highest in spring, as plant inputs are consistent throughout winter and spring months, this spring spike may be due to the spring-thaw effect, notable as a time when chambers are typically placed on soils to capture N_2O emissions as soils thaw (Butterbach-Bahl *et al.*, 2013), though this may not be significant for Ireland. Soil temperature purportedly explains 86% of the variations in N_2O emissions in European forest soils (Schindlbacher *et al.*, 2004), leading to the expectation that emissions would be highest during the summer months, however this is clearly not the case. The spatial pattern of N_2O emissions (Figure 6.17) is similar to from that of NO_3 (Figure 6.16) with upland areas having low emissions, though the variation in emissions is much greater regarding NO_3 with ranges from 0-90 kg N ha^{-1}, while N_2O emissions vary from under 0.15 to over 0.18 kg N ha^{-1}. Methane emissions simulated by the model are zero or below during each season, and CH_4 sequestration is highest during summer months, an unusual finding as methane emissions are known to increase as soil temperatures increase (van Hulzen *et al.*, 1999; Oertel *et al.*, 2016). Areas with highest C content (Figure 6.11) are also the areas with highest CH_4 sequestration (Figure 6.20).

6.4.3 *Modelled Emissions and National Emissions Inventory Estimates*

It is difficult to compare model outputs for grassland and cropland in relation to the tier 1 and 2 inventory-based methods undertaken by Duffy *et al*., (2018), as their assumptions are that cropland remaining cropland and grassland remaining grassland are not C sources and may well be C sinks where management practices are well established. Duffy *et al.* (2018) estimate croplands to be C sinks of -131.93 kt CO_2eq, with a combined uncertainty estimation of 72.15%, while grasslands are sources of 5.77 kt CO_2eq due to N_2O emissions, CO_2 emissions are presumed to be zero. Modelled results indicate Irish croplands are a CO_2 source of 14.50 kt C. The 2.32% decline of SOC content over time indicates that Irish croplands are C sources, while the inclusion of other greenhouse gases reinforces this as cropland fluxes remain positive when all GHGs are examined, though emissions are lower than when examining CO_2 alone. Management related activities including ploughing, sowing and fertilizer application are a typical feature of croplands and are not simulated by the model at regional scale. Improved measurement/monitoring protocols are required to quantify these management related disturbances (Osborne *et al.*, 2010), before these processes can be included in model simulations.

Irish grasslands are observed to be carbon sinks in research (Kiely *et al.*, 2017) yet ECOSSE model outputs shows them as CO_2 sources, which agrees with Duffy *et al*. (2018), indicating further research into grassland emissions is needed. The model only simulates soil respiration, and therefore does not factor in C sequestration, though this can be estimated from examining the SOC content over time, which is in steady decline for Irish grasslands (Figure 6.22). According to the model outputs grassland SOC is declining at a rate of 0.153% per year, though the decline appears to slow down during the later years of the model run. Examining all GHGs together (Figure 6.23) shows most Irish grasslands are GHG sources, though some areas are shown to be sinks, emphasising the importance of including gases other than CO_2 when modelling soil fluxes, particularly CH_4 and N_2O (Tian *et al.*, 2015). Global ECOSSE does not include the application of fertilizers and other management practices which may be occurring to enhance C or N in the soil, while the assumptions of the tier-1 method that cropland remaining cropland on well managed land may also be erroneous. More observational evidence on different land-use and soil types is vital if we are to have confidence in either tier-1 or tier-3 methodologies. Once the observations are in place to compare the model outputs to, the model must also allow for the inclusion of typical management practices based on the observations, in order to calibrate it as accurately as possible for simulating emissions.

Smith *et al.* (2010d) outline the multitude of factors which must be accounted for in order to accurately estimate the carbon budget of croplands, from field to continental scale. They find that the diversity and complexity of croplands makes it impractical to attempt to upscale from individual sites to continental scale, and argue that the intricate data at field or farm scale can be useful to parameterise or validate ecosystem models, which can be combined with continental-scale datasets to estimate fluxes over large areas. Xu and Shang (2016) estimate the global average Rs from croplands to be 0.704 kg C m^2 yr^{-1}, lower than grasslands at 0.841 kg C m^2 yr^{-1}, and forests at 0.907 kg C m^2 yr^{-1}, with the low values for croplands attributed to lower C inputs to soil as a result of the removal of aboveground biomass when the crop is harvested. Average grassland emissions for Ireland as projected by the ECOSSE model are also higher than croplands, and significantly above the estimates from Xu and Shang (2016) as average Global ECOSSE grassland CO_2 emission estimates are 2.81 kg C m^2 yr^{-1} and cropland are 1.6 kg C m^2 yr^{-1}. Examination of all GHGs does indicate that some Irish grasslands are sinks, which agrees with Kiely *et al.* (2017) though further integration of observations and model processes is necessary to have strong confidence in model outputs.

Irish grassland emissions are assumed to be net zero or sinks on the basis of the implementation of well-established management practices such as appropriate fertiliser usage, manure management and managed grazing (Duffy *et al.*, 2018) – it is not possible to factor these management practices in to the ECOSSE model regional runs as they use the limited data mode, and as the model does not simulate sequestration it is difficult to compare these results. These issues highlight the uncertainties associated with attempting tier-3 modelling for grassland and cropland and emphasise the need for models which can incorporate more advanced management practices, and the integration of models with actual farm practices. For models to be useful to estimate national emissions it is essential that more observational data is recorded and published for modelled emissions to be evaluated, the inclusion of management practices into models to reflect real-world behaviour is also recommended.

While the use of biogeochemical models to assess the carbon cycle is expanding, there is still a need for improvement of these models (Robertson *et al.*, 2015). This analysis shows that the significant uncertainties inherent in data partitioning and model parameterisation can complicate the evaluation procedure, and that transparency around the type of partitioning and the uncertainties in model evaluation are often absent in the literature and should be highlighted. Further complexities are introduced when running a limited-data model for a country and comparing it to very limited point-scale observations. Ideally, the model outputs would be compared to a range of CO_2, N_2O, NO_3 and CH_4 data in order to assess the usefulness of the model across land-use types and times of year. The maps presented in the results section serve mainly as an indication of model performance, rather than a definitive national emissions estimation. Availability, accessibility and openness of data is to be encouraged in order to evaluate models with a higher degree of confidence.

While models may not provide accurate estimates of amounts, and it is difficult to assess accuracy when the range in observations is so large, they could still be useful for providing information on relative differences, and on the reaction of the soil system to changes in climate, particularly resulting from extreme events. To examine this, the next chapter describes the process of generating extreme climate scenarios which are used to drive the model, and are compared to a 'normal' climate.

7 Simulated Response of Extreme Weather Events on Soil GHG Emissions

This chapter aims to assess the impact of extreme weather events on emissions of GHGs from Irish soils. To achieve this a novel block resampling methodology was developed which assesses the observed climate sequence and extracts extreme seasons for temperature and precipitation, then generates a new sequence which can be used to drive the GlobalECOSSE model. The data and methods of analysis are described, and results are presented for a series of theoretical extreme scenarios. These results are then discussed, and limitations are outlined.

7.1 Introduction

The response of the terrestrial biosphere to climate extremes has been widely discussed in the literature (Reichstein *et al.*, 2013; Frank *et al.*, 2015), climate extremes have the potential to disrupt carbon dynamics, the global energy balance and the structure of ecosystems themselves, with consequences for C sequestration, radiative forcing and the global climate (Bahn *et al.*, 2015). It is virtually certain that the incidence of extreme events will increase in future, with increases in frequency and intensity of extremes highly dependent on the degree to which humans reduce GHG emissions (Seneviratne *et al.,* 2012). These enhanced extreme events will impact the entire carbon cycle and will have a notable impact on soil physical and chemical characteristics and soil respiration (Reichstein *et al.*, 2013). The observational record shows that the occurrence of prolonged hot, dry weather (heat-waves and droughts) can significantly impact the ability of the terrestrial biosphere to sequester and store carbon; four years' worth of C sequestration was undone in just one summer during the 2003 European heat-wave (Ciais *et al.*, 2005). The response of ecosystems to extreme events is far from linear, and can vary depending on the ecosystem and antecedent conditions (Bastos *et al.*, 2013), and events may be lagged, so the effects of a climate extreme on an ecosystem may take seasons or years to express itself fully, while responses may exceed the duration of the extreme event (Frank *et al.*, 2015). Examples of this include reduced productivity in the years following drought, increased pest mortality as a result of a climate extreme, loss of biomass due to fire, or loss of soil carbon due to heavy precipitation (*ibid*).

This chapter seeks to investigate the impact of various notional extreme events on Irish soils, their C contents, and GHG emissions. Though the ECOSSE model has proven to be problematic in the temporal simulation of GHG fluxes at both site and regional scales, this chapter will explore the use of the model as a tool to investigate the potential impact of extreme events, focusing in particular on relative changes associated with different storylines of extreme events. A proportional indication of the response of the soil system to climatic shocks is still useful to give an indication of potential relative change, as a study investigating these events on emissions of greenhouse gases from Irish soils has yet to be undertaken.

7.1.1 *Climate Extremes*

An extreme weather event is described by the IPCC as 'the occurrence of a value of a weather or climate variable above (or below) a threshold value near the upper (or lower) ends of the range of observed values of the variable' (Seneviratne *et al.,* 2012 pp. 557). A small change in the mean or variance of a climate variable can lead to disproportionately large changes in the frequency of extreme events, making hitherto infrequent extreme temperature and precipitation events more likely (Nicholls and Alexander, 2007). Along with climate change, it is important to consider the potential impact extreme events have on soil GHG quantity, as soils are known to respond strongly to extreme events (Ciais *et al.*, 2005) and extreme events are more likely to occur in future (Seneviratne *et al*., 2012). Changes in the climate system are already evident, not just with changes in the mean climate but also in changes in both the frequency and intensity of extreme events (Mora *et al.*, 2018). Climate extremes are hard to predict, and future simulations of extremes typically have high uncertainties associated with them or are not well resolved spatially (e.g. drought, heavy precipitation) (Seneviratne *et al.,* 2012). Temperate regions are highly susceptible to temperature and precipitation extremes, droughts and storms and their associated impacts (Frank *et al.*, 2015).

7.1.1.1 *Observations*

The effects of extreme events such as heat-waves on ecosystems has come to prominence as a result of the high frequency of warm events in the first decade of the 21st century (Bastos *et al.*, 2014), where along with warm summers in 2002, 2006 and 2007 and 2018, Europe experienced two 'mega-heatwaves' of extreme magnitude, extent and duration in the years 2003 and 2010. These events were so extreme they are thought to have broken 500-year-long seasonal temperature records, the 2010 event being so warm that temperatures over 4 standard deviations above the mean were recorded, causing increases in human mortality, wildfires, ecosystem and crop impacts (Barriopedro *et al.*, 2011). The 2003 heat-wave had significant impacts on the European C cycle. Europe's terrestrial biosphere is an annual sink of between 135 and 205 Tg C yr^{-1}, equivalent to 7-12% of European anthropogenic C emissions (Janssens *et al.*, 2003). Current C sinks in temperate ecosystems could become C sources as the frequency of extreme events increases (Ciais *et al.*, 2005).

The mechanisms of C release in response to extreme weather are not fully understood, and indeed depend on the nature of the extreme event itself. Analysis of vegetation productivity data from MODIS showed that moisture deficits combined with high temperatures were the main causes of the extreme response of vegetation in 2003, while in 2010 the sole driver of the reduced productivity appeared to be the extremely high temperatures (Bastos *et al.*, 2014). Though the impact of extreme events on the carbon cycle are not fully known, increasing temperatures are thought to increase terrestrial C uptake (carbon enrichment effect), though droughts and storms can cause the release of terrestrial C via a reduction in primary productivity and leaching of carbon, potentially negating this enhanced C uptake (Reichstein *et al.*, 2013).

7.1.1.2 *Future Projections of Climate Extremes*

The frequency and intensity of extreme events is expected to increase with temperatures, leading to ecosystem responses which could accelerate further climate change (Rolinski *et al.*, 2015). According to Seneviratne *et al*. (2012) it is virtually certain that the frequency and magnitude of warm daily temperature extremes and decreases in cold temperature extremes will increase by the end of the 21st century across the globe, and it is very likely that heat waves will increase in both length, frequency and intensity over most land areas, where areas in southern Europe will experience 1-in-20 year events at the frequency of 1-in-2 year events, with the exception of high northern latitudes where they are likely to become 1-in-5 year events. In terms of temperature, a global increase of just 1.5°C will lead to a 3°C increase in temperature on extreme hot days in the mid-latitudes, with the number of hot days increasing across most global land regions, with the scale of temperature increase dependant the degree of collective human action to reduce emissions (IPCC, 2018). Precipitation extremes are also likely to increase, particularly in winter in northern mid-latitudes, there is medium confidence that these increases in heavy precipitation will occur alongside decreases in overall precipitation, resulting in increased intensity (Seneviratne *et al*., 2012). The risks from extreme precipitation events are projected to be higher at 2°C warming than 1.5°, though there is medium confidence in this (IPCC, 2018). As projections are uncertain and models are unable to capture all processes which influence these events (e.g. sub grid-scale), there is low confidence in changes in fluvial flooding, and medium confidence that droughts will increase in frequency and intensity (Seneviratne *et al*., 2012). Christidis *et al.* (2015) analyse the likelihood of extreme hot summers following the 2003 European heatwave, and conclude that the temperature increase of 0.81 K since 2003 enhances the probability of extreme events such that an event that would occur twice every 100 years would occur twice every ten years under new climate conditions. Depending on the emissions scenario chosen, the distribution of the future state of temperature differs, with warmer (high radiative forcing) scenarios increasing the chances of more frequent extremes like the heat wave of 2003 (IPCC, 2018).

Heatwaves, droughts and high temperatures can have combined or separate effects on carbon fluxes, and their effects on respiration in different land cover types may differ (Bastos *et al*., 2014). As is to be expected with modelling complex ecosystems, establishing a simple relationship between driver and responder variables is far from easy. Different ecosystems also respond differently to drought, with southern European ecosystems under major threat, more so than ecosystems in northern Europe as only ~1/5th of total European land area is vulnerable to extreme drought (Rolinski *et al.*, 2015). As the feedbacks from extreme events can be nonlinear, a small shift in the severity or frequency of climate extremes can substantially reduce the carbon sink potential of an ecosystem and could result in positive climate feedbacks, shifting a previous C sink into a source (Reichstein *et al.*, 2013).

There is a need for targeted assessments in regions vulnerable to climate extremes in order to understand the vulnerabilities of unique areas, to prepare the most appropriate tailored response (Reichstein *et al*., 2013). Current models are not complex enough to include all these feedbacks and dynamic responses – and are constrained by the lack of observational evidence of ecosystem responses to change. Without this prior knowledge it is difficult to include these factors in analyses, nevertheless this research will continue based on what data is available.

Smith *et al.* (2015) acknowledge that the future brings increased climatic variability with more precipitation extremes and high severity of droughts, leading to stresses in soil function, and therefore recommend research into the interactions between these extremes and the soil. Reichstein *et al.* (2013) suggest future research should address the effect of these extreme events on the mechanisms driving C cycling at ecosystem scale. Frank *et al.* (2015) emphasise the need for regional investigations of the interactions between the carbon cycle and extreme events, to allow for global upscaling of the impacts of climate extremes on carbon-climate feedbacks. This study aims to add to this growing area of research.

7.2 Data & Methods

7.2.1 *Observed Climate Data*

EObs data (outlined in the previous chapter) was utilised with Ireland extracted for ease of processing. The land area representing Ireland was extracted to reduce the file size and to increase processing speed when generating extreme scenarios, and to ensure extremes were analysed for Ireland only, as temperature and precipitation ranges are much greater in European countries, and extremes are experienced differently across Europe.

7.2.2 *Observed Soil Data*

HWSD soil data (outlined in Section 6.2.4) is used by the Global ECOSSE model to determine soil carbon content. The ECOSSE model has not been validated against N emissions in this study, but has previously been shown to adequately simulate N emissions across European sites (Bell *et al.*, 2011).

7.2.3 *Generating Climate Extremes: Block Resampling*

In order to investigate the potential impacts future extreme weather events may have on soil carbon stocks in Ireland several methods of analysis were considered. These included stochastic weather generation, future climate model runs and block resampling methodologies.

While future climate model runs have sometimes been considered the 'most reliable and robust method available' (Prudhomme and Davies, 2009; Murphy *et al.*, 2004), model projections are limited by the large range of climate model outputs across emissions scenarios and model intercomparison projects, which often does not serve as an adequate driver of factors which affect regional or local scale processes (e.g. rainfall) and can have significant uncertainties associated with it, which increase as further granularity is added (a 'cascade of uncertainty'; Wilby and Dessai, 2010). These uncertainties have not been improved upon in the CMIP5 range of models when compared to CMIP4, as the addition of more processes and observations to the models did not result in a reduction in uncertainties (Knutti and Sedláček, 2013). While our understanding of the systems has increased, the modelling of these additional processes means the models are now more complex and represent a more intricate understanding of the climate system, there remains an inability to perfectly model the hugely complex atmospheric processes which affect and are affected by climate change (Knutti and Sedláček, 2013). The ranges of output by different climate models across future climate scenarios have significant uncertainty and display large variability, and projections can be complicated to the point of being contradictory when choosing one model over another, they are also computationally expensive to run and take up large amounts of storage. Reichstein *et al.* (2015) call for an improved experimental approach which measures impacts at plant and ecosystem levels in order to delineate the differential responses of ecosystem components including soils. Frank *et al.* (2015) call for future experiments to assess the lagged and legacy effects of extreme events on ecosystems, including the response of systems to multiple climate extremes, in order to elaborate on the mechanisms and processes at large, this information would serve to improve biogeochemical models and their treatment of extreme events.

For the purposes of this analysis a block resampling methodology similar to that of Prudhomme and Davies (2009) was employed using EObs climate data from 1951-2017. Prudhomme and Davies (2009) argue that three-month (seasonal) resampling is preferable to 1-month resampling in order to maintain the seasonal structure of variables sampled. This method is utilised in the present research to better represent soil moisture. Analysis is performed on the data to extract extreme seasons for warm, cold, wet or dry seasons based on percentiles above 0.8 for extreme hot/wet, and below 0.2 for extreme cold/dry, so that the 'extreme' seasons are only those which are anomalous to the observed record, meaning the extremes are realistic for the location as they have occurred in the past. Those seasons which are not extreme are also available to select from as 'normal' seasons. The methodology allows for selection of deterministic sequences of seasons or years, making it possible to choose 'normal' or 'extreme' years or seasons in whatever order the user desires. After a block is resampled it remains available to be sampled again, ensuring there is always data available for any length of a new series. A new climate series is then derived from a random selection of seasons, respecting the annual sequence. For example, to test the influence of a heat wave the sequence of 10 'normal' years followed by an anomalously hot summer could be generated, along with any permutations of warm, wet, dry and cold seasons can be selected in whatever order desired. A comprehensive example of the block resampling code is printed in Appendix B for Temperature, the full code in the form of jupyter notebooks (Python 2.7) is available here (https://github.com/podgeflat/block-resampling). The process can be summarized as follows:

- EObs NetCDF data from 1950-2017 for temperature and precipitation downloaded
- Each year divided into seasons (3-month blocks: DJF, MAM, JJA, SON) using December from the previous year as the first winter month, to respect the climatological sequence.
- Observed series separated into four sub-series containing 3-month blocks of the same season (winter, spring, summer, autumn).
- Each block consists of daily rainfall or temperature, which the model uses to calculate PE using the Thornthwaite method (Thornthwaite, 1948).
- Anomalies are calculated based on differences in seasonal averages/sums of temperature/precipitation compared to the long-term averages/sums.
- Quantiles are used to determine which seasons can be considered 'extreme', if a seasonal anomaly falls below 0.2 or above 0.8, the season is considered 'extreme' and is noted in a list.
- The methodology allows for the sampling to be entirely random, or entirely deterministic, for example it is possible to select a number of random 'normal'

years, or a number of random 'extreme' years, or a combination of the two, depending on the requirements of the investigation.

- The selections respect the annual sequence (i.e. a spring block selected after a winter block). Though this can be changed if the user desires.
- Each seasonal block is selected independently from the preceding one so that two consecutive blocks may not be selected from the same year they were recorded.
- After a block is resampled, it is put back into the corresponding sub-series (winter, spring, summer, autumn) so that the same block can be selected more than once, and some blocks may not be used at all.
- Changes in multi-season extremes are facilitated by allowing observed blocks (even the largest) to be resampled more than once in a resampled series.
- New extreme datasets are then joined to existing EObs data using a utility tool provided with GlobalECOSSE.

This method only resamples observations from 1950-2017 and may not capture historical natural variability for the same location outside the records, or variability for different locations. It also excludes possible future extreme seasons which are outside the range of extremes that have already been observed.

7.2.3.1 *Extreme Storylines*

In future under a warmer climate extreme events will increase (Seneveritne *et al*., 2012), the incidence of extreme events is highly dependent on the changes in radiative forcing associated with the pathways of human activity (IPCC, 2018). Due to computational limitations it is not possible to run numerous climate scenarios to get a range of potential responses of Irish soils to future climate change. It is still useful to assess the potential impacts extreme events will have on soil carbon emissions, particularly when the response of soil to warming is still a widely debated topic in soil science (e.g. van Gestel *et al.*, 2018; Crowther *et al.*, 2018; Xiao *et al.*, 2018; Hicks Pries *et al.*, 2018), and the models are not yet capable of accurately representing responses to future warming as we still do not understand the entire soil system. Running multiple climate model scenarios will therefore give a range of outputs, with very little confidence in any, and will not be useful for policy prescriptive purposes. We do, however, know that soil responds strongly to extreme events (Reichstein *et al.*, 2013) and that these extreme events will be more likely in future as changes in the mean climate will result in changes in the extremes (Seneveritne *et al.,* 2012), for that reason it is still very useful to investigate the potential impact climate extremes will have on soil GHG fluxes, in order to anticipate the degree of shock which may be felt from a range of different extreme scenarios.

For the purposes of this analysis, several possible extreme climate storylines were defined and compared to a notional baseline climate in order to investigate the impact of potential shocks. These storylines select randomly from the climate series meaning temperature and rainfall regimes are realistic as they have previously occurred in the observed record. As the incidence of cold extremes is highly likely to decline in future, storylines will be based on high temperature extremes along with both 'normal' and 'extreme' precipitation. This analysis will thus compare a control climate set consisting of 10 years of 'normal' precipitation and temperature data to the impact of 10 years of:

1. Hot climate
2. Very hot climate
3. Hot and dry climate
4. Hot and wet climate

Where 'hot' consists of seasons where the average temperature anomaly is greater than the 80th percentile, very hot is greater than the 90th, hot and dry has temperatures greater than the 80th percentile and rainfall below the 20th percentile, while hot and wet consists of temperatures and rainfall greater than the 80th percentile. Tian *et al.* (2015b) argue that large increases in both CH_4 and N_2O emissions are likely in future and therefore these GHGs along with CO_2 must be considered simultaneously when evaluating effective, efficient mitigation policy. These variables were therefore converted from their atomic to molecular mass (CO_2: 44/12, CH_4: 16/12, N_2O: 44/28) and then to their 100-year global warming potential (GWP) value by multiplying by a factor from IPCC (2007) values (CO_2: 1, CH_4: 23, N_2O: 296).

7.3 Results

7.3.1 *Observed Changes in Temperature Extremes*

Figure 7.1 illustrates observed changes in extremely warm summers and cold winters from the EObs climate dataset. Warm summers are increasing and cold winters are decreasing over the observed period, with notable warm summers 1995 and, as well as the winter of 2010, the coldest winter for 50 years, and the cold winter of 2011 (Met Éireann, 2018a).

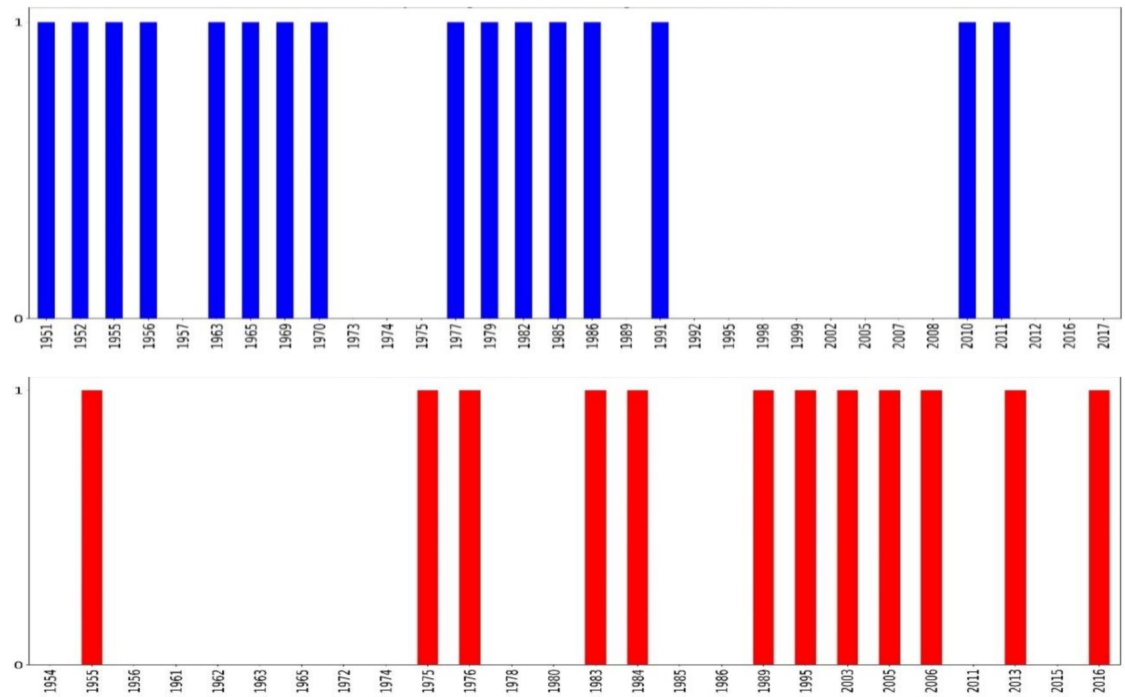


Figure 7.1: Occurrence of extremely cold winters (top) and warm summers (bottom) over the period 1950-2016, 'extreme' seasons are defined as those which are >0.8 or <0.2 percentiles from the mean value.

7.3.2 *Observed Changes in Precipitation Extremes*

Changes in precipitation extremes are less seasonally distributed than temperature and can occur at different times of the year, they are therefore presented as annual seasonal sums (counts of extreme seasons in each year), and are shown here (Figure 7.2) as extremes of wet and dry. Again this allows for testing of the veracity of the methodology used, by comparing to annual reports from Met Éireann (Met Éireann, 2018b), where on examination of the annual report for 2012 it is clear that one season had particularly high rainfall (summer 2012) while the others had below average rainfall, this is reflected in Figure 7.2 where one extremely wet and three extremely dry seasons are evident.

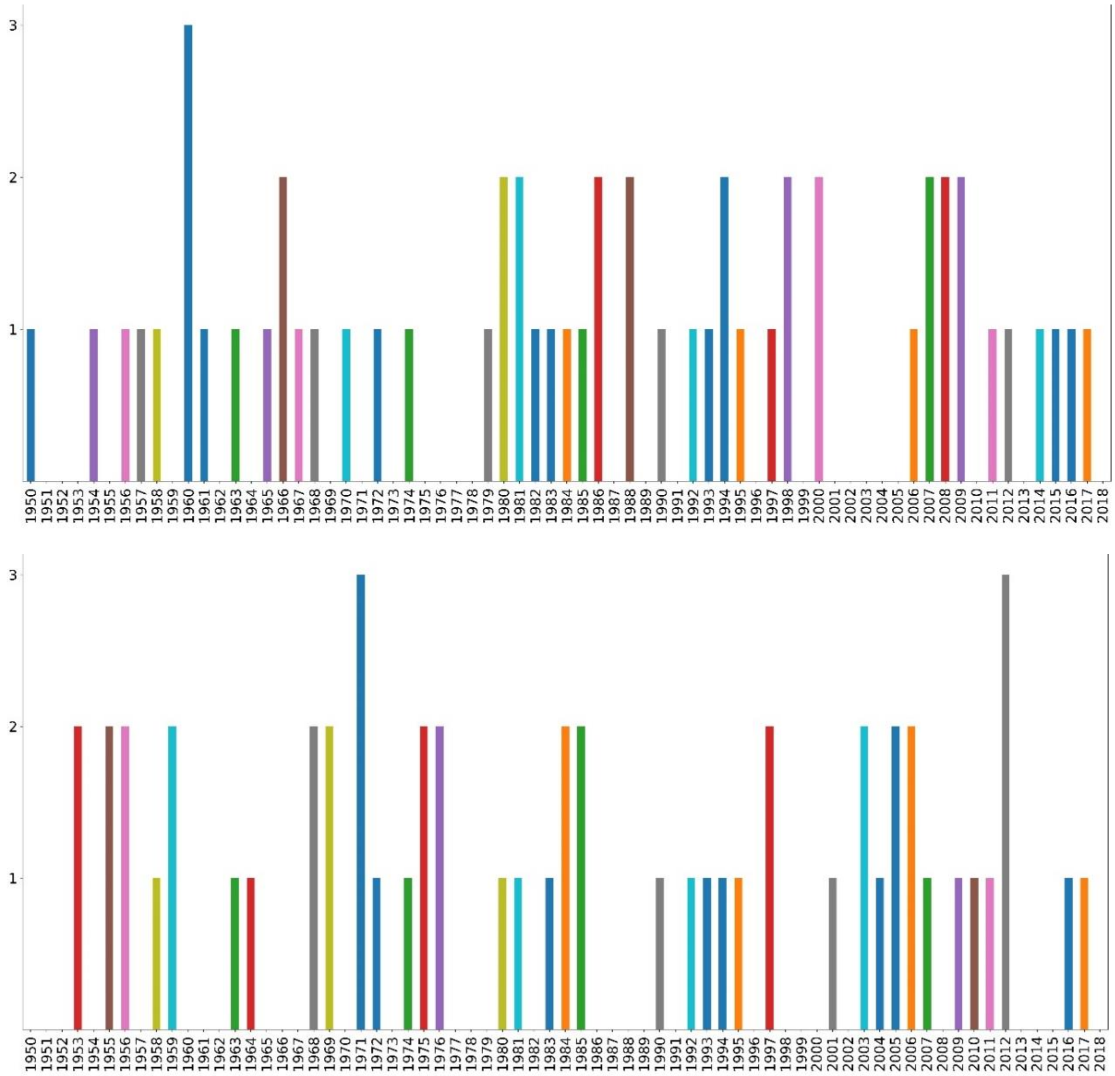


Figure 7.2: Occurrence of wet (top) and dry (bottom) extreme seasons on an annual basis for the period 1950-2017, 'extreme' seasons are defined as those which are >0.8 or <0.2 percentile values above or below the mean values

7.3.3 *Assessment of Extreme Events*

7.3.3.1 *Normal Temperature & Precipitation (control)*

Figure 7.3 outlines the annual CO_2 emissions when the Global ECOSSE model is run using 'normal' weather, where most years show relatively low CO_2 emissions. This is used as the 'control' climate, and extreme scenarios are differenced from this control to determine the relative response. Figure 7.4 outlines the seasonal pattern of different GHG emissions, with highest CO_2 emissions during summer, and lowest in spring and autumn, NO_3 emissions are consistent throughout the year, N_2O emissions peaking during spring, and CH_4 sequestration highest in summer with emissions highest during winter.

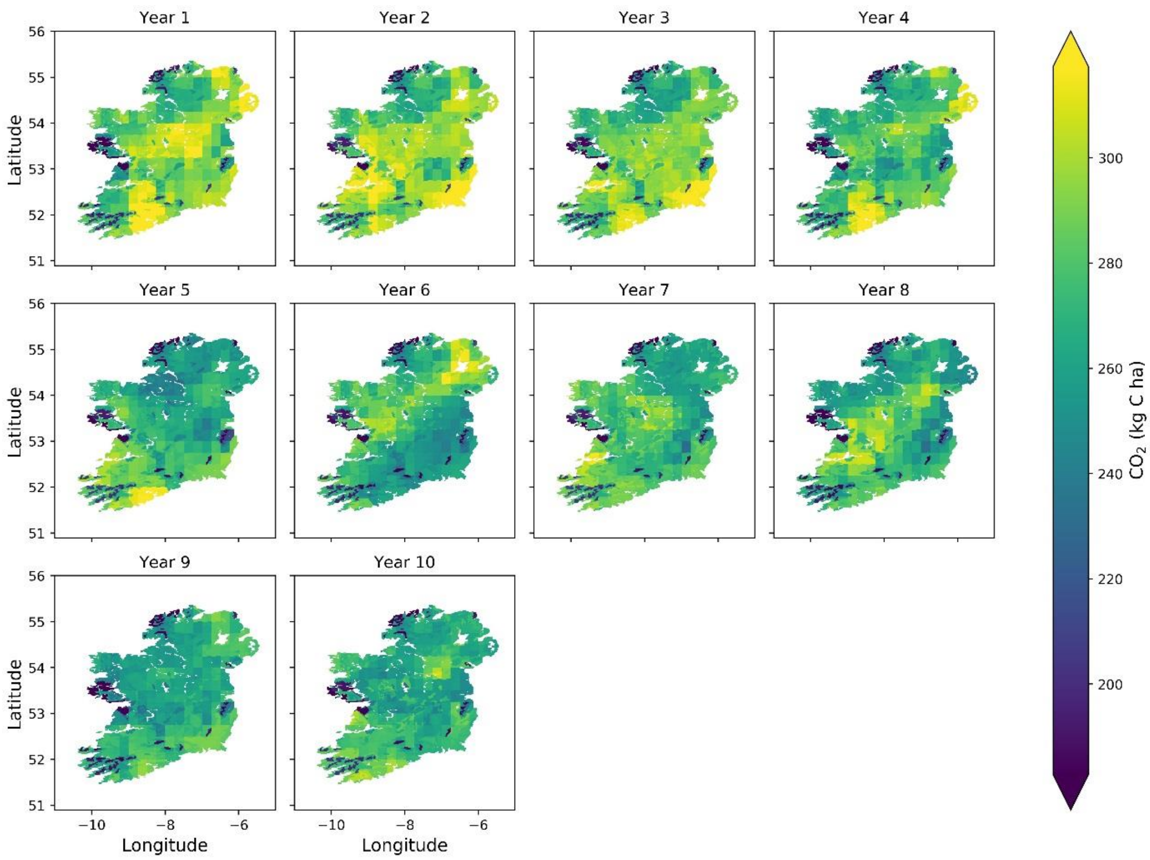


Figure 7.3: CO_2 output running 10 'normal' years of data where seasons within the 0.2 and 0.8 percentiles were selected at random to run the model

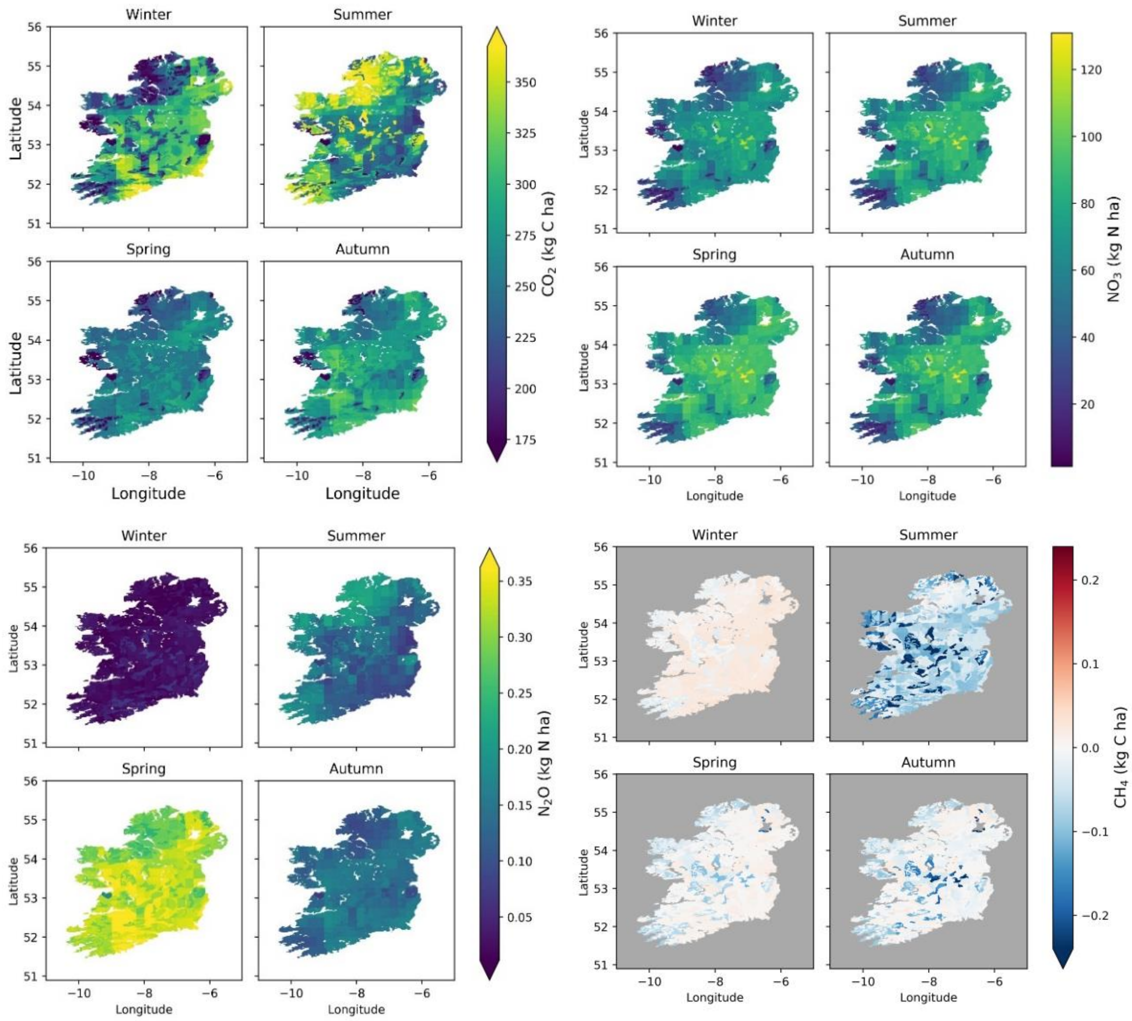


Figure 7.4: Average seasonal GHG model outputs for CO_2, NO_3, N_2O and CH_4 from running the model using 'normal' data for 10 years. CH_4 uses a different colour ramp to illustrate sequestration and emission.

Figure 7.5 shows average CO_2 emissions for the 10-year period with highest emissions observed in the midlands, south and southeast, and lowest emissions in the northwest and upland areas. Examining the average SOC across the country in year 1 and year 10 (Figure 7.6) indicates that SOC does not fall significantly over the period, over the 10 years average annual SOC declined by 0.31%. This equates to 0.031% per year and is lower than the grassland decline calculated in Section 6.3.8.1, as the extremes which naturally occurred during those years are not included in this dataset. Emissions for the 10 'normal' years are consistently lower than those outlined for the years 2001-2017 in the previous chapter (Figure 6.13), as the extremes experienced in those years have not been included in this control version.

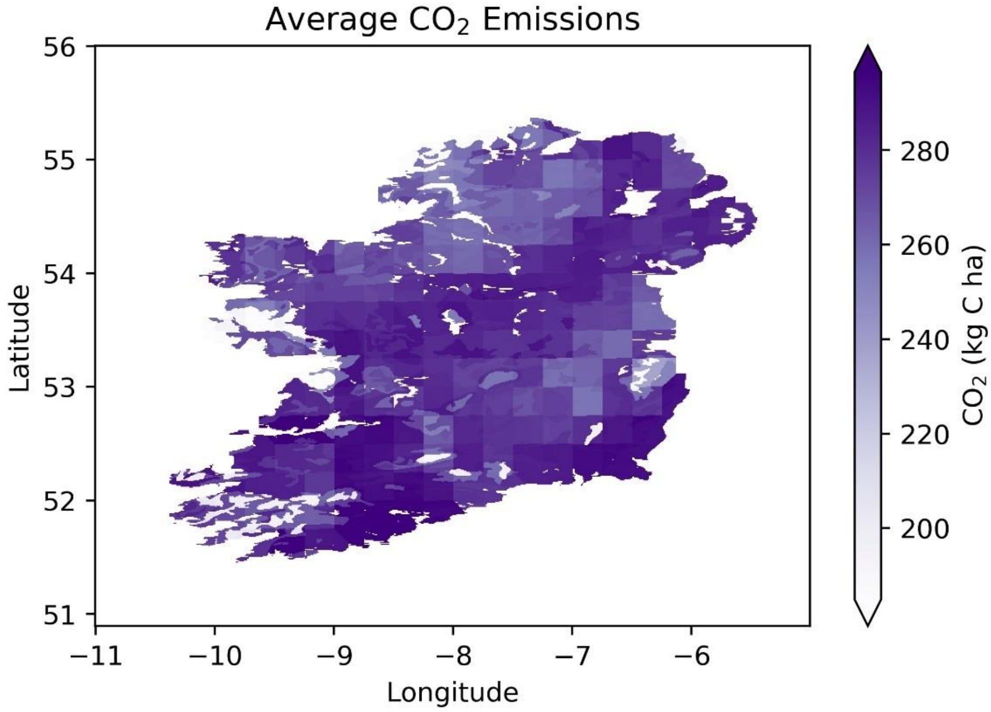


Figure 7.5: The average in CO_2 emissions over the 10-year period of normal weather

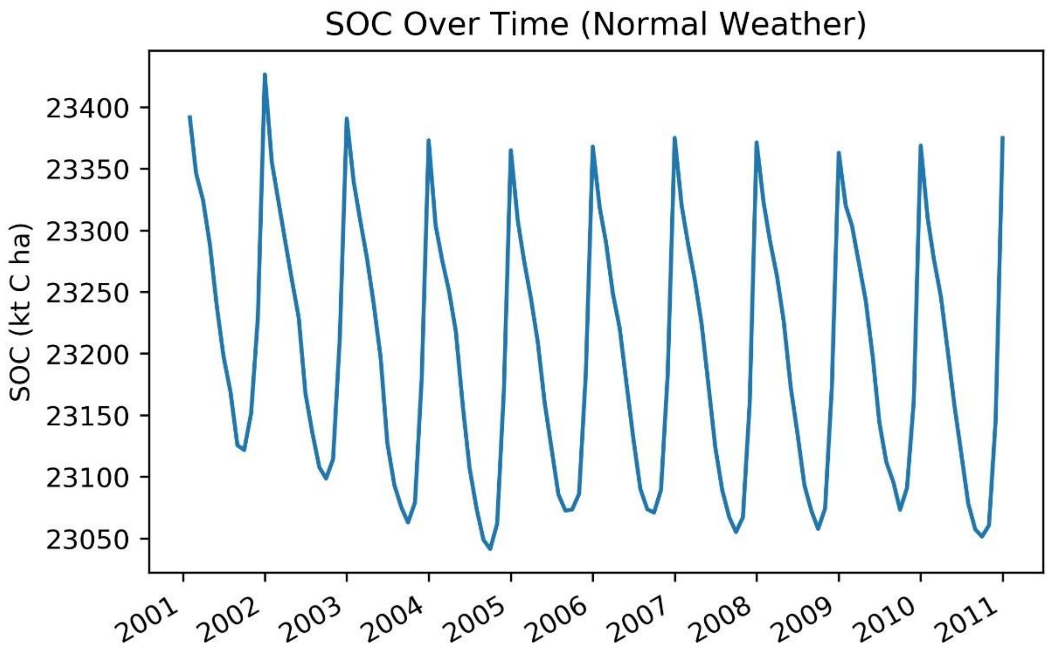


Figure 7.6: Average SOC from Irish soils over time for the control model run using 'normal' non-extreme weather

7.3.3.2 *Hot Temperature, Normal Precipitation*

The model was run using hot temperature data where seasonal average temperatures are greater than the 80th percentile. Precipitation data is within the 20th to 80th percentiles. Figure 7.7 illustrates the 10-year average seasonal responses of different modelled variables to hot temperatures, showing CO_2 increases are highest in winter (indicating winter temperatures no longer suppress respiration) and show decreases during summer, which may be due to excessive drying of the soil with extreme temperatures. NO_3 increases are consistent throughout the year but strongest in autumn. N_2O increases are most significant during spring, while CH_4 does not change significantly in most seasons, except for summer when CH_4 sequestration is higher in soils with high C content.

Figure 7.8 indicates that increases in emissions are most prevalent in the west and northwest of the country, with relatively smaller increases in the east and southeast. Hot weather increases emissions by over 30kg/ha in the most extreme areas. SOC losses over the 10-year period with hot weather extremes are 1.00%, over three times that of 'normal' weather at 0.31%.

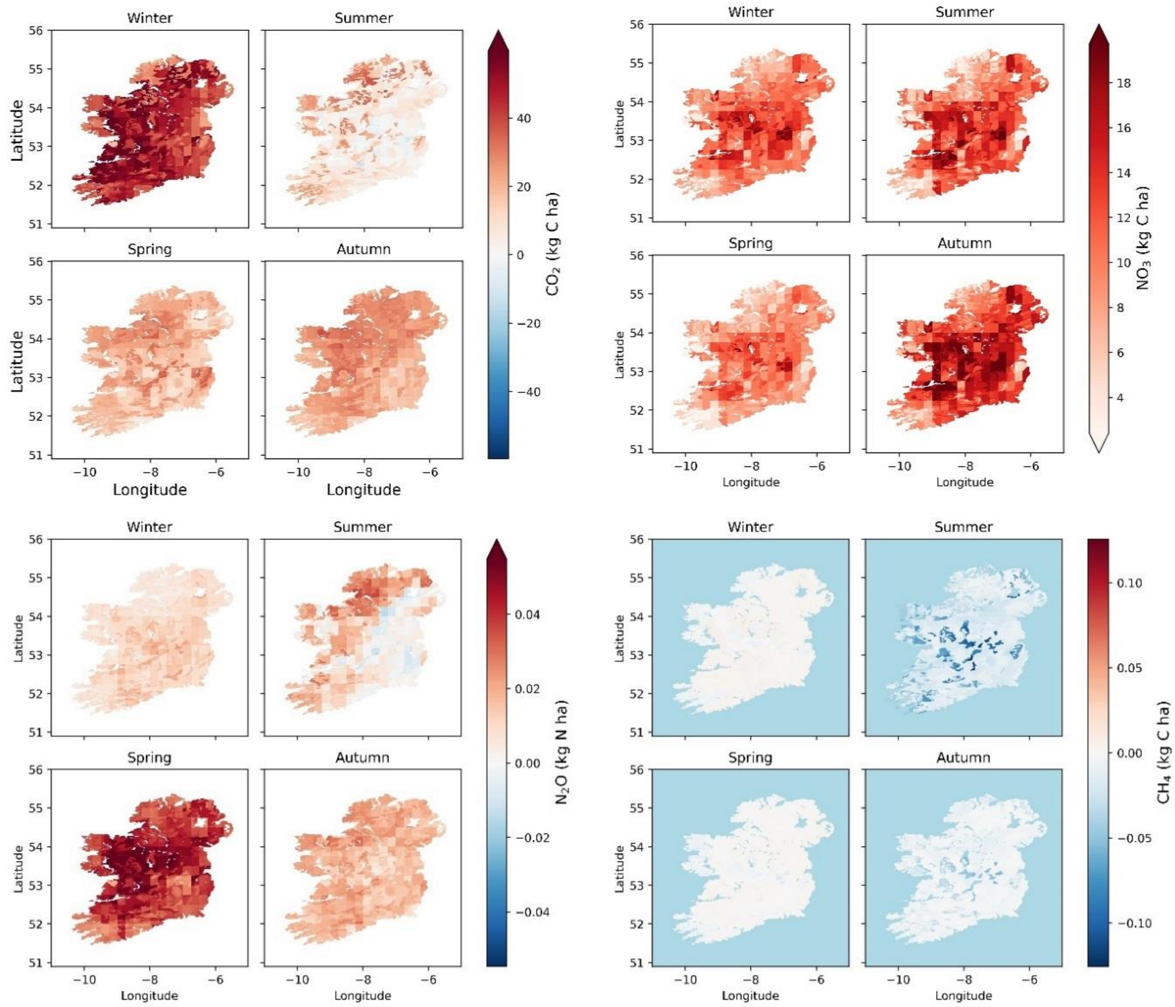


Figure 7.7: GHG model outputs for CO_2, NO_3, N_2O and CH_4 from running the GlobalECOSSE model using extreme hot temperature and non-extreme precipitation data

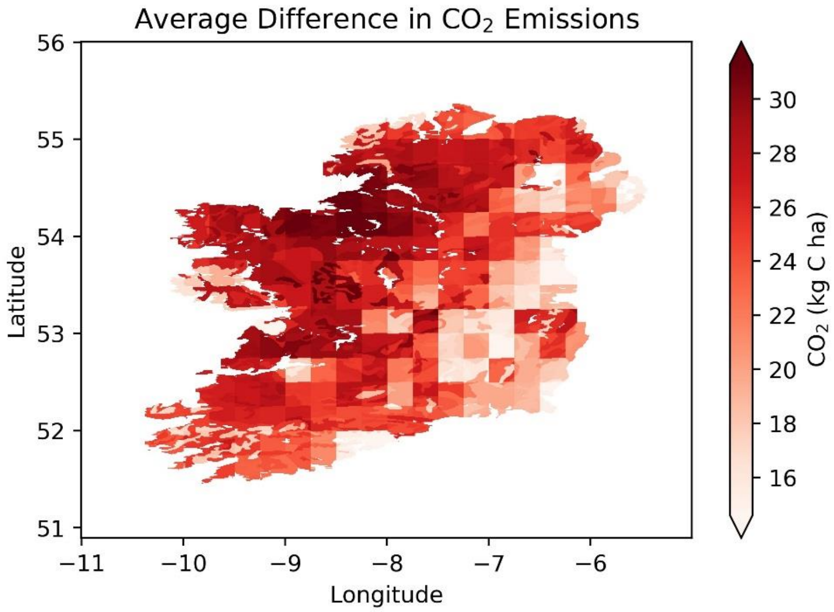


Figure 7.8: The average difference in CO_2 emissions over the 10-year period of hot extreme weather in comparison to the control run.

7.3.3.3 *Very Hot Temperature, Normal Precipitation*

To further test the model's sensitivity to temperature and to investigate the impact of warmer extremes, 'very hot' extreme temperatures were used to run the model, where 'very hot' seasons are those where the seasonal average temperature anomaly is above the 90^{th} percentile.

Figure 7.9 shows the seasonal responses of modelled variables to extreme hot temperatures, comprised of seasons with temperature anomalies greater than the 90^{th} percentile. Results show enhanced emissions during winter, spring and autumn for CO_2 and lower emissions during summer, likely due to excessive soil drying. NO_3 emissions are higher across all seasons, N_2O emissions see the largest increases during spring, increases during winter and autumn, and decreases in some areas during summer. Very hot weather enhances CH_4 sequestration during summer and autumn and has little effect during winter and spring. CH_4 fluxes in Figure 7.9 indicate that temperature drives higher sequestration levels, though the scale of sequestration is relatively small (between -0.08 and +0.08 kg C ha^{-1}) compared to CO_2.

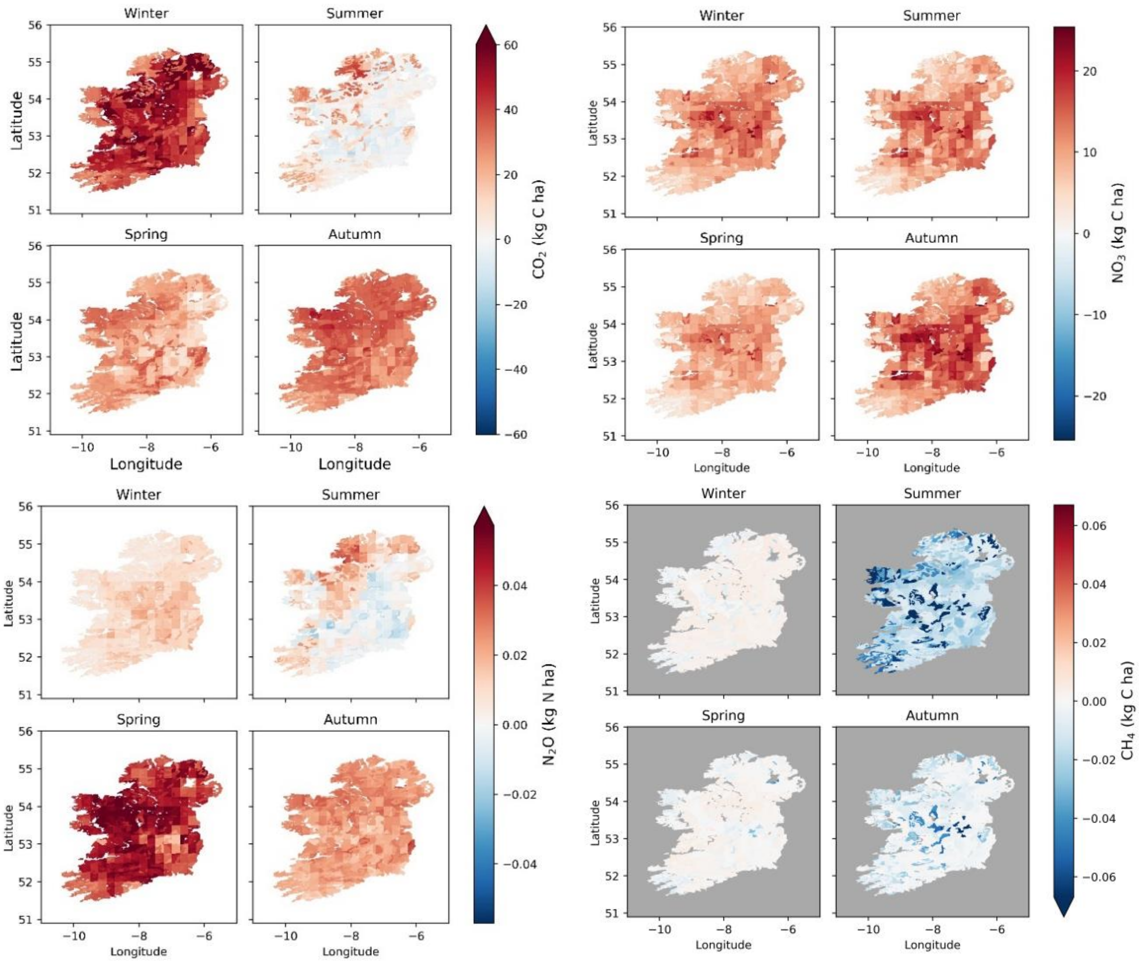


Figure 7.9: GHG model outputs for CO_2, NO_3, N_2O and CH_4 from running the model using very hot extreme temperature and normal precipitation data

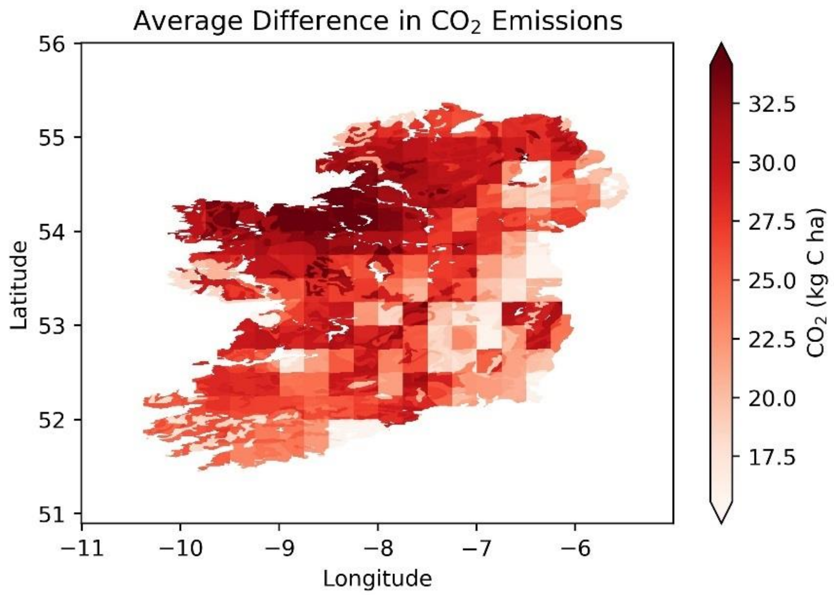


Figure 7.10: The average difference in CO_2 emissions over the 10-year period of very hot extreme weather in comparison to the control run.

Figure 7.10 shows the average difference in CO_2 emissions of very hot extreme weather compared to the control. The scale of these emissions is higher than that of the hot extremes shown in Figure 7.8, indicating that even though emissions are lower in summer, the overall increase in emissions for very hot extreme weather outweighs the decrease in the summer months. Calculating the loss of SOC from year 1 to year 10 of the simulation reflects this, as 1.1% of total SOC was lost over the 10-year period, slightly higher than the 1.00% lost from the '*Hot Temperature, Normal Precipitation'* storyline.

7.3.3.4 *Hot & Dry*

Figure 7.7 shows apparent reductions in emissions during extremely hot weather and normal precipitation during the summer months, perhaps due to excessive drying of the soil. To further test this reaction the model was run using 10 years of extreme hot and extreme dry weather, where seasonal temperature anomalies are above the 80th percentile and seasonal rainfall anomalies are below the 20th percentile. Figure 7.11 shows seasonal responses of modelled GHGs to hot/dry temperature extremes. For CO_2, emissions are significantly lower in summer, autumn and spring for most areas, and are slightly higher during the winter months. This is due to respiration being inhibited due to the lack of water, similar to the reduced fluxes resulting from dry soils in Chapters 4 & 5.

The north-west of the country (Figure 7.11) appears to have higher emissions during most seasons, suggesting that soils here do not dry out as much, or that enough rainfall happens in these regions even in extreme drought conditions for the country, that soils do not dry out enough for respiration to be inhibited. The west coast of Ireland sees increasing emissions during winter, spring and autumn, as the west coast receives more rainfall than the rest of the country. Increases in respiration during winter are likely due to the high rainfall during the winter months, even when an extremely dry season is chosen, it is not dry enough for respiration to be inhibited during winter. NO_3 emissions are higher across all seasons, with significant increases in the high C soils in the midlands of the country, over 80 kg N ha^{-1} higher than the control period. Emissions of N_2O are higher in winter and much lower in spring and summer, while the majority of areas are lower in autumn. CH_4 emissions are very similar in winter and spring, with enhanced sequestration during summer and autumn, particularly in high-C soils.

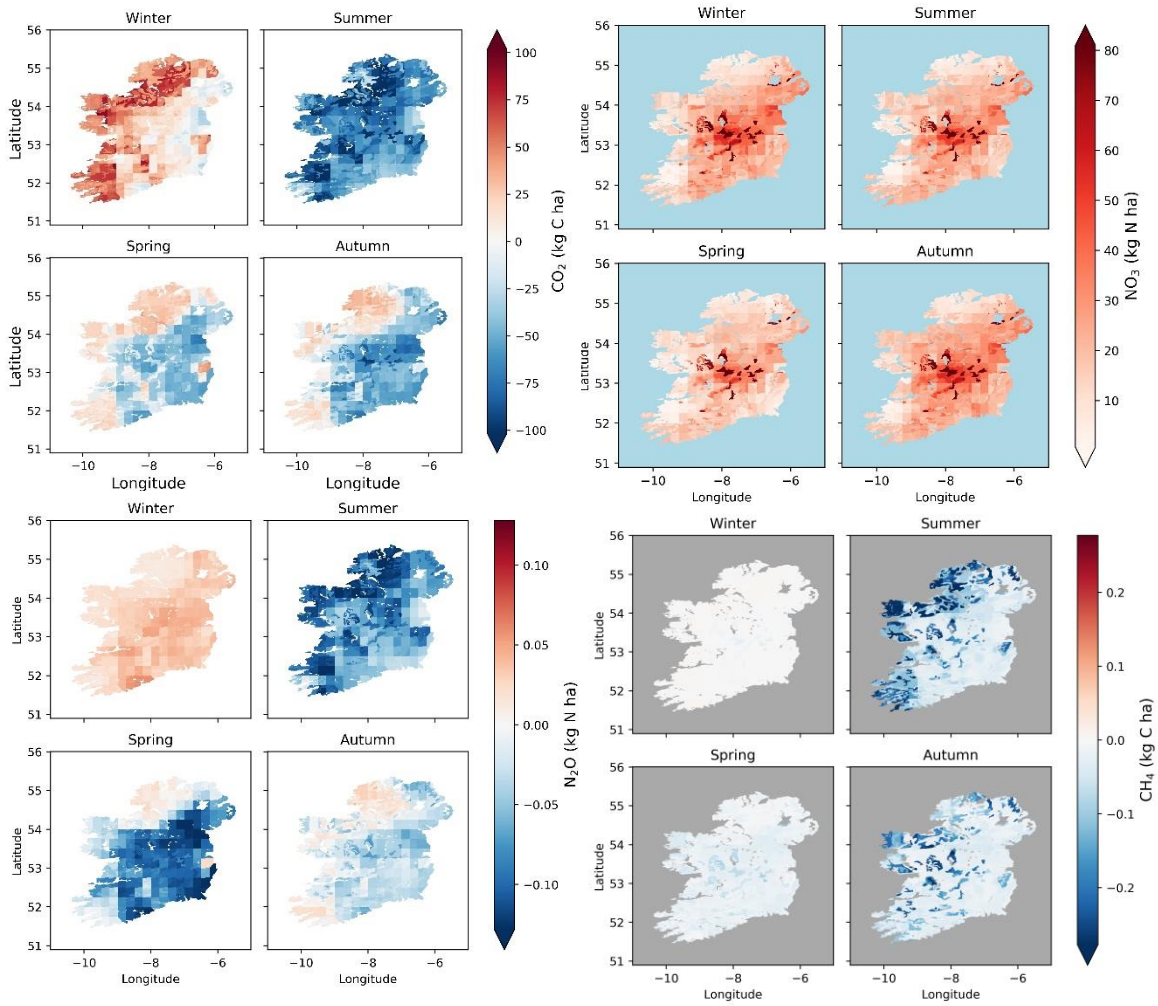


Figure 7.11: GHG model outputs for CO_2, NO_3, N_2O and CH_4 from running the GlobalECOSSE model using hot and dry extreme weather data.

Figure 7.12 shows the average difference in CO_2 emissions between the control and the hot/dry scenarios, where CO_2 emissions are higher in the northwest, west and southwest, and significantly lower in the rest of the country. The dry weather clearly inhibits soil respiration in most areas except for those areas which receive high enough rainfall levels for soil respiration to continue uninhibited. Hot/Dry extremes caused losses of 0.84% over the period, less than hot and very hot extremes, but still higher than the 0.31% from normal climate data.

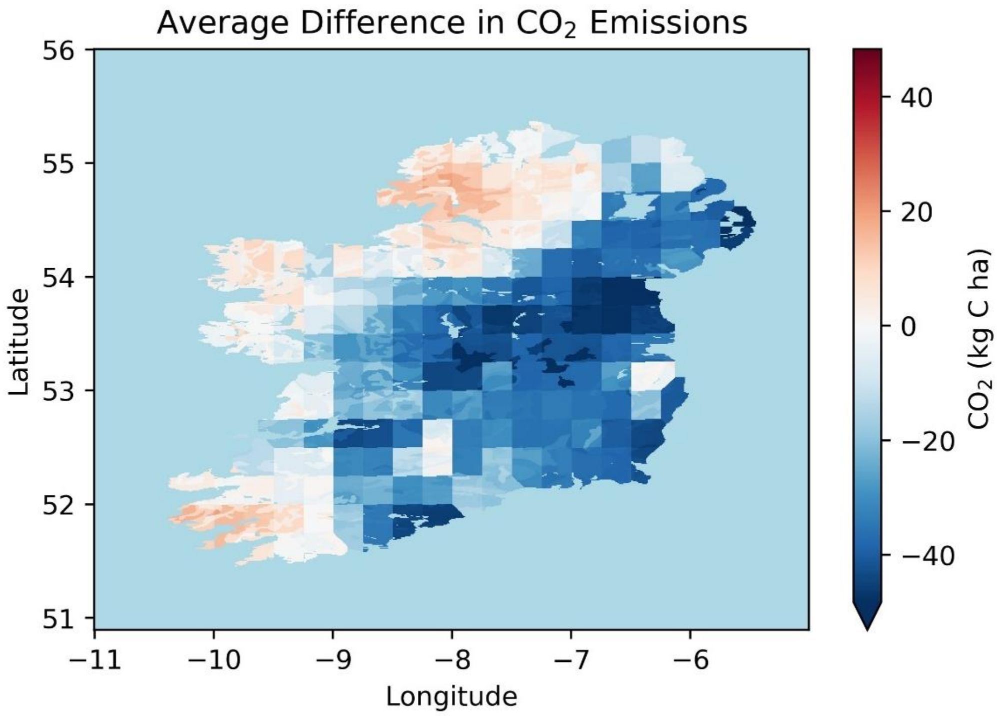


Figure 7.12: The average difference in CO_2 emissions over the 10-year period of very hot extreme weather in comparison to the control run

7.3.3.5 *Hot & Wet*

As very hot extreme temperatures (Section 7.3.3.3) and dry temperatures (Section 7.3.3.4) caused emissions to be lower in certain areas, this is likely due to drier soils inhibiting respiration, to test this the model was run using extreme hot and wet weather (temperature and rainfall seasonal anomalies greater than the 80th percentile) to investigate the modelled responses. Emissions are higher than the control for most GHGs in most seasons with the exception of NO_3 (Figure 7.13). Figure 7.14 shows the differences between the control run and the hot/wet run, with emissions in most areas much higher than observed in all other scenarios, with differences in emissions of over 150 kg C ha^{-1} in this case compared to over 60 kg C ha^{-1} for the hot and very-hot scenarios. This indicates that the increased rainfall does not allow the soil to dry out and therefore emissions are enhanced. This increase is most pronounced during summer in the southeast of the country. NO_3 emissions are more varied, with emissions decreasing during spring and summer, and increasing during winter and autumn, though these increases are not observed in the west and northwest of the country where decreased emissions are evident. The scale of difference in emissions here is lower than observed during the hot/dry extreme sequence, as increases and decreases are no higher than ~25 kg N ha^{-1} compared to the increases of > 80 kg N ha^{-1} from the hot/dry sequence. N_2O emissions during winter are not significantly different from the normal run, with increases highest during summer, then spring, then autumn. Changes in CH_4 emissions are negligible in winter and spring, with increased emissions observed during summer and autumn, again in soils with high C content.

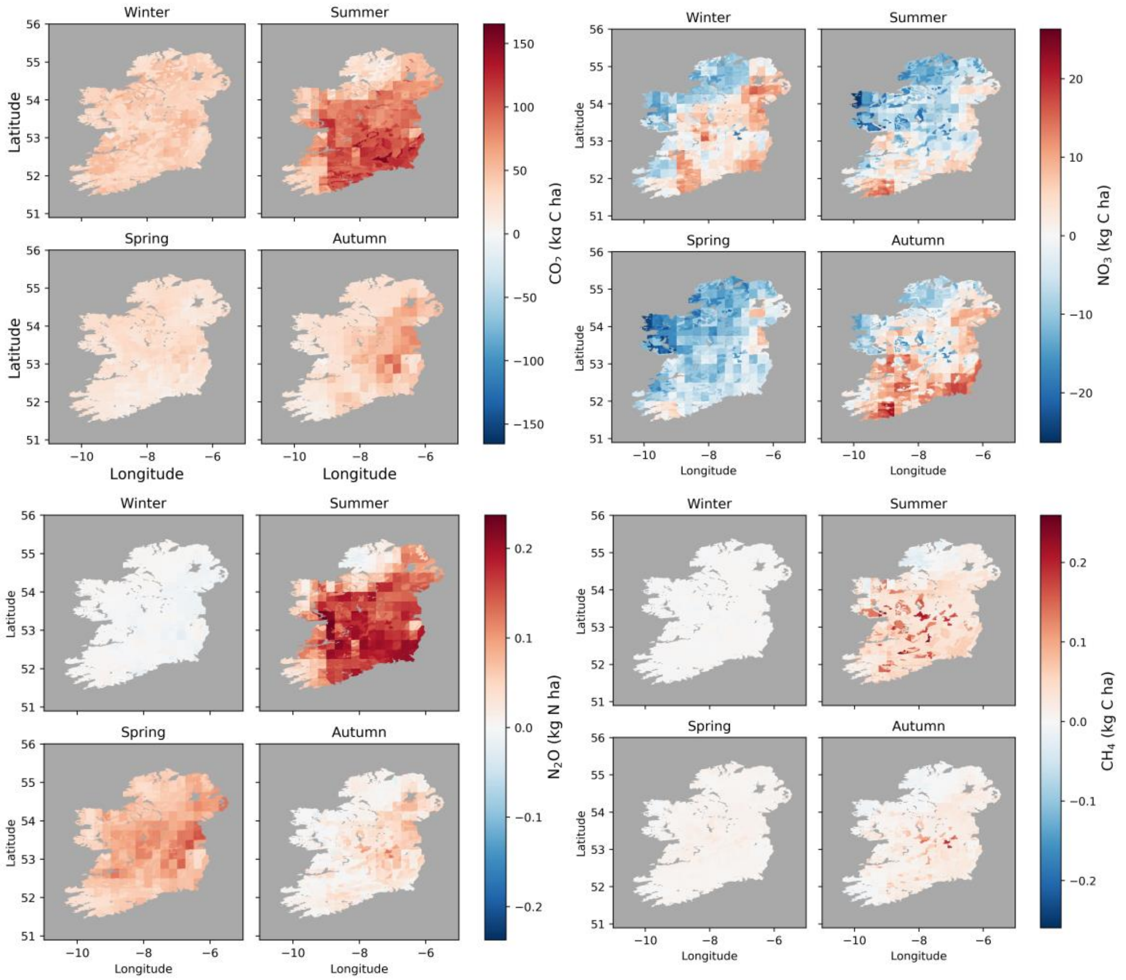


Figure 7.13: GHG model outputs for CO_2, NO_3, N_2O and CH_4 from running the GlobalECOSSE model using hot and wet extreme weather data

Figure 7.14 shows the average difference in CO_2 emissions between the control and the hot/dry scenarios, where CO_2 emission increases in all areas, but increases are lower in the northwest, west and southwest, and higher in the rest of the country. The wet weather does not allow soil respiration to be inhibited, leading to much higher annual average fluxes. Hot/Wet extremes caused losses of 2.1% over the period, well above hot and very hot extremes, and significantly higher than the 0.31% from normal climate data.

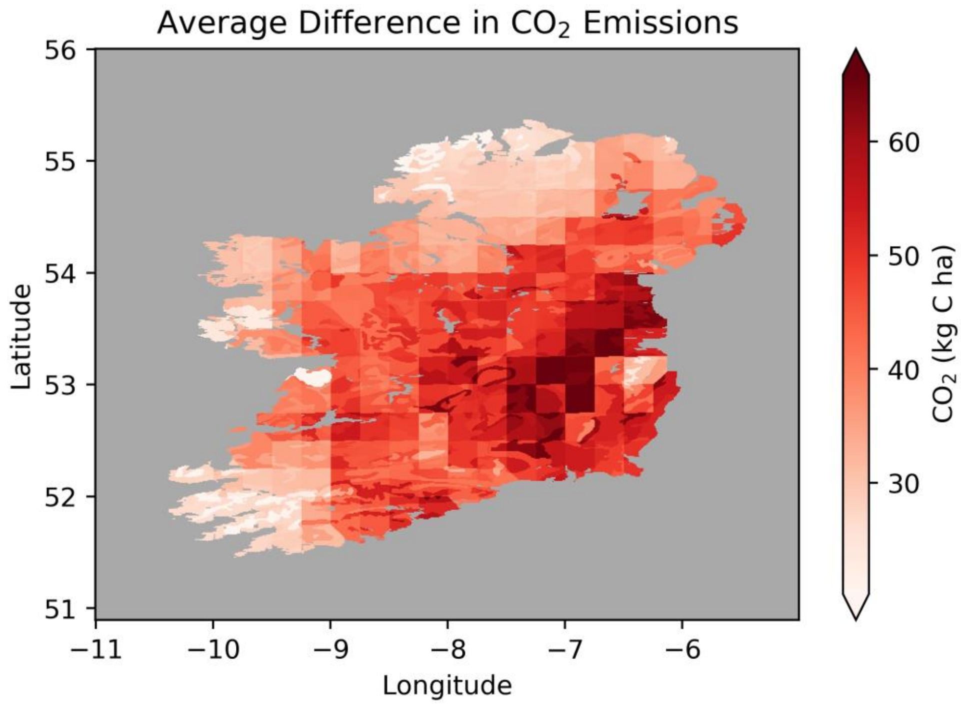


Figure 7.14: The average difference in CO_2 emissions over the 10-year period of hot and wet weather in comparison to the control run

7.3.3.6 *CO_2 Equivalent Maps for Each Run*

Figure 7.15 illustrates the results of calculating CO_2 equivalent values for all GHGs, which follow the pattern of individual emissions with highest emissions from the hot/wet scenario and lowest from the 'normal' scenario. The GHG maps give a better picture of the fluxes of GHGs, normal climate sees most of the country as a GHG sink, while the hot and very hot scenarios show increasing GHG emissions across the country, and the hot/dry scenario showing reductions in emissions due to the inhibition of respiration and other GHG fluxes. The hot/wet scenario sees most of the country become a source of GHGs. The normal climate sees more sequestration than averages in the previous chapter, showing the influence of removing extremes.

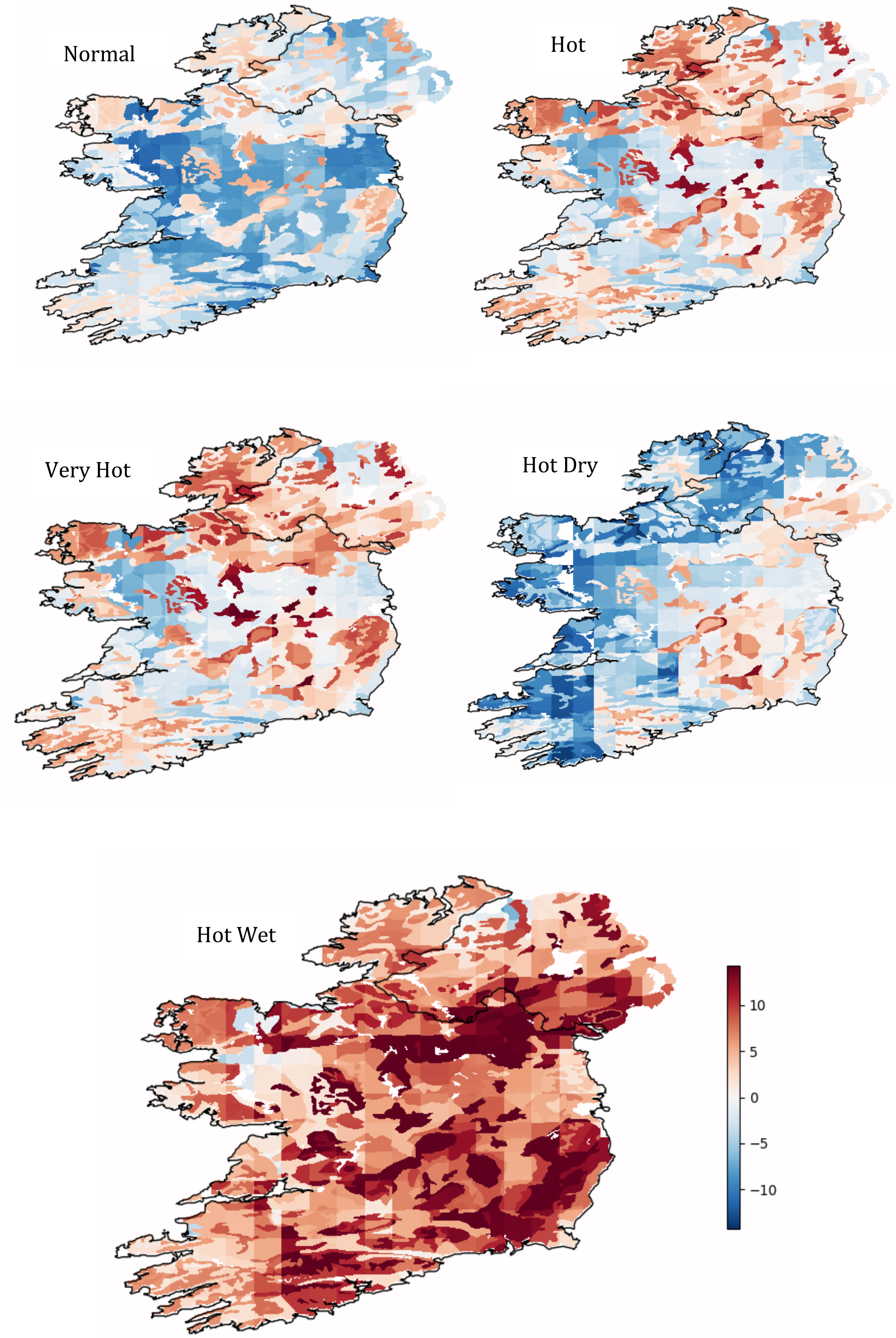


Figure 7.15: GHG CO_2 equivalent fluxes for normal and extreme weather runs, units in kg C ha-1, scale is identical for all maps.

7.4 Discussion & Conclusion

In Ireland the incidence of extremely warm summers is increasing, while the incidence of extremely cold winters is decreasing according to analysis of the EObs dataset (Figure 7.1), agreeing with observed trends in Irish climate (Walsh and Dwyer, 2012). This also agrees with global trends towards a shift in the mean climate towards a warmer state, with more frequent and intense hot extremes, and fewer cold extremes (Seneviratne *et al.,* 2012).

7.4.1 *Carbon*

The climate observations were used to create scenarios of changes in extremes to assess potential responses of Irish soils to extreme events. The findings indicate that soil carbon emissions will increase when temperature alone increases, as is to be expected as respiration typically increases with increasing temperatures in all climates and land-use types (Lloyd and Taylor, 1994; Bond-Lamberty and Thomson, 2010; Wu *et al.*, 2011). Running the model for hot/dry scenarios showed respiration is inhibited strongly in summer, likely due to excessive drying of the soil, and is enhanced in winter as even dry winters in Ireland do not appear to be dry enough to inhibit respiration, particularly on the west coast (Figure 7.11). Soil respiration is typically lower in dry conditions and increases to a maximum at intermediate moisture then declines when oxygen becomes excluded (Xu and Shang, 2016), and the typical positive relationship between soil respiration and temperature is known to be constrained by the availability of soil moisture (Wood *et al.*, 2013), indicating that the model is responding correctly to environmental changes. Reichstein *et al.* (2013) note that ecosystem respiration declined during the 2003 heat wave, though GPP also declined causing the reduction in sequestration observed (Ciais *et al.*, 2005).

7.4.2 *Nitrogen*

Experimental evidence shows increases in soil nitrogen mineralisation in response to increasing temperature, to a point of 25°C, and that N mineralisation is highest when soil moisture content is between 80-100% of field capacity (Guntiñas *et al.*, 2012), indicating that N emissions should increase as temperature and moisture increase. Modelled results show increases in both NO_3 and N_2O for the hot and very hot scenarios in all seasons except summer, where some decreases in emissions compared to the normal run are observed. N leaching is shown to be enhanced with increasing temperatures, particularly with increases 2°C above normal (Jabloun *et al.*, 2015). When hot-dry emissions are examined (Figure 7.11) emissions are significantly enhanced for nitrate, and are reduced in all seasons but winter for nitrous oxide, indicating that N_2O fluxes are more moisture dependent and are inhibited when moisture is limited, as is the case in reality where water filled pore space is positively correlated with increased N_2O emission (Smith *et al.*, 1998b; Unger *et al.,* 2010). Hot/wet temperatures saw increases in N_2O emissions in all seasons except winter, again behaving as is expected (*ibid*). Changes in N_2O emissions across scenarios are relatively small (±0.1 kg N ha^{-1}) as they are typically enhanced by agricultural fertilizer use, an activity not included in these model runs. NO_3 emissions under the hot/wet scenario are variable, with increases in winter and autumn on the east coast and decreases in the west, the opposite spatial pattern in summer, and decreases across most of Ireland during spring, making interpretation of these results difficult. NO_3 emissions are highest from high-C soils, during the hot, very hot and hot/dry scenarios, which is known to occur in N mineralisation studies (Liu *et al.*, 2017). The pattern is less apparent during the hot/wet simulation. The ECOSSE model was observed by Zimmermann *et al.* (2018) to perform well on grasslands but strongly overestimated N fluxes on arable sites, which should also be acknowledged when interpreting these results as N_2O emissions may also be underestimated here. As manure and fertilizer applications are not simulated it is highly likely that modelled N_2O emissions are lower than they would be in reality.

7.4.3 *Methane*

Hot and dry weather acts to enhance CH_4 sequestration during the warmer months, a finding contrary to observations which show methane emissions increase significantly with temperature where water is non-limiting (Yvon-Durocher *et al.*, 2014), indicating that even on peat soils the model may be drying excessively. Hot, very hot, and hot/dry extreme scenarios enhanced methane sequestration, however the hot/wet scenario showed emissions to increase on the same soils, indicating that the lack of moisture may be inhibiting CH_4 emission in the model, though this does not seem to be the case in observations where methane production is observed to increase with increasing temperatures (van Hulzen *et al.*, 1999). It has been observed that soil hydrology is a significant control on methane emission, with methane uptake increasing as soil moisture decreased, while emissions are high when water table depth is low in typically wet soils (Christiansen *et al.*, 2016), likely explaining why methane emissions are so prominent in the high C soils of Ireland under hot and wet conditions. Changes in methane emissions across scenarios are relatively small also, with ranges from ± 0.2 kg C ha^{1}, indicating that these fluxes may not be very significant. Renou-Wilson & Wilson (2018) assess the potential impact of climate change on Irish peatlands in future, projections indicate that CO_2 emissions from peatlands will be enhanced on drained peat soils causing a positive feedback on climate change, while rewetted peat soils have lower CO_2 emissions and some are likely to remain as sinks under future climate change. This enhanced CO_2 emission as a response to warmer temperatures from peatlands is not shown in the Global ECOSSE spatial simulations, indicating that improvements to the simulation of emissions from peat soils need to be considered in future model developments. In order to fully assess the potential impacts of rewetting and drainage of peat soils it may be useful to allow for the categorisation of peat into categories of drained/rewetted for simulations to account for these effects. The findings of Renou-Wilson & Wilson (2018) also indicate that rewetting of peatlands is to be prioritised as an adaptation measure to protect peat soils from increased emissions resulting from warming temperatures and extreme events.

7.4.4 *CO_2 Equivalents*

Examination of global warming potential files showed the importance of converting emissions to GHG equivalents and highlights the radiative forcing importance of GHGs other than CO_2 as it is evident that most Irish soils under normal climate are sinks of GHGs, but extreme temperatures can turn these areas from sinks to sources, particularly when hot/wet extremes are combined. This is highlighted by Tian *et al.* (2015) who acknowledge the importance of including the three major GHGs (CO_2, CH_4 and N_2O) simultaneously when evaluating climate change mitigation policy. These gases can have amplifying or suppressing effects on the total GHG flux, and are affected differently by changes in management, climate and land-use, meaning their inclusion is essential if a realistic estimate of the ecosystem response is to be made.

Drought conditions enhance GHG sequestration across most of the country, particularly on the west coast (Figure 7.15), a result which may give an incorrect indication of the response of soils to this type of extreme. Lagged effects such as changes to soil microbial community structure and activity (Frank *et al.*, 2015), the initial pulse of respiration after re-wetting of soils (Davis *et al.*, 2010), and enhanced respiration one year after a warm event (Arnone III *et al.,* 2008) are not simulated by the model. Additionally, the suppression of fluxes within the model as a result of dry conditions may not be accurate due to the excessive drying of soils and issues with the water modifier (Chapter 4).

The calculation of GHG equivalents has recently been revised by Etminan *et al.* (2016) who reassess the conversion factors of greenhouse gases to CO_2eq, particularly methane which has a greater warming potential in its short-wave spectrum, meaning previous estimates of GHG projections may have underestimated the impact of CH_4. Methane's 100-year global warming potential is revised upwards by 14% compared to the IPCC (2013), and uncertainties for CO_2 and N_2O emissions are ±10%, indicating that regular revision of GWP calculations is necessary as knowledge advances.

7.4.5 *Uncertainties and Improvements*

As the future climate data used here are sequences of observed past extreme events, it is possible that temperature and precipitation amounts are too low for future scenarios, as future warming may shift the climate into a state where extremes are outside those previously experienced in the observed record. The response of the soil to warming and to warm/wet and drought conditions may be more extreme than the model projections presented here. The definition of what constitutes an 'extreme' event has been questioned by Reichstein *et al.* (2013) who find that defining extremes based on climate statistics alone is not the most ideal way of assessing impacts on ecosystems and the carbon cycle, as what may be considered 'extreme' climatologically may not stimulate an 'extreme' response from the ecosystem. Ecosystems may be affected by different degrees of 'extreme', Reichstein *et al.* (2013) argue that an extreme event should be determined based on the severity of the ecosystem response, not the climatic drivers. Their full definition is "conditions where an ecosystem function (such as carbon uptake) is higher or lower than a defined extreme percentile during a defined time period and over a certain area, traceable to single or multivariate anomalous meteorological variables" (Reichstein *et al.,* 2013, pp. 288). Rolinski *et al.* (2015) outline their methodology for redefining ecosystem vulnerability as "hazardous conditions when the ecosystem is losing carbon over a long time" (pp. 1823), rather than previous popular definitions which focus on weather conditions that form a hazard for an ecosystem (Van Oijen *et al.*, 2014). This method recognises that all ecosystems respond differently to change, and that an ecosystem-specific approach which uses observations to recognise the factors which cause vulnerability for that ecosystem is a better way of assessing the impact of potential future shocks than assuming a generic response to climate changes. The ecosystem-specific approach (if observed data are available) also allows for the linking of ecosystem processes to driver changes, elucidating the complexities of each ecosystem and allowing for more accurate estimation of responses to potential shocks. While the use of ecosystem responses as an indicator of what constitutes extreme is laudable and sensible, unfortunately a lack of observations means this process is not often possible, for example Vicca *et al.* (2014) investigate whether observed soil moisture responses can be used to simulate CO_2 efflux under altered precipitation regimes, finding that it is not possible, likely due to a lack of high-frequency measurements on which to base the projections.

Frank *et al.* (2015) outline the potential direct impacts of droughts on soil respiration and find changes in microbial community and structure are both a direct and indirect effect of drought, while peatland-carbon decomposition due to a reduced water table is regarded as a potential indirect effect. Analysis of the sensitivity of different ecosystem factors to extreme drought found GPP and NPP are typically more sensitive than ecosystem respiration, with the sensitivity increasing as drought severity increased, with a lack of rainfall attributed to the reduction in GPP and NPP, and a lack of moisture in the soil, reduced C input and a drought-induced reduction in soil C content being the causes of the reduction in Rh. As drought severity increased, the response of Rh increased to resemble that of NPP and GPP, and responses varied across mesic and xeric sites showing that the reactions of Rh to extreme drought can vary in magnitude, timescale and can be exacerbated by different mechanisms (Shi *et al.*, 2014).

The response of an ecosystem to a climatic shock may not always be immediate, Zona *et al.* (2014) find a delayed response to extremely warm and dry conditions one year after the initial event, highlighting the complexity of individual ecosystem responses and the need for further investigation of extremes and multiple extreme scenarios (compound events). The impact of drought extremes can have direct impacts on the carbon cycle by affecting plant physiology and soil microbial activity, and lagged impacts including changes to soil microbial community structure and activity (Frank *et al.*, 2015). Drought is known to decrease the rate of soil respiration, though observations have shown that rain events which end the drought stimulate a pulse of soil respiration in mineral soils, this effect varied by site and the degree of soil drainage, the main determinant of soil respiration across sites with different degrees of drainage is still mainly temperature (Davis *et al.*, 2010). Though recent research is indicating that soil moisture and photosynthesis may be more important than previously thought (Zhang *et al.,* 2018). Arnone III *et al.* (2008) find grassland respiration is enhanced one year after an anomalously warm season, offsetting the net ecosystem carbon uptake. The GlobalECOSSE model does not simulate these interactions and feedbacks, which is potentially a source of error in these simulations.

According to the results in Section 7.3, future warming on the west coast of Ireland is more likely to enhance soil respiration during winter due to higher levels of precipitation allowing for respiration to continue uninhibited, however in most areas during the other seasons soil respiration during drought conditions is expected to decrease. Heavy precipitation events (expected to increase as the climate warms; Seneveritne *et al.,* (2012)) can also affect the long-term productive capacity of soils and can cause crop damage/failure as a result of waterlogged soils moving to an anaerobic state (Reichstein *et al.,* 2015). Hot, very hot and hot & dry extreme events are predicted to increase NO_3 emissions, N_2O emissions are expected to increase under hot, very hot and hot/wet extreme events, and decrease under hot/dry extreme events, as grassland are the largest source of N_2O by land-use (Oertel *et al.*, 2016), and grasslands dominate Irish land-use, this should be considered in future extreme analysis studies. CH_4 emissions are expected to decrease during hot, very hot and hot/dry extremes while hot/wet extreme scenarios can be expected to enhance emissions or reduce sinks, particularly in high-C soils. These GlobalECOSSE model runs do not account for changes in land-use or for the implementation of management practices such as changing the cropping regime, irrigation or fertilizer application, which would likely result in changes to these projections, and which should be considered in any future work.

Tian *et al.* (2015a) argue that extensive manipulated experiments are needed to assess the magnitude, distribution and response of Rh to changes in climate, land-use and extreme events to serve as a benchmark for reducing model uncertainty, this data is essential in order to fully assess whether the ECOSSE model is correctly simulating the responses to extremes. In response to the myriad uncertainties associated with these projections, this research recommends the approach of Smith *et al.* (2015) who argue that although more knowledge is needed and more experiments/modelling studies need to be performed to protect soils in the long-term, the best practices for protecting and enhancing soils is already known and many can be immediately implemented. A key recommendation of this chapter is that amid significant uncertainties policy-makers and stakeholders must build resilience into systems to reduce their vulnerabilities to potential shocks. Resilience can be built by increasing soil carbon content in simple ways such as using cover crops and crop rotation, incorporating straw and manure, and moving toward reduced/minimum tillage.

8 Thesis Discussion & Conclusion

8.1 Introduction

This chapter summarises the findings of the thesis, and includes further discussion of soil and greenhouse gases, difficulties in modelling, and interactions between variables which make modelling a challenge. Uncertainties in the modelling process are highlighted, along with directions for potential future research.

The research questions this thesis attempted to answer were:

A. Is it possible to use models to improve national emission estimates for soils and move towards a tier-3 reporting methodology?
B. What is the potential impact of future extreme events on emissions of greenhouse gases from soils?

The aims and associated objectives identified to answer these questions were 1. To investigate whether it is possible to simulate soil carbon emissions from Irish soils by comparing modelled soil carbon emissions to observations at an Irish site, 2. To upscale these emissions to national scale using the GlobalECOSSE model, and 3. To investigate the impact of extreme weather events on quantities and fluxes of GHGs by creating extreme scenarios adapted from observations.

8.2 Summary of Research

Chapter 1 outlined the motivation underlying soil carbon modelling, the links between the global carbon cycle and climate change, and the legal frameworks which emerged from these links. This chapter also described the importance of soil in relation to the carbon cycle and emissions inventories with a focus on Ireland, along with the potential for sequestration. Chapter 2 was an in-depth description of theory, observations and methods of modelling soil GHG emissions. Chapter 3 discussed process-based modelling of greenhouse gas emissions from soils in detail, outlining various models and modifiers and the equations that drive them. Chapter 4 outlined the process of simulating soil CO_2 emissions for an Irish site using the ECOSSE model and assessed model parameters to identify potential causes for the offset between simulations and observed data. Chapter 5 delved deeper into these issues by deconstructing the ECOSSE model to its modifiers, finding the simulation of water by the ECOSSE model to be problematic, along with the simulation of evaporation. Chapter 6 discussed the upscaling of the model from site to national scale, introduced the GlobalECOSSE model, and compared its outputs to observations before simulating GHG emissions for Irish soils. Chapter 7 outlined the potential response of Irish soils to extreme weather events generated using a novel block resampling methodology. Chapter 8 summarises the thesis, outlines limitations and uncertainties, discusses policy implications, and outlines potential directions for future work. As a result of the findings in Chapters 4-7, the following conclusions can be drawn from the research aims:

8.2.1 Aim 1 (*Research Question A)*: To assess the ability of a model to simulate soil carbon emissions at a selected Irish site.

An offset between observations and model outputs is evident, which cannot be overcome by changing model parameters (Chapter 4). Running the ECOSSE model for an arable site and comparing model outputs to flux and chamber measurements showed a discrepancy between model outputs and observations during the growing season. On a cumulative basis model performance is good in year one, underestimates in year two, and overestimates in year three. Adjustments to various model parameters including crop, water, soil and pH did not overcome the issues observed. Removing crops entirely allowed the soil to stay moist, but CO_2 fluxes were significantly reduced due to the lack of plant inputs to the soil. The model was responsive to changes in crop type, with magnitudes of fluxes changing, likely due to changes in plant inputs from different crops, though the timing issues remained. Alterations to water parameters did not significantly affect modelled CO_2 fluxes, and the soil still dried out when changes to available water parameters were implemented, meaning the fluxes were still inhibited. Similarly changes to soil parameters including sand, silt, clay, bulk density and pH exhibited little change in output, motivating further research into the source of the issue.

The simulation of water by the ECOSSE model is the apparent cause of the difference with observations, while potential evaporation causes excessive drying in comparison to actual evaporation (Chapter 5). Further investigation into the offset identified in Chapter 4 first prompted examination of potential natural causes for the offset. Radiation, temperature and leaf area index indicated that a natural offset is present as plant growth is strongly linked to radiation while the modelled emissions are linked to temperature, however the natural offset is small and doesn't account for the discrepancy highlighted in Chapter 4. Following this, components of the ECOSSE model in terms of its fundamental modifiers for temperature, water, crop and pH are analysed. Application of the ECOSSE temperature modifier along with temperature modifiers from different studies indicated that the modifier is performing as expected and is not the source of the offset. Including the water modifier in simulations (using water content to 25cm outputted by the ECOSSE model) showed a significant decline in respiration, as simulated water content was so low during the growing season that a modifier of 0.2 was applied, inhibiting respiration by 80%. Changes to the crop parameter reduced respiration by 40% during the growing season by applying a modifier of 0.6, while the pH is static so the modifier had no effect. Deconstruction of the ECOSSE model in this way produced output similar to the model itself, indicating that the process of simplifying the model was successful. Results indicate that the simulated drying of the soil by the model is not realistic. Soil water content measurements available at the site were used as inputs to the water modifier which showed significant improvement over the model simulations. The water modifier of the ECOSSE model therefore functions correctly when observed soil water content is used, but the simulation of water by the ECOSSE model allows the soil to dry unrealistically compared to reality, erroneously inhibiting respiration. The ECOSSE model is therefore deficient at simulating soil moisture at this site at least. Changes to the weather data inputted to the model can overcome this by using actual rather than potential evaporation, which allows more moisture to remain in the soil, though this may only be true for this arable site on well-drained sandy soil.

8.2.2 Aim 2 (*Research Question A)*: To upscale site emissions to national scale.

Irish soils respond as expected to weather events according to model simulations on a seasonal and annual basis, with results indicating that Irish grasslands and croplands are sources of CO_2, though some grasslands are overall GHG sinks when all GHGs are included (Chapter 6). Though there is an offset present in the model, which is due to the water modifier, issues with the ECOSSE water modifier have been identified before (Bell *et al.*, 2012; Zimmermann *et al.*, 2018), and ECOSSE performs well at certain sites (Zimmermann *et al.*, 2018). The SoilR model is introduced in this chapter which confirms the strong influence water can have, and allows for assessment of the ability of the ECOSSE model to be scaled temporally. A pre-release spatial version of the ECOSSE model (GlobalECOSSE) was used to simulate GHG emissions from Irish soils using the HWSD soil database and EObs temperature and precipitation data, with PE calculated using the Thornthwaite method. GlobalECOSSE is used here to assess the ability of the model to simulate national emissions, producing the first GHG emission maps for Ireland. Model outputs align with theory as warm temperatures increase respiration, and soils with the highest C content have the highest CO_2 emissions during warm temperatures, along with the highest sequestration of CH_4. The importance of including all GHGs, not just CO_2 is emphasised by the agricultural simulations, where croplands are exclusively GHG sources, while grasslands have much lower emissions, and some are CO_2 sinks. Though the model is likely to underestimate emissions on well-drained sandy soils due to issues with the water component, these model outputs are a baseline of simulations on which future work can build. Increased observations are essential in order to evaluate model performance, and it is important to have consistency across observations as partitioning of flux and chamber data introduce large error ranges, with no optimum method available. It is possible to upscale emissions to national scale, but it is difficult to have confidence in these estimates due to issues with both the model and observations.

8.2.3 Aim 3 (*Research Question B)*: To investigate the impact of extreme weather events on quantities and fluxes of greenhouse gases in Irish soils.

Soils respond as expected to extreme events, with warmer temperatures increasing emissions, though the interactions between temperature and moisture are important, as hot and dry extremes reduce respiration due to issues previously highlighted with the water modifier, meaning hot and wet extreme conditions show the largest GHG emissions. There are clearly uncertainties associated with the national emissions projections, nevertheless it remains a useful exercise to assess the response of Irish soils to extreme events, to get an indication of potential future change. The model was ran using new sequences of weather data derived from seasonal extremes, results indicated enhanced respiration in response to warming, reduced respiration during drought and significantly enhanced respiration during hot and wet extreme conditions. Reduced respiration during drought is to be expected based on the results from Chapters 5 & 6, where dry conditions inhibit respiration, though this is uncertain as some modelled soils may dry excessively compared to reality. The importance of including multiple GHGs is emphasised in the CO_2 equivalent maps (Figure 7.15) where most Irish soils are GHG sinks under 'normal' or non-extreme conditions, and under hot and dry conditions, while hot and wet conditions show most Irish soils to be GHG sources. Feedbacks, legacy effects, and delayed reactions are not simulated by the GlobalECOSSE model, and ought to be included in future simulations. Model outputs are indicative only, as uncertainties are significant, this output serves an initial assessment which can be built upon in future, and emphasises the need for building resilience into the soil system as the response to potential shocks is so uncertain.

8.3 Limitations of the Research

Considering the findings of this thesis, this section details the intricacies and uncertainties in the relationship between soil and climate change, and the limitations imposed on the research because of these uncertainties.

8.3.1 *Soil & Greenhouse Gases*

It has long been noted that soil stores a significant amount of carbon which is vulnerable to changes in temperature and precipitation as a result of climate change. Contradictory empirical and modelling studies highlight complex interactions between SOM decomposition and changes in environmental variables (temperature and rainfall) creating uncertainty around both current stocks and future projections (Davidson and Janssens, 2006).

Enhanced carbon absorption by terrestrial ecosystems as temperatures increase (CO_2 fertilization effect) can be offset by the increased release of CO_2 by soils in temperate regions (Bellamy *et al.*, 2005), and the magnitude of release dependent on efficiency of soil microbe carbon use (Allison *et al.*, 2010). The response of soils to warming under experimental conditions is similar, as warming soils by 4°C increased annual soil respiration by 34-37% to 100cm depth (Hicks Pries *et al.*, 2017). The future timing and magnitude of soil C release and its response to different combinations of forcing factors such as temperature, rainfall and land management remains uncertain. Amid this uncertainty the estimated direction of change globally is assumed to be the same – studies show that warming will cause soil carbon losses, these losses depend strongly on the initial soil C stocks, meaning high latitudes are most vulnerable as they have the highest soil C stocks and are projected to experience the greatest temperature increases (Crowther *et al.*, 2016). These claims have been challenged with the inclusion of more studies, which indicate that the change in soil C stocks in response to warming is not significantly different from zero across studies, emphasising the need for more local assessments as there appear to be no hard-and-fast rules for assessing soil C responses to warming (van Gestel *et al.*, 2018).

Though this thesis finds enhanced respiration as a response to warming, the response of soils to warming is a hotly debated topic in soil science, with papers challenging the estimates of other researchers, showing the vitality and dynamism of the topic and the lack of consensus on this important issue (van Gestel *et al.*, 2018; Crowther *et al.*, 2018; Xiao *et al.*, 2018; Hicks Pries *et al.*, 2018). As the climate changes, soil carbon stocks are projected to change, yet the magnitude of this change is uncertain, even the direction of change varies across studies, and remains unclear (Jackson *et al.*, 2017). It is vital that this process is understood correctly in order to project potential future emissions accurately. Some researchers argue that decomposition rates (and therefore emissions) do not vary with temperature (Giardina and Ryan, 2000), some suggesting NPP and therefore soil C content will increase as a result of warming (Cao and Woodward, 1998) and others suggesting the effect of warming on soil C will increase NPP but also encourage microbial activity which enhances soil C decomposition and causes greater C losses (Drake *et al.*, 2011; Phillips *et al.*, 2012). Others suggest that soil C loss will be more pronounced than previously thought, as a result of non-labile SOC being more sensitive to temperature changes (Knorr *et al.*, 2005). Despite this debate, it has been acknowledged that increasing temperatures result in increased decomposition of organic matter, and as a consequence, greater CO_2 is released to the atmosphere (Powlson, 2005). The results from this thesis agree with this, as higher emissions are observed during warmer temperatures, however the interactions between temperature and moisture are vital to acknowledge, as drought conditions strongly inhibit respiration and can lead to enhanced C sequestration according to these results (Section 7.3.3.6). Some studies attempt to link increasing temperatures to SOC losses (Bellamy *et al.*, 2005) though the confidence in these links is undermined by factors other than climate change, urging caution when interpreting results (Smith *et al.*, 2007).

According to the IPCC (Ciais *et al*., 2013) around half of the emissions arising from fossil fuel burning and land-use change have remained in the atmosphere since pre-industrial times. The other half has been sequestered and stored by sinks in the global carbon cycle, namely the ocean (155 ± 30 Pg C), and vegetation biomass and soils not affected by land-use change (160 ± 90 Pg C). Examining all greenhouse gases in the terrestrial biosphere *together* is important as global land CO_2 uptake from 2001 to 2010 is outweighed by the warming capacity of biogenic methane and N_2O emissions by a factor of two. This is emphasised by the results of Chapter 6 where land can change from a source to a sink when all GHGs are included in analysis. The terrestrial biosphere is therefore a source of GHGs at the rate of 3.9±3.8 (top down) and 5.4±4.8 (bottom up) CO_2eq (Tian *et al.*, 2016). These large ranges reflect the uncertainties inherent in modelling complex biogeochemical systems and emphasise the importance of measurement-based approaches to quantification and modelling of GHGs.

8.3.2 *Projected Changes*

Smith *et al.* (2005) investigated projected changes in carbon stocks of European (defined as EU25 countries plus Norway and Switzerland) croplands and grasslands up to 2080 with areas for cropland and grassland as 126.5 Mha and 62.7 Mha respectively. Technology improvements are expected to increase soil carbon stock by increasing inputs to the soil, this is thought to be more effective for cropland as grassland is typically extensively managed and less likely to benefit from yield enhancing technologies, though the potential for Irish grasslands to store more carbon is highlighted by Kiely *et al.* (2017), who argue a conservative estimate of 48 t C ha^{-1} to 50cm is available, and recommend the potential for Irish soils to sequester carbon be included in GHG emissions inventories.

Smith *et al.* (2005) suggest average European SOC stocks across multiple SRES scenarios are projected to increase by 1-7 t C ha^{-1} in croplands and 3.2-6.2 t C ha^{-1} in grasslands, this is without factoring in potential changes in land-use. The projected land-use changes include reductions in cropland and grassland, and when they are factored in to the estimates the SOC stocks decline in all scenarios for cropland, and in all-but-one scenario for grassland. Regional changes are different under each scenario, emphasising the importance of studies which focus on specific locations to guide regional policymaking. Lugato *et al.* (2014) use the CENTURY model to project organic carbon stock changes in European agricultural soils and find increases across north-western Europe with decreases in carbon at lower latitudes and towards the east. These increases are attributed to enhanced NPP and C input due to atmospheric C enrichment, they also find SOC losses in vulnerable soils in south and eastern Europe are limited in magnitude suggesting resilience in SOC. Though GHG sequestration is simulated by the model in some cases in Chapter 6, the direction of change in SOC is downward for Irish cropland and grasslands, disagreeing with the CENTURY model projections for north-west Europe, though the addition of fertilizer applications and land management could alter these results. Impacts of extremes are 'difficult to be predicted and simulated' (Lugato *et al.,* 2004 pp. 324) and it is recommended they be included in future, Chapter 7 assessed the potential response of Irish soils to extreme events and found they agreed with the theoretical understanding of the response of soil carbon to temperature and moisture, and that a warmer/wetter climate will see the greatest increase in emissions.

Crowther *et al.* (2016) synthesise 49 studies to investigate the responses of global soil carbon to warming and find losses of 30 ± 30 Pg C to 203 ± 161 PgC under one degree of warming, and under business as usual emissions a loss of 55 ± 50 Pg C by 2050. These considerable uncertainties largely stem from a lack of understanding of how soil communities take to acclimatise to warming, if the effects are realised slowly the losses by 2050 will be closer to 200 Pg C, if soils acclimatise more rapidly the estimates will be toward the lower end of the estimate (50 Pg C). The losses are strongly associated with initial soil C stocks, with losses beginning to occur in areas with 2-5 Kg C m^{-2} and losses becoming considerable in soils with >7 Kg C m^{2}. This vulnerability is presumed to result from the high temperature sensitivity of C decomposition and biogeochemical limits on the potential C inputs to the soil. Claims made by Crowther *et al.* (2016) about the importance of initial soil C stocks and the direction of change as a response to warming were challenged by van Gestel *et al.* (2018), who performed a similar analysis on a larger number of datasets (94), and found the importance of initial stocks were not replicated in their larger sample, and the direction of change under warming was not statistically significant from zero, similar to Lu *et al.* (2013). van Gestel *et al.* (2018) recommend future experimental work to focus on underrepresented regions of the global database, as most studies come from mid-latitude countries and are predominantly from the USA, mainland Europe and China. It is also recommended that data is integrated more with process-based models, as is undertaken in this thesis. In response, Crowther *et al.* (2018) acknowledged the significance of including more sites, and argued the inclusion of yet more data may well adjust the relationship again, but maintain their conclusions on the potential loss of C from areas with initially high C content still stand, though it may be processes underlying the development of C stocks which are good predictors for response to warming, rather than the C stocks themselves. They echo van Gestel *et al.* (2018) in calling for the inclusion of more data from under-sampled regions of the globe, and highlight the importance of further research in this area to get a more definitive perspective on the responses of soil C to warming. It is clear that more data will help to elucidate the responses of soils to warming in different regions, an issue which has been previously highlighted (Smith, 2012).

8.3.3 *Confounding Interactions*

Projecting changes in SOM and SOC, along with GHG emissions from soils under climate change is a complex and multifaceted process, made more difficult by responses of different variables which can reinforce or counteract one another. For example, increased plant productivity resulting from higher levels of atmospheric C has been found to stimulate both C and N cycling in forests, as the increase in plant inputs in the upper soil layers is not stored in the soil for long due to accelerated decomposition by microbes (Phillips *et al.*, 2012). This means that although more C may be inputted into soils as atmospheric CO_2 increases resulting from increased productivity, this may not necessarily translate to higher C storage as microbial activity counteracts or outweighs the C inputs. In contrast to this, in a meta-analysis of experimental responses of soils to artificially induced warming, Lu *et al.* (2013) found that although litter decomposition, soil respiration and DOC leaching are enhanced under warming, implying the turnover rate of C will increase, the ecosystem storage of C could remain stable due to the increased plant-derived C influx counteracting the enhanced soil efflux as the climate warms. The increase of soil respiration is estimated at 9%, comparable to the 12% increase estimated by Wu *et al.* (2011). When the effect of experimental warming is tested over the whole soil profile the increase in respiration is much higher at 34-37%, albeit for one soil type in a forest ecosystem (Hicks Pries *et al.*, 2017), suggesting other studies do not account for substantial increases in fluxes by not warming soils deeper, and that models do not accurately represent SOC sensitivity as the

Q_{10} found at depth is higher than that used by most ESMs (Todd-Brown *et al.,* 2013; Hicks Pries *et al.,* 2017). Similar to Crowther *et al.* (2016), responses of soil C stocks to warming were observed independently of environmental factors such as latitude, MAT and MAP, and forcing factors such as the magnitude of warming and experimental duration. The experimental methods used by Hicks Pries *et al.* (2017) were criticised by Xiao *et al.* (2018) who pointed out that warming the soil profile in its entirety is not realistic as surface warming would gradually heat the soil profile with a thermal lag from shallow to deep soils. Xiao *et al.* (2018) also criticised the removal of certain Q_{10} values as 'outliers' when they may have been reactions to the unrealistic warming, and the non-removal of the CO_2 data which corresponded to these outliers. By reanalysing the data using a different methodology and including outliers Xiao *et al.* (2018) found surface soil layers to be more responsive to warming with a much higher temperature sensitivity than deeper soil layers. Hicks Pries *et al.* (2018) respond to the criticism with claims that over climatic timescales soils have been shown to warm at the same rate throughout the profile (with the exception of permafrost), and that the experiments cited by Xiao *et al.* (2018) do not show warming in the entire profile due to lateral heat transfer, and argue that their warming of the entire profile to 1m by 4°C is more realistic. Hicks Pries *et al*. (2018) argue the outliers they removed were likely due to differences in substrate availability and microbial communities, not warming. They also emphasise that their conclusions were different only in magnitude compared to Xiao *et al.* (2018), and that the direction of change found by both research teams was the same. CO_2 production increased across all depths, and though changes in deep soils may only make up 10% of the response to warming, this is a significant amount when scaling from site to global scale. These uncertainties again emphasise the need for using observed data, with long-term field measurements of warming induced changes to soil C stocks recommended in order to improve our understanding of soil C dynamics and our projections.

Wu *et al.* (2010) find increased temperatures enhanced plant biomass and productivity, respiration and ecosystem photosynthesis, but did not affect overall C uptake, increased precipitation enhanced respiration and ecosystem photosynthesis, leading to higher overall C uptake seen in increased plant biomass and productivity. Reductions in precipitation constrained aboveground biomass and productivity, soil respiration, photosynthesis and net C uptake, as is observed during dry conditions in Section 7.3.3.4. Overall Wu *et al.* (2010) find C fluxes were more sensitive to increased precipitation than reduced precipitation, and when both warming and precipitation were altered, the responses of ecosystems were smaller than single-factor effects. This finding is echoed by Suseela *et al.* (2012) who point out the complex interactions between soil respiration and altered warming and precipitation and find seasonal variation of the temperature sensitivity of microbial respiration in the field. An independent analysis of the global soil respiration database (SRDB) found the contribution of global Rh to be increasing (Bond-Lamberty *et al.,* 2018), the authors posit two possible explanations for the increase in Rh, either GPP increases resulting in higher C uptake by ecosystems and therefore greater detritus production and substrate availability for soils (thereby enhancing respiration), but this theory is hampered by the fact that substrate inputs are not rising fast enough to match the increases in Rh. The second explanation Bond-Lamberty *et al.* (2018) posit is that climate changes and increased temperatures have enhanced SOC mineralization, as the increase in global Rh of 1.2% in 25 years concurrent with temperatures rising by 0.7°C is consistent with results from experimental warming studies (Crowther *et al.*, 2016; Lu *et al.*, 2013; Zhou *et al.*, 2016; Wang *et al.*, 2014). Bond-Lamberty *et al*. (2018) warn of the difficulty of observing a statistically significant increase in Rh at a certain site, even if 25 years of perfect Rh observations were available as the climate driven increase (particularly at one site) is small compared to the interannual variation of Rh.

Further complexities in projecting future emissions are exemplified by the possible countervailing impacts of reducing emissions of one greenhouse gas unintentionally leading to increases in other GHGs, which may offset the initial reduction. For example, soil carbon sequestration can lead to enhanced N_2O emissions with 100 year GWPs that offset 75-310% of the sequestration (Li *et al.*, 2005). The ability of soil carbon in arable land to significantly mitigate against climate change has been questioned due to enhanced N_2O emissions from C management practices, with findings showing short-term sequestration potential can be offset by increased N_2O emissions in the long-term, with soils eventually becoming a GHG source when N-fixing cover crops are used, and remaining a small sink when crop residue retention and low soil disturbance is practiced (Lugato *et al.*, 2018). Alternative management practices such as manure application may well increase SOC content, but associated increases in N_2O emissions can largely offset the benefits, even in warm temperate climates, acidic soils, and soil textures of sandy and clay loams (Zhou *et al.*, 2017).

The potentially confounding effects of N_2O increases as a result of SCS are highlighted by van Groenigen *et al.* (2017) who point out that the typical C:N ratio is 12:1, and the sequestration rate of agricultural soils would have to be 1200 Tg C yr^{-1} according to the 4/1000 initiative, meaning 100 Tg N yr^{-1} would be required to meet demand, calling for an increase of ~75% of global N production, or N_2 fixation rates twice that of the current rate. Theoretically surplus N would be enough to meet this demand, but it is not evenly spatially distributed across the planet, and N surpluses are likely to decline in the coming decades (Zhang *et al.*, 2015). Soil chemistry constraints therefore reduce the likelihood of the 4/1000 initiative meeting its goals, leading van Groenigen *et al.* (2017) to call for a more localised mitigation framework via a spatially explicit action plan for agricultural soils, where soils with low C stock and high nutrient availability (degraded soils in nutrient-rich areas) should concentrate on increasing SOC, others should focus on reducing non-CO_2 GHGs and improving N retention. This emphasises the importance of looking at both C and N together when performing mitigation analysis, as N has the potential to confound the C sequestration potential of soils, as is shown in Chapters 6 & 7 where C, CH_4 and N emissions together can change soils from overall GHG sources to sinks.

8.3.4 *Model Uncertainties*

The uncertainties stemming from modelling fluxes from the soil carbon pool are comparable to those related to cloud feedbacks, widely regarded as the biggest uncertainty in climate modelling (Jones & Falloon, 2009). As soil carbon is such a vital part of the global carbon cycle (Stockmann *et al.*, 2015) with LULUCF being responsible for ~25% of anthropogenic GHG emissions, 10-14% from agricultural production (mainly soils and livestock management) and 12-17% from land-use change including deforestation (Paustian *et al.*, 2016), the contribution of soil C can account for 10% of the C in the atmospheric pool (Raich and Potter, 1995), it is therefore vital that Earth System Models (ESMs) capture this cycle accurately as it is a major source of the uncertainty.

Nishina *et al.* (2014) examine seven terrestrial biome models and find SOC stocks initially vary from 1090 to 2650 Pg C in historical periods, when forced using the four RCPs uncertainties are then amplified, RCP 8.5 is projected to change from a net sink of 347 Pg C to a source of 122 Pg C. The potential sink is attributed to increased fertilization and NPP from higher atmospheric CO_2 levels stimulating soil C accumulation. Crowther *et al.* (2016) suggest IPCC (Ciais *et al.*, 2013) assessments which project increased soil C under warming at high latitudes due to increased plant productivity are inaccurate, due to increased efflux from respiration and DOC leaching as temperatures increase. Projections of soil C dynamics in CMIP5 models vary greatly (as discussed in Section 3.3.4) and while the estimated stocks are relatively accurate at the biome scale, they correlate poorly to observations at the grid scale, with differences in SOC content observed by ESMs not due to structural differences between the models, rather due to differences in simulated NPP and soil decomposition (Todd-Brown *et al.*, 2013; Todd-Brown *et al.*, 2014).

Todd-Brown *et al.* (2014) examined changes in SOC by 2100 using 11 ESMS from CMIP5 for the RCP 8.5 scenario and found ranges from a loss of 72 Pg C to a gain of 253 Pg C (mean gain of 65 Pg C). These gains are attributed to increases in NPP and uncertainties are largest in tundra and boreal regions where models project losses of 37 Pg C to gains of 146 Pg C (mean gain of 39 Pg C). These differences are largely attributed to initial SOC stock estimates between models, with decomposition dominated by changes in Q_{10} factors, decomposition rate and soil temperature changes. It is acknowledged that most models perform poorly in estimating changes in high latitudes, as modelled accumulations are not matched by empirical studies which project serious losses of SOC at these latitudes (Koven *et al.,* 2011; Todd-Brown *et al.* 2013). Permafrost dynamics in northern latitudes are also poorly represented, as are constraining effects on SOC storage like priming and nutrient availability. It is suggested that the inclusion of these limiting effects will estimate lower SOC storage than models currently project (Todd-Brown *et al.*, 2014). Uncertainties are complicated by different estimates of soil carbon stocks at high latitudes, with ranges from 290 Pg C (HWSD) to 380-620 Pg C (NCSCD) (Todd-Brown *et al.*, 2013).

8.4 Policy Implications

This thesis attempted to assess the ability of models to improve GHG reporting for national emissions inventories by moving toward a tier-3 reporting methodology. Considering the findings and the limitations outlined above, the results indicate that more work is needed for a tier-3 methodology to be successfully employed. Though the ECOSSE model has been recommended ahead of others for simulating emissions from Irish soils in the past (Khalil *et al.*, 2016), rigorous testing found the model simulation of water on a well-drained sandy soil to be deficient, resulting in erroneously inhibited fluxes. Though not all Irish soils are well-drained, it is important that this issue is rectified in the model structure before it is possible to have confidence in results from well-drained soils, particularly as climate is likely to exacerbate soil drying in future, and before models can be used to accurately inform policy.

To move toward a tier-3 reporting methodology it is vital that simulations are evaluated against observations, though as shown in the findings of the thesis and the limitations discussed in Section 8.3, observations have significant uncertainties associated with them. Measurements can be taken in multiple different ways, and post-processing which introduces uncertainties is also often required. More observations are required before spatial model simulations can be used for national greenhouse gas emission estimates, as current model outputs cannot be adequately evaluated without observations to compare them to. These observations need to cover multiple land-uses and soil types, should span large timescales, and include fluxes of all GHGs. The importance of including all GHGs cannot be overstated, as simulation results in Chapter 6 show their inclusion can turn land from a

GHG sink to a source. For ECOSSE or similar models to be used for tier-3 reporting there also needs to be consistency across observations. A combination of complementary flux and chamber measurements combined with experiments which isolate the heterotrophic component of respiration are required, as model outputs must be evaluated against data which has robust provenance. Significant investment in infrastructure would be required for this to take place.

Considering the limitations outlined above, the simulation of extreme events by the model (Chapter 7) is still useful in informing current policy, as results indicate that increased warm, wet weather will enhance the emission of GHGs by soils, with higher emissions observed with warmer temperatures. Observations of emissions over long periods of time which span extreme events are required to have strong confidence in these results however. It is also important that models begin to incorporate complexities such as lagged and legacy effects of extreme events, again informed by observations across a wide range of soil types. Nevertheless, the results of extreme event simulations lead to the recommendation that policy ought to be prescribed in accordance with the IPCC's Special Report on Global Warming of 1.5°C (IPCC, 2018), to limit emissions as much as possible with the aim of restricting global warming to 1.5°C, as soil emissions are likely to be enhanced as temperatures and precipitation increase. This requires immediate drastic action on behalf of government and industry to reduce emissions by 45% compared to 2010 levels by 2030, and to net zero by 2050 (IPCC, 2018). As Ireland is already poised to miss less ambitious targets set by the EU, significant political effort is needed for emissions reductions to be achieved.

Avoiding increased emissions from soils is essential if Ireland is to achieve its mitigation obligations. Robust adaptation measures which enhance soil carbon quantity can sequester atmospheric CO_2 but also improve crop yield and soil health, therefore these strategies ought to be encouraged. It is also vital that monitoring networks which examine the holistic response of soils to these measures are set up, and that all GHGs are examined together to assess potential confounding interactions as outlined above.

8.5 Future Research

To improve modelling studies in future it is essential that observations improve in quantity and quality, as models cannot be accurately assessed without improvements in measurements. A national network of soil respiration measurements across soil types and land-uses over long time periods is essential for model outputs to be adequately evaluated. Data and metadata must be made freely available and readily accessible. It is vital that observations and model outputs are directly comparable, as some observations (such as

NEE measured by eddy covariance) must be partitioned into the relevant components for comparison to be possible. Various methods of partitioning fluxes are practiced, which all introduce uncertainties when partitioning NEE into ecosystem respiration (Stoy *et al.*, 2006) and when partitioning ecosystem respiration into its autotrophic and heterotrophic components (Koerber *et al.*, 2010; Khalil *et al.*, 2013). Partitioning of chamber data also introduces uncertainties, with ranges for the heterotrophic component from 3% to 99% across biomes and land-uses, and 27-90% for temperate grasslands (Subke *et al.*, 2006), emphasising the uncertainties introduced when choosing a method of partitioning. Ideally multiple measurements which are comparable to one another ought to be used in order to determine the most accurate representation of the C flux, as it is difficult to be confident in model assessments when comparing to observations with such large variation. Ideally on-site experiments which partition fluxes into autotrophic and heterotrophic components would be used, though the experimental method also introduces uncertainties (Subke *et al.*, 2006), a standardised methodology is now recommended (Hoffmann *et al.*, 2017). Standardisation of methods is desirable for model and observation inter-comparison studies to be possible, yet this may not be feasible as different methods of partitioning may work better in different situations, and on-site root-exclusion experiments are expensive and time-consuming. It is difficult to foresee a universally applicable measurement and partitioning framework, even though improvements to chamber estimations have been suggested (He *et al.*, 2016).

Increased knowledge about soil carbon turnover and fluxes remains to be fully implemented in ESMs (Bradford *et al.*, 2016). Nevertheless, the projected direction of global change (soil carbon loss) is consistent across warming scenarios, with most C losses occurring at high latitudes due to both the initial high levels of C in their soils and the projected fast rates of warming in these regions, leading to a positive feedback to the global carbon cycle and enhancing climate change. These losses at high latitudes far outweigh potential increases in soil C at lower latitudes, contradicting projections from the IPCC (2013) who projected increases in soil C at high latitudes due to increasing plant productivity (Crowther *et al.*, 2016). The potential impacts of shocks resulting from increased frequency and intensity of extreme weather are not discussed, though this study suggests that extreme temperature increases will lead to SOC losses if enough moisture is present to allow for respiration to continue uninhibited.

Sequestered soil C is also vulnerable to future changes in management, temperature and rainfall, as carbon sequestered in soil is vulnerable to management practices e.g. when plant residue retention (returning plant litter to the soil) was halved, soil C was lost, with similar consequences when N fertilizer was changed. These losses were further exacerbated with increasing temperature and/or rainfall. The effect of rainfall change is moderate, and depends on the direction of change, meaning local management strategies for C sequestration and retention are advised (Luo *et al.*, 2016).

Amid these estimates it is also important to note that the complex nature of SOM and SOC means it is very difficult to predict what is going to happen to stocks in the future, with contradictory results from field and lab experiments leading to researchers questioning the intricacies of the SOC response to warming. Conant *et al.* (2011) note that experimental differences may have resulted from studies which minimised the influence of SOM availability found that slow processes responded more to changes in temperature, indicating that low quality substrates are more responsive to temperature regarding depolymerization, or that temperature increases affect enzymes which degrade low-quality polymers more than others. The dearth of knowledge regarding these processes led the researchers to call for experiments which focus on the impact of temperature on microbial efficiency and enzyme production, as well as long-term low-cost experiments giving field-level data on SOC responses to warming. Similarly Todd-Brown *et al.* (2014) call for inclusion of priming, nutrient availability, mineral surface stabilization and aggregate formation in models, and predict that this will constrain increases in SOC as the climate warms. The contribution of Rh to Rs is highly variable, and in-situ observations (ideally with exclusion experiments) are preferable to identify the contribution of the heterotrophic component of respiration (Bond-Lamberty *et al.*, 2004). The desirability of accurate point-scale observations also creates problems, as Bond-Lamberty *et al.* (2018) highlight the uncertainty regarding the sensitivity of Rh to changes in temperature, precipitation and organic matter inputs is directly due to the infrequent, small scale and variable nature of Rh observations. These limitations are intrinsic to work which attempts to represent the complex global soil infrastructure and bridging the gap between small and large-scale will remain a research challenge. Robust adaptation is essential in the face of uncertainty, and resilience must be built into systems now to protect against any future shocks.

The EU climate and energy package 2020 prohibits the use of the LULUCF sector to offset national emissions, yet there is potential for change here for the period 2020 to 2030 to allow states to achieve their emissions reduction targets (European Commission, 2016). Schulte *et al.* (2016) assessed Ireland as an example of an Atlantic climate zone and considered 5 elements of the SOC cycle relevant to similar pedoclimatic regions recommending the following processes as best-practices for maintaining and increasing Irish soil C content:

1. *Maintenance of SOC stocks.* 53-75% of SOC in Ireland is stored in peat soils, estimated at 1500 to 1500 Mt C.
2. *Reduction of existing SOC emissions.* The largest source of SOC emissions on Irish soils comes from artificially drained wet soils, denoted as 'emission hotspots' they are typically intensively managed drained histic soils (peaty O horizon, overlying mineral soil or rock) (SIS Technical Report, 2008). 59% of emissions from land drainage arises from these hotspots, even though they make up only 18% of the Wetlands Supplement land area, and 6% of the total agricultural area.
3. *Preventing new CO_2 emissions.* Milk quota abolition has led to an expansion of dairying in Ireland resulting in poorly drained fertile soils being drained, leading to oxidation and SOC losses. Cost benefit analysis by O'Sullivan *et al.* (2015) found financial benefits from drainage and increased productivity outweighed the increased GHG emissions financial penalties, however, using new figures from 2030 price projections this relationship is reversed for some areas. It could be argued that considering purely financial consequences of increased emissions is myopic at best and recklessly irresponsible at worst, as much more than financial penalties are at stake where GHG emissions are concerned.
4. *Enhanced long-term sequestration in grasslands.* Grasslands in Ireland are thought to be net carbon sinks on balance (Abdalla *et al*., 2013) with the potential for enhanced SCS (Kiely *et al.*, 2017)
5. *Enhanced sequestration through land-use change (afforestation).* Ireland has the lowest forest cover of any EU member state at 11%. Since all land is not suitable for afforestation, Farrelly and Gallagher (2015) highlight that 0.9m ha of potentially suitable Irish land is subject to habitat conservation, 2.4m ha of productive agricultural land will probably be the focus of agricultural intensification in accordance with the FoodWise 2025 strategy, leaving 1.3m ha of 'marginal agricultural land' where competition for other land-uses is low.

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10 Appendix A: IPCC Accounting Methodology

To find which method to use (tier 1 – tier 3) countries are obliged to follow the decision trees shown in Figure 10.1 and Figure 10.2 for mineral and organic soils.

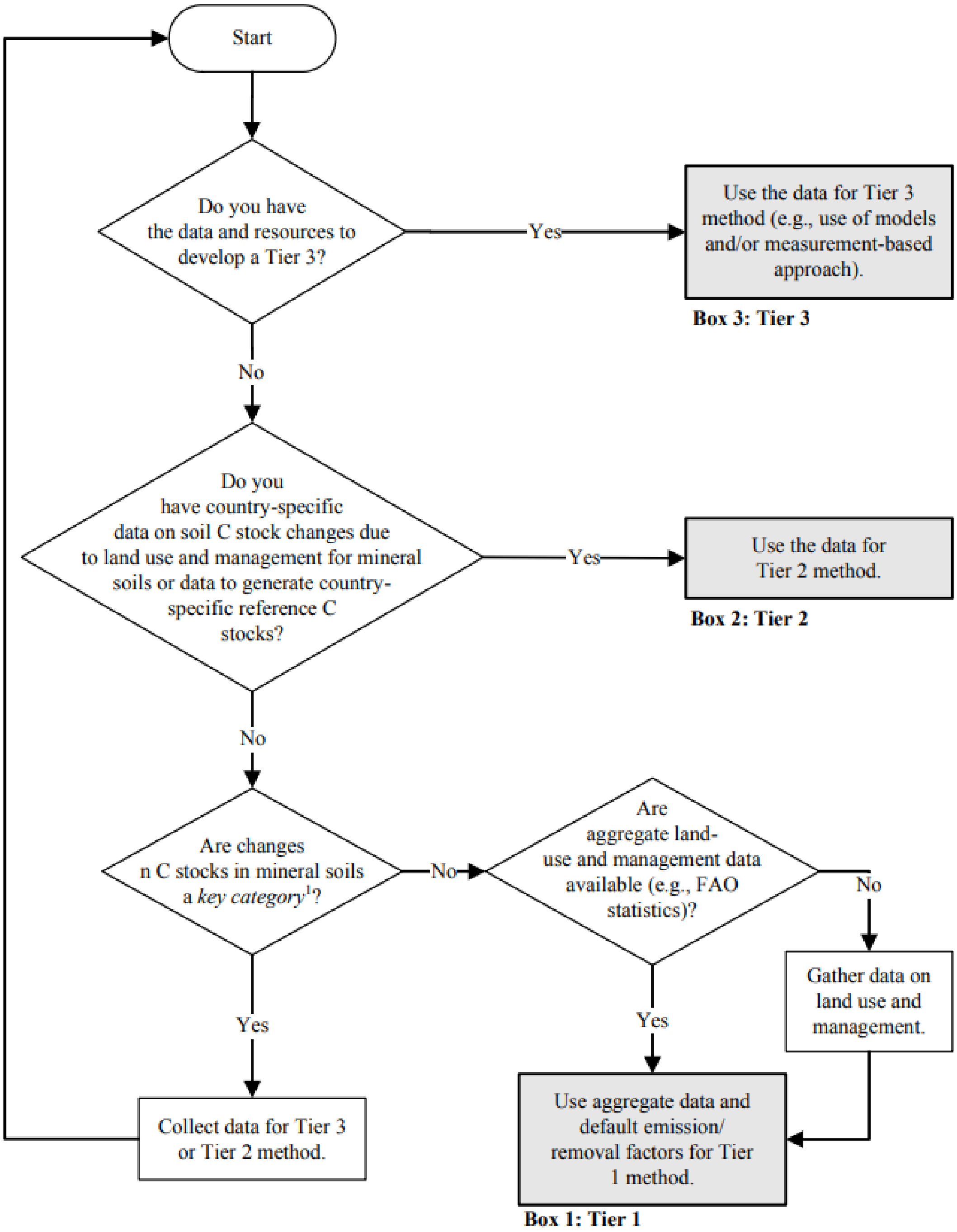

Figure 10.1: Generic decision tree to determine the appropriate tier to estimate changes in carbon stocks in mineral soils by land-use category (from IPCC, 2006)

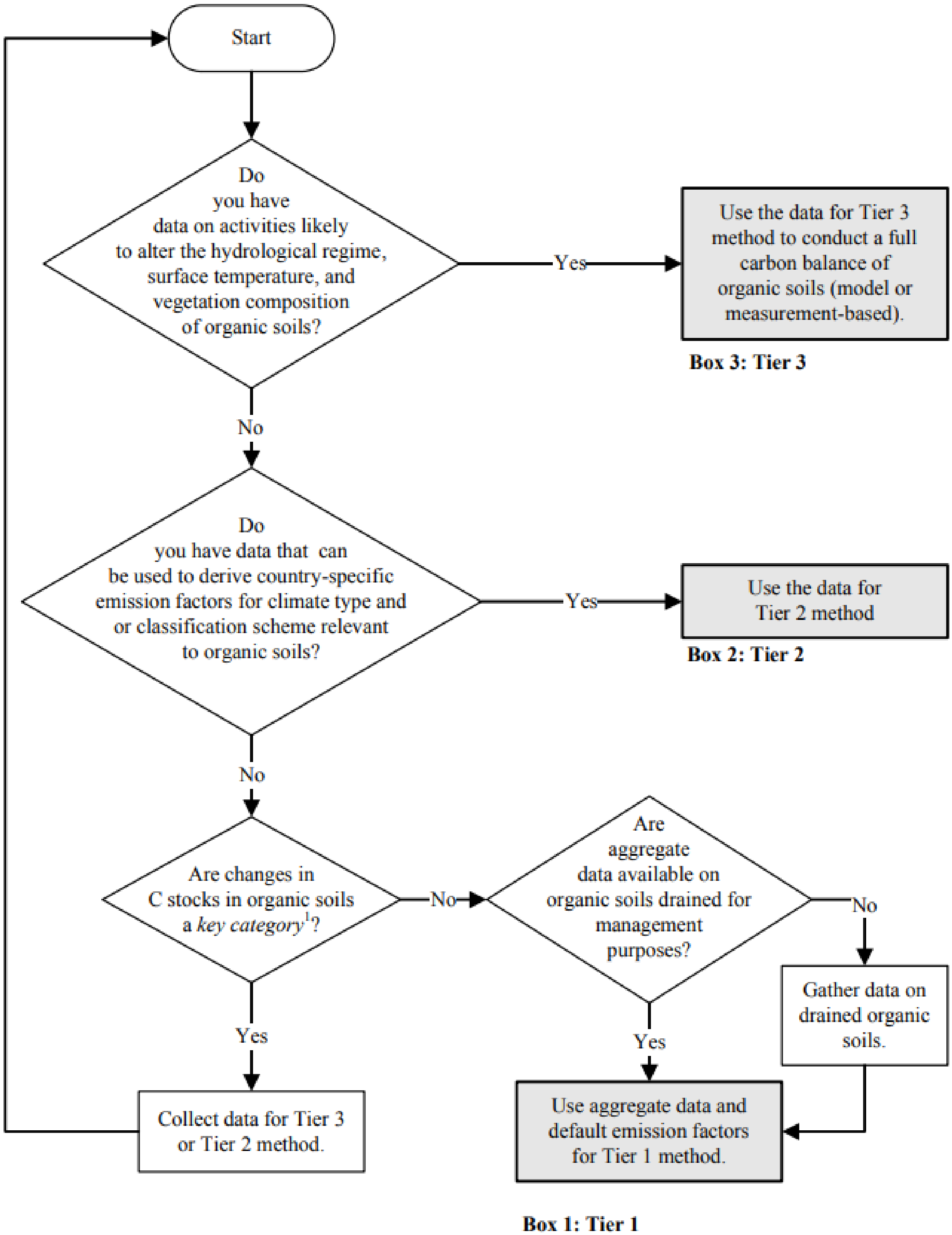

Figure 10.2: Decision tree to determine the appropriate tier to estimate change in carbon stocks in organic soils by land-use category (from IPCC, 2006)

Default reference SOC stocks for mineral soils are outlined in Chapter 2 of the IPCC (2006) guidelines and are separated into High Activity Clay (HAC), Low Activity Clay (LAC), Sandy, Spodic, Volcanic and Wetland soils for multiple climate regions. These stocks are derived from soil databases (Jobbágy and Jackson, 2000), and mean values are presented with nominal error estimate of 90%.

Cropland emissions are estimated using tier 1 method for estimating changes in SOC stocks in mineral soils using Equation 10.1 to estimate changes in SOC stocks by subtracting C stocks in the last year of an inventory time period from the stock at the beginning of the inventory time period, with annual changes estimated as difference in stocks over time divided by the time dependence of cropland stock change factors, taken from 2006 IPCC Guidelines, Volume 4, Chapter 5 (IPCC, 2006).

$$\Delta C_{Mineral} = \frac{(SOC_0 - SOC_{(0-T)})}{D} \qquad \text{Equation 10.1}$$

$$SOC = \sum_{c,s,i} (SOC_{REF_{c,s,i}} \bullet F_{LU_{c,s,i}} \bullet F_{MG_{c,s,i}} \bullet F_{I_{c,s,i}} \bullet A_{c,s,i}$$

Where:

$\Delta C_{Mineral}$ = Annual C stock change in mineral soils, t C yr^{-1}
SOC_0 = SOC stock in the last year of an inventory period, t C
$SOC_{(0-T)}$ = SOC stock at the beginning of the period, t C
SOC_0 and $SOC_{(0-T)}$ are calculated using the SOC equation where the reference carbon stocks and stock change factors are assigned according to the land-use and management activities and corresponding areas at each of the points in time (time = 0 and time = 0-T)
T = number of years over the inventory time period
c = represents the climate zones, s the soil types, and i the set of management systems that are present in a country
SOC_{REF} = the reference carbon stock, t C ha^{-1}
F_{LU} = stock change factor for land-use systems or sub-system for a particular land-use, dimensionless
F_{MG} = stock change factor for management regime, dimensionless
F_I = stock change factor for input of organic matter, dimensionless
A = land area of the stratum being estimated, ha. All land in the stratum should have common biophysical conditions (i.e., climate and soil type) and management history over the inventory time period to be treated together for analytical purposes.

Stock changes in cropland soils for different management activities are estimated for tier 1 methodologies using Table 5.5 in Chapter 5 of the IPCC (2006) guidelines, shown as Tables 10.1 and 10.2 below.

Table 10.1: Relative stock change factors for different management activities on cropland from IPCC (2006)

Factor value type	**Level**	**Temper-ature regime**	**Moist-ure regime**[1]	**IPCC defaults**	**Error**[2,3]	**Description**
Land use (F_{LU})	Long-term culti-vated	Tem-perate/ Boreal	Dry	0.80	± 9%	Represents area that has been continuously managed for >20 yrs, to predominantly annual crops. Input and tillage factors are also applied to estimate carbon stock changes. Land-use factor was estimated relative to use of full tillage and nominal ('medium") carbon input levels.
			Moist	0.69	± 12%	
		Tropical	Dry	0.58	± 61%	
			Moist/ Wet	0.48	± 46%	
		Tropical montane[4]	n/a	0.64	± 50%	
Land use (F_{LU})	Paddy rice	All	Dry and Moist/ Wet	1.10	± 50%	Long-term (> 20 year) annual cropping of wetlands (paddy rice). Can include double-cropping with non-flooded crops. For paddy rice, tillage and input factors are not used.
Land use (F_{LU})	Peren-nial/ Tree Crop	All	Dry and Moist/ Wet	1.00	± 50%	Long-term perennial tree crops such as fruit and nut trees, coffee and cacao.
Land use (F_{LU})	Set aside (< 20 yrs)	Tempe-rate/ Boreal and Tropical	Dry	0.93	± 11%	Represents temporary set aside of annually cropland (e.g., conservation reserves) or other idle cropland that has been revegetated with perennial grasses.
			Moist/ Wet	0.82	± 17%	
		Tropical montane[4]	n/a	0.88	± 50%	
Tillage (F_{MG})	Full	All	Dry and Moist/ Wet	1.00	NA	Substantial soil disturbance with full inversion and/or frequent (within year) tillage operations. At planting time, little (e.g., <30%) of the surface is covered by residues.
Tillage (F_{MG})	Re-duced	Tem-perate/ Boreal	Dry	1.02	± 6%	Primary and/or secondary tillage but with reduced soil disturbance (usually shallow and without full soil inversion). Normally leaves surface with >30% coverage by residues at planting.
			Moist	1.08	± 5%	
		Tropical	Dry	1.09	± 9%	
			Moist/ Wet	1.15	± 8%	
		Tropical montane[4]	n/a	1.09	± 50%	
Tillage (F_{MG})	No-till	Temperat e/ Boreal	Dry	1.10	± 5%	Direct seeding without primary tillage, with only minimal soil disturbance in the seeding zone. Herbicides are typically used for weed control.
			Moist	1.15	± 4%	
		Tropical	Dry	1.17	± 8%	
			Moist/ Wet	1.22	± 7%	
		Tropical montane[4]	n/a	1.16	± 50%	

Table 10.2: Part 2 of relative stock change factors for different management activities on cropland from IPCC (2006)

Factor value type	Level	Temper-ature regime	Moist-ure regime[1]	IPCC defaults	Error[2,3]	Description
Input (F_I)	Low	Tem-perate/ Boreal	Dry	0.95	± 13%	Low residue return occurs when there is due to removal of residues (via collection or burning), frequent bare-fallowing, production of crops yielding low residues (e.g., vegetables, tobacco, cotton), no mineral fertilization or N-fixing crops.
			Moist	0.92	± 14%	
		Tropical	Dry	0.95	± 13%	
			Moist/ Wet	0.92	± 14%	
		Tropical montane[4]	n/a	0.94	± 50%	
Input (F_I)	Med-ium	All	Dry and Moist/ Wet	1.00	NA	Representative for annual cropping with cereals where all crop residues are returned to the field. If residues are removed then supplemental organic matter (e.g., manure) is added. Also requires mineral fertilization or N-fixing crop in rotation.
Input (F_I)	High with-out manure	Tem-perate/ Boreal and Tropical	Dry	1.04	± 13%	Represents significantly greater crop residue inputs over medium C input cropping systems due to additional practices, such as production of high residue yielding crops, use of green manures, cover crops, improved vegetated fallows, irrigation, frequent use of perennial grasses in annual crop rotations, but without manure applied (see row below).
			Moist/ Wet	1.11	± 10%	
		Tropical montane[4]	n/a	1.08	± 50%	
Input (F_I)	High – with manure	Tem-perate/ Boreal and Tropical	Dry	1.37	± 12%	Represents significantly higher C input over medium C input cropping systems due to an additional practice of regular addition of animal manure.
			Moist/ Wet	1.44	± 13%	
		Tropical montane[4]	n/a	1.41	± 50%	

[1] Where data were sufficient, separate values were determined for temperate and tropical temperature regimes; and dry, moist, and wet moisture regimes. Temperate and tropical zones correspond to those defined in Chapter 3; wet moisture regime corresponds to the combined moist and wet zones in the tropics and moist zone in temperate regions.

[2] ± two standard deviations, expressed as a percent of the mean; where sufficient studies were not available for a statistical analysis to derive a default, uncertainty was assumed to be ± 50% based on expert opinion. NA denotes 'Not Applicable', where factor values constitute defined reference values, and the uncertainties are reflected in the reference C stocks and stock change factors for land use.

[3] This error range does not include potential systematic error due to small sample sizes that may not be representative of the true impact for all regions of the world.

[4] There were not enough studies to estimate stock change factors for mineral soils in the tropical montane climate region. As an approximation, the average stock change between the temperate and tropical regions was used to approximate the stock change for the tropical montane climate.

The steps for estimating SOC changes over time using a tier 1 methodology for cropland remaining cropland on mineral soils using the equation and information above are (IPCC, 2006):

- **Step 1:** Sort the data into inventory time periods using the years in activity data were collected (e.g., 1990 to 1995, 1995 to 2000, etc.)
- **Step 2:** Determine the amount of Cropland Remaining Cropland by mineral soil types and climate regions in the country at the beginning of the first inventory time period. The first year of the inventory time period will depend on the time step of the activity data (0-T; e.g., 5, 10 or 20 years ago).
- **Step 3:** Classify each Cropland into the appropriate management system using the decision tree in the guidance document.

- **Step 4:** Assign a native reference C stock values (SOC_{REF}) from based on climate and soil type.
- **Step 5:** Assign a land-use factor (F_{LU}), management factor (F_{MG}) and C input levels (F_I) to each Cropland based on the management classification and Tables 10.1 and 10.2 (Step 2).
- **Step 6:** Multiply the factors (F_{LU}, F_{MG}, F_I) by the reference soil C stock (SOC_{REF}) to estimate an 'initial' soil organic C stock ($SOC_{(0-T)}$) for the inventory time period.
- **Step 7:** Estimate the final soil organic C stock (SOC_0) by repeating Steps 1 to 5 using the same native reference C stock (SOC_{REF}), but with land-use, management and input factors that represent conditions for each cropland in the last (year 0) inventory year.
- **Step 8:** Estimate the average annual change in soil organic C stocks for Cropland Remaining Cropland ($\Delta C_{Mineral}$) by subtracting the 'initial' soil organic C stock ($SOC_{(0-T)}$) from the final soil organic C stock (SOC_0), and then dividing by the time dependence of the stock change factors (i.e., 20 years using the default factors). If an inventory time period is greater than 20 years, then divide by the difference in the initial and final year of the time period.
- **Step 9:** Repeat steps 2 to 8 if there are additional inventory time periods (e.g., 1990 to 2000, 2001 to 2010, etc.).
- Grassland soils use the same equation and methods as croplands (Equation 10.1), though it is recommended for tier 1 approaches that data on grassland management activity should be obtained and classified into appropriate land-management systems, then stratified by IPCC climate regions and soil types. Tier 1 methods use Table 10.3 (from IPCC, 2006) to determine relative stock change factors for managed grasslands, these values are for management effects on the top 30cm of the soil profile.

Table 10.3: Relative stock change factors for grassland management (From IPCC, 2006)

Factor	Level	Climate regime	IPCC default	Error [1,2]	Definition
Land use (F_{LU})	All	All	1.0	NA	All permanent grassland is assigned a land-use factor of 1.
Management (F_{MG})	Nominally managed (non –degraded)	All	1.0	NA	Represents non-degraded and sustainably managed grassland, but without significant management improvements.
Management (F_{MG})	Moderately degraded grassland	Temperate /Boreal	0.95	± 13%	Represents overgrazed or moderately degraded grassland, with somewhat reduced productivity (relative to the native or nominally managed grassland) and receiving no management inputs.
		Tropical	0.97	± 11%	
		Tropical Montane[3]	0.96	± 40%	
Management (F_{MG})	Severely degraded	All	0.7	± 40%	Implies major long-term loss of productivity and vegetation cover, due to severe mechanical damage to the vegetation and/or severe soil erosion.
Management (F_{MG})	Improved grassland	Temperate /Boreal	1.14	± 11%	Represents grassland which is sustainably managed with moderate grazing pressure and that receive at least one improvement (e.g., fertilization, species improvement, irrigation).
		Tropical	1.17	± 9%	
		Tropical Montane[3]	1.16	± 40%	
Input (applied only to improved grassland) (F_I)	Medium	All	1.0	NA	Applies to improved grassland where no additional management inputs have been used.
Input (applied only to improved grassland) (F_I)	High	All	1.11	± 7%	Applies to improved grassland where one or more additional management inputs/improvements have been used (beyond that is required to be classified as improved grassland).

[1] ± two standard deviations, expressed as a percent of the mean; where sufficient studies were not available for a statistical analysis a default, based on expert judgement, of ± 40% is used as a measure of the error. NA denotes 'Not Applicable', for factor values that constitute reference values or nominal practices for the input or management classes.

[2] This error range does not include potential systematic error due to small sample sizes that may not be representative of the true impact for all regions of the world.

[3] There were not enough studies to estimate stock change factors for mineral soils in the tropical montane climate region. As an approximation, the average stock change between the temperate and tropical regions was used to approximate the stock change for the tropical montane climate.

Note: See Annex 6A.1 for estimation of default stock change factors for mineral soil C emissions/removals for Grassland.

In order to estimate SOC stocks and stock changes it is the same steps as listed above for cropland are followed, for full details see IPCC (2006).

Tier 2 methods use equation 10.1 along with country-specific information on reference C stocks, climate regions, soil types and/or land-management classification systems, effectively updating Table 10.3 using values derived for more detailed country-specific classification schemes of management, climate and soil types, and following the same methodology. A tier 3 approach uses dynamic models and/or detailed inventory approaches in the same way as croplands, with the same caveats for choice of model. Uncertainties in GHG inventory assessments can help identify issues with SOM models, with the expectation that future research will help to improve these areas by reducing the uncertainties, however it is first important to quantify these errors and uncertainties before they can be reduced (Campbell and Paustian, 2015).

11 Appendix B: Block Resampling Code

NOTE: This code is for temperature data, full code for temperature and precipitation data is available online in the form of jupyter notebooks at github.com/podgeflat/block-resampling

```python
# # Block Resampling

# This code resamples a NetCDF file using percentiles.
# ### User-Defined Variables
# Change these values for the degree of extreme you want - but be careful, if you go to high you won't have enough data for each season, so some trial and error may be necessary

upperlimit = 0.8 #this method uses percentiles, if this number is 0.9 the top 10% of data will be considered 'extreme' and so on
lowerlimit = 0.2

# ### Load Necessary Packages
import pandas as pd # data manipulation
import numpy as np  # maths library
import os  # interacts with the operating system
import matplotlib.pyplot as plt  # draws graphs
get_ipython().magic(u'matplotlib inline') # shows graphs in jupyter as code runs
import matplotlib  # plotting library
#additional NetCDF things:
import xarray  # Excellent library for data with 3+ dimensions
np.set_printoptions(precision=3, linewidth=100, edgeitems=2)  # make numpy less verbose

# ### Read in & display climate data
# Read in netCDF for Ireland
ds = xarray.open_dataset('C:/Path/ToFile/IrelandEObsMonthly.nc')
ds #check it

#plot a slice to see if it is what it's supposed to be
temp = (ds.tg).isel(time=4)
temp.plot()

#convert to dataframe
df = ds.to_dataframe()
df.head()
#df.to_csv('E:/Temp/dfexplore.csv') #write to csv to explore (optional)
df = df.reset_index()
df.head(n=440)

#convert datetime from unix time to readable date (https://stackoverflow.com/questions/19231871/convert-unix-time-to-readable-date-in-pandas-dataframe)
df['time'] = pd.to_datetime(df['time'],unit='s')
df.head()
df.tail()

# Find start and end year of the data
no_of_years = df['time'].dt.year #creates a variable for the year column
no_of_years = list(no_of_years) #turns it into a list

startyear = no_of_years[0] #gets the first value
print startyear

endyear = no_of_years[-1] #gets the last value
print endyear

# Split data into seasons based on months
# Winter = 1, Spring = 2, Summer = 3, Autumn = 4
```

```python
#create a season function to split data into seasons
def get_season(row):
    if row['time'].month >= 3 and row['time'].month <= 5:
        return '2'
    elif row['time'].month >= 6 and row['time'].month <= 8:
        return '3'
    elif row['time'].month >= 9 and row['time'].month <= 11:
        return '4'
    elif row['time'].month <= 2 or row['time'].month >= 12:
        return '1'
    else:
        return '-9999'

# Apply the season function to the data
df['Season'] = df.apply(get_season, axis=1)
df.tail()

# Create 'Year' column from the 'date' column
df['Year'] = df['time'].dt.year
df.head()

# Make December of previous year part of winter for current year (to keep climatolgical year)
#Everywhere the month is '12', the year column gets increased by 1.
df.loc[df['time'].dt.month == 12, 'Year'] += 1
df.head()

# Create a new dataframe indexed by Year and Season
#how to multiindex from here: http://stackoverflow.com/questions/33435971/selecting-time-series-data-in-a-specific-sequence-using-pandas/33437422#33437422
df2 = df.set_index(['Year', 'Season'], inplace=False)
df2.head()

# # Temperature Extremes
# Calculate mean values for each season
seasmean = df['tg'].groupby(df['Season']).mean()
print seasmean.head() #check the averages - do they seem correct?

# Calculating differences between each season overall season means
df2['seasdif'] = df2['tg'].groupby(level=['Year','Season']).mean() - seasmean #creates an anomaly column
seasdif = df2['tg'].groupby(level=['Year','Season']).mean() - seasmean #creates a series
seasdif

# # Extracting extreme seasons
# Create a copy of the dataframe and two blank lists for hot and cold extremes
seasdif2 = pd.DataFrame(seasdif)
warm = []
cold = []
seasdif2

# ### [Quantiles/ Percentiles](http://pandas.pydata.org/pandas-docs/stable/generated/pandas.DataFrame.quantile.html)
# (works in the same way as [numpy.percentile](http://docs.scipy.org/doc/numpy-dev/reference/generated/numpy.percentile.html))
seasdif2['warm'] = 0 #add a blank column for warm
seasdif2['cold'] = 0 #add a blank column for cold

seasdif2.loc[seasdif2['tg'] > seasdif2['tg'].quantile(upperlimit), 'warm'] = 1 # adds 1 for hot percentile
seasdif2.loc[seasdif2['tg'] < seasdif2['tg'].quantile(lowerlimit), 'cold'] = 1 # adds 1 for cold percentile
seasdif2

# count the extremes
```

```
extremecount = seasdif2[['warm','cold']]
extremecount

# ### Select out combinations of extremes
#identify columns with  extremes
extremeseasons = seasdif2.loc[(seasdif2.cold==1) | (seasdif2.warm==1)]
extremeseasons

# Examine the frequency of extremes, are warm summers increasing? Are cold winters decreasing?
matplotlib.rcParams['figure.figsize'] = (20.0, 10.0) #change plotting params

extremewinters = extremeseasons.xs('1', level='Season')
extremesprings = extremeseasons.xs('2', level='Season')
extremesummers = extremeseasons.xs('3', level='Season')
extremeautumns = extremeseasons.xs('4', level='Season')

# make the plots for winter
extremewinters[['cold']].plot(kind='bar', title = 'Frequency of extremely cold winters')
extremesummers[['warm']].plot(kind='bar', title = 'Frequency of extremely warm summers')
extremewinters[['cold']].plot(kind='bar', title = 'Frequency of Extremely Cold Winters', color = 'blue')
plt.title('Frequency of Extremely Cold Winters', fontsize = 30)
plt.legend().remove()
plt.tick_params(labelsize = 20)
plt.xlabel('')
plt.yticks(np.arange(0, 2, step=1.0))
plt.tight_layout()
#save it
os.chdir('E:\Location')
plt.savefig('ColdWinterFreq.jpeg', format = 'jpeg', dpi = 400)

# summer
extremesummers[['warm']].plot(kind='bar', title = 'Frequency of Extremely Warm Summers', color = 'red')

plt.title('Frequency of Extremely Warm Summers', fontsize = 30)
plt.legend().remove()
plt.tick_params(labelsize = 20)
plt.xlabel('')
plt.yticks(np.arange(0, 2, step=1.0))
plt.tight_layout()
#save it
os.chdir('E:\Location')
plt.savefig('WarmSummerFreq.jpeg', format = 'jpeg', dpi = 400)

# Create new index for extremes
df2.index.tolist()

# Count extreme values in each year
extremecount = seasdif2.groupby(level=[0]).sum()
extremecount.drop(extremecount.columns[[0]], axis=1, inplace=True)
extremecount

# ## Plot frequency of extremes
extremecount['cold'].plot(kind='bar')

# ### Create new extreme dataframes to sample from
#cold
extremecold = seasdif2.loc[(seasdif2.cold==1)]

#hot
extremehot = seasdif2.loc[(seasdif2.warm==1)]

```

```
#normal
normal = seasdif2.loc[(seasdif2.cold == 0) & (seasdif2.warm==0) & (seasdif2.dry==0) & (seasdif2.wet==0)]

#extreme
extreme = seasdif2.loc[(seasdif2.cold == 1) | (seasdif2.warm==1) | (seasdif2.dry==1) | (seasdif2.wet==1)]

#test
extreme

# **Get the index to re-index the dataframes later **
#cold
coldindex = extremecold.index.tolist()

#hot
hotindex = extremehot.index.tolist()

#normal
normalindex = normal.index.tolist()

#extreme
extremeindex = extreme.index.tolist()

#test
extremeindex

# Create indices from the dataframes
#cold
extremecold = df2.loc[coldindex]

#hot
extremehot = df2.loc[hotindex]

#normal
normal = df2.loc[normalindex]

#extreme
extreme = df2.loc[extremeindex]

#test view
extreme

# ### Resample the data and create a new sequence
df3 = df2
df3.head()

# ### Separate years into seasons for each extreme variable
#Cold years
coldsample = [[],[],[],[]] #empty list of lists
for (yr,se) in coldindex:
    coldsample[int(se)-1] += [yr] #function which gives the years which have extreme seasons [[1],[2],[3],[4]]
coldsample

#hot years
hotsample = [[],[],[],[]] #empty list of lists
for (yr,se) in hotindex:
    hotsample[int(se)-1] += [yr] #function which gives the years which have extreme seasons [[1],[2],[3],[4]]

#normal years
normalsample = [[],[],[],[]] #empty list of lists
for (yr,se) in normalindex:
```

```
    normalsample[int(se)-1] += [yr] #function which gives the years which have extreme seasons [[1],[2],[3],[4]]

#extreme years
extremesample = [[],[],[],[]] #empty list of lists
for (yr,se) in extremeindex:
    extremesample[int(se)-1] += [yr] #function which gives the years which have extreme seasons [[1],[2],[3],[4]]

#test
hotsample

# ### Check if extreme indices have enough data to sample from
#
# Checks the data to see if there are enough extreme years and prints an error otherwise - if there are no errors you can assume there is at least one full year of data for each extreme type.
#
# If there is an error - you will not be able to generate that variable (tends to happen for short datasets and combinations of extremes (cold/wet, warm/dry etc).
#
# To overcome this you can change your threshold for extremes (quantiles) or find longer data. You can also comment out the variables in the code below if there is not enough data.

#cold years
cold_ctr = 0 #variable to count from (1 is winter, 2 spring, 3 summer, 4 autumn)
coldseq = [] #blank list
try:
    for yrlist in coldsample:
        ran_yr = np.random.choice(yrlist, 1) #choose a randomly sampled year from previous cell
        cold_ctr += 1 # increment cold_ctr variable by 1
        coldseq += [(ran_yr[0], cold_ctr)] #populate coldseq with a random year and a random season (in order)
except:
    print('coldseq (cold extremes) does not have enough extreme data for a full year, it contains: ' + str(coldsample))

#############################################################################################################################
#hot years
hot_ctr = 0 #variable to count from (1 is winter, 2 spring, 3 summer, 4 autumn)
hotseq = [] #blank list
try:
    for yrlist in hotsample:
        ran_yr = np.random.choice(yrlist, 1) #choose a randomly sampled year from previous cell
        hot_ctr += 1 # increment counter variable by 1
        hotseq += [(ran_yr[0], hot_ctr)] #populate blank sequence with a random year and a random season (in order)
except:
    print('hotseq (hot extremes) does not have enough extreme data for a full year, it contains: ' + str(hotsample))

#############################################################################################################################
#Normal years
normal_ctr = 0 #variable to count from (1 is winter, 2 spring, 3 summer, 4 autumn)
normalseq = [] #blank list
```

```
try:
    for yrlist in normalsample:
        ran_yr = np.random.choice(yrlist, 1) #choose a randomly sampled year from previous cell
        normal_ctr += 1 # increment counter variable by 1
        normalseq += [(ran_yr[0], normal_ctr)] #populate blank sequence with a random year and a random season (in order)
except:
    print('normalseq (non-extreme data) does not have enough data for a full year, it contains: ' + str(normalsample))

##############################################################################################################################
#extreme years
extreme_ctr = 0 #variable to count from (1 is winter, 2 spring, 3 summer, 4 autumn)
extremeseq = [] #blank list
try:
    for yrlist in extremesample:
        ran_yr = np.random.choice(yrlist, 1) #choose a randomly sampled year from previous cell
        extreme_ctr += 1 # increment counter variable by 1
        extremeseq += [(ran_yr[0], extreme_ctr)] #populate blank sequence with a random year and a random season (in order)
except:
    print('extremeseq (extreme data) does not have enough data for a full year, it contains: ' + str(extremesample))

# If the output above says there is not enough extreme data for a full year - omit the extreme from your analysis (you will hit errors which will prevent you from using it anyway)

# ## Annual resampling
#normal years
normal_ctr = 0 #variable to count from (1 is winter, 2 spring, 3 summer, 4 autumn)
normalseq = [] #blank list

#extreme years
extreme_ctr = 0 #variable to count from (1 is winter, 2 spring, 3 summer, 4 autumn)
extremeseq = [] #blank list

#cold years
cold_ctr = 0 #variable to count from (1 is winter, 2 spring, 3 summer, 4 autumn)
coldseq = [] #blank list

#hot years
hot_ctr = 0 #variable to count from (1 is winter, 2 spring, 3 summer, 4 autumn)
hotseq = [] #blank list

# Comment/uncomment sections here to alter the way you choose data

# ## Seasonal Resampling
# First - convert the annual dataframes into seasonal dataframes
#normaldata
normalwinter = normalsample[0]
normalspring = normalsample[1]
normalsummer = normalsample[2]
normalautumn = normalsample[3]

#extreme data
extremewinter = extremesample[0]
```

```python
extremespring = extremesample[1]
extremesummer = extremesample[2]
extremeautumn = extremesample[3]

#cold data
coldwinter = coldsample[0]
coldspring = coldsample[1]
coldsummer = coldsample[2]
coldautumn = coldsample[3]

#hot data
hotwinter = hotsample[0]
hotspring = hotsample[1]
hotsummer = hotsample[2]
hotautumn = hotsample[3]

# ### Define annual functions (for generating normal and extreme years)
def normalyear(projection, years):
''''Function takes 2 arguments: 'projection' is the dataframe you will generate and populate with your data, 'years' is the number of output years'''
    normal_ctr = 0 #variable to count from (1 is winter, 2 spring, 3 summer, 4 autumn)
    normalseq = [] #blank list
    for i in range (years): #change number here for number of years
        for yrlist in normalsample:
            ran_yr = np.random.choice(yrlist, 1) #choose a randomly sampled year from previous cell
            normal_ctr += 1 # increment cold_ctr variable by 1
            normalseq += [(ran_yr[0], normal_ctr)]
        for item in normalseq: #item is a tuple with year and season, coldseq is all extreme cold year and season pairs
            projection.append(normal.query("Year == %d and Season == '%d'" % item))
            normalseq = [] #reset coldseq to an empty list so it samples from a new random year
            normal_ctr = 0 #reset counter to 0 so seasons stay as 1,2,3,4

def extremeyear(projection, years):
''''Function takes 2 arguments: 'projection' is the dataframe you will generate and populate with your data, 'years' is the number of output years'''
    extremeseq = [] #reset to an empty list so it samples from a new random year
    extreme_ctr = 0 #reset counter to 0 so seasons stay as 1,2,3,4
    for i in range (years): #change number here for number of years
        for yrlist in extremesample:
            ran_yr = np.random.choice(yrlist, 1) #choose a randomly sampled year from previous cell
            extreme_ctr += 1 # increment counter variable by 1
            extremeseq += [(ran_yr[0], extreme_ctr)]
        for item in extremeseq: #item is a tuple with year and season, coldseq is all extreme cold year and season pairs
            projection.append(extreme.query("Year == %d and Season == '%d'" % item))
            extremeseq = [] #reset to an empty list so it samples from a new random year
            extreme_ctr = 0 #reset counter to 0 so seasons stay as 1,2,3,4

def hotyear(projection, years):
''''Function takes 2 arguments: 'projection' is the dataframe you will generate and populate with your data, 'years' is the number of output years'''
    hotseq = [] #reset to an empty list so it samples from a new random year
    hot_ctr = 0 #reset counter to 0 so seasons stay as 1,2,3,4
    for i in range (years): #change number here for number of years
        for yrlist in hotsample:
            ran_yr = np.random.choice(yrlist, 1) #choose a randomly sampled year from previous cell
```

```
            hot_ctr += 1 # increment counter variable by 1
            hotseq += [(ran_yr[0], hot_ctr)]
        for item in hotseq: #item is a tuple with year and season, coldseq is all extreme cold year and season pairs
            projection.append(extremehot.query("Year == %d and Season == '%d'" % item))
            hotseq = [] #reset to an empty list so it samples from a new random year
            hot_ctr = 0 #reset counter to 0 so seasons stay as 1,2,3,4

# ### Define seasonal functions
def futurewinter(projection, data, input_list):
'''''function takes 3 arguments, projection is the dataframe you will write your data to, data is the dataset you are sampling from (e.g. extreme contains all extreme data), and input_list is the list of years for your variable(e.g. extreme winter contains all years with extreme winters).'''
    items = [] #blank list to populate with year/season pairs
    ran_yr = np.random.choice(input_list, 1) #chooses a random year
    items += [(ran_yr[0], 1)] #takes the random year and appends number 1 (to denote winter)
    for item in items:
        projection.append(data.query("Year == %d and Season == '%d'" % item))

def futurespring(projection, data, input_list):
    items = [] #blank list to populate with year/season pairs
    ran_yr = np.random.choice(input_list, 1) #chooses a random year
    items += [(ran_yr[0], 2)] #takes the random year and appends number 2 (to denote spring)
    for item in items:
        projection.append(data.query("Year == %d and Season == '%d'" % item))

def futuresummer(projection, data, input_list):
    items = [] #blank list to populate with year/season pairs
    ran_yr = np.random.choice(input_list, 1) #chooses a random year
    items += [(ran_yr[0], 3)] #takes the random year and appends number 3 (to denote summer)
    for item in items:
        projection.append(data.query("Year == %d and Season == '%d'" % item))

def futureautumn(projection, data, input_list):
    items = [] #blank list to populate with year/season pairs
    ran_yr = np.random.choice(input_list, 1) #chooses a random year
    items += [(ran_yr[0], 4)] #takes the random year and appends number 4 (to denote autumn)
    for item in items:
        projection.append(data.query("Year == %d and Season == '%d'" % item))

# ## All possible year and season combinations
#
#To generate your final sequence you can choose combinations of years and seasons, i.e. you can have 5 'normal' years followed by a cold winter,a wet spring, a dry summer and a wet autumn. Do this by copying and pasting the relevant code
#
# **WARNING: IF SECTIONS OF CODE DON'T RUN IT IS DUE TO LACK OF DATA COMBINATIONS**

projection = [] #sample blank dataframe so code runs

#normal year
normalyear(projection, 1) #one normal year for example

#extreme year
extremeyear(projection, 1) #one extreme year

#hot year
hotyear(projection, 1) #one extreme hot year
```

```

# **Winter Functions**

#normal winter
futurewinter(projection, normal, normalwinter)

#extreme winter
futurewinter(projection, extreme, extremewinter)

#wet winter
#futurewinter(projection, extremewet, wetwinter)

#dry winter
#futurewinter(projection, extremedry, drywinter)

#hot winter
futurewinter(projection, extremehot, hotwinter)

#cold winter
futurewinter(projection, extremecold, coldwinter)

# **Spring Functions**
#normal spring
futurespring(projection, normal, normalspring)

#extreme spring
futurespring(projection, extreme, extremespring)

#hot spring
futurespring(projection, extremehot, hotspring)

#cold spring
futurespring(projection, extremecold, coldspring)

# **Summer Functions**
#normal summer
futuresummer(projection, normal, normalsummer)

#extreme summer
futuresummer(projection, extreme, extremesummer)

#hot summer
futuresummer(projection, extremehot, hotsummer)

#cold summer
futuresummer(projection, extremecold, coldsummer)

# **Autumn Functions**
#normal autumn
futureautumn(projection, normal, normalautumn)

#extreme autumn
futureautumn(projection, extreme, extremeautumn)

#hot autumn
futureautumn(projection, extremehot, hotautumn)

#cold autumn
futureautumn(projection, extremecold, coldautumn)

# ## Generate your new sequence
#
# Simply copy and paste the functions above (following seasonal sequence) to generate your future climate.
# The example below shows 2 'normal years', followed by 2 'extreme' years, a cold winter, wet spring, hot/dry summer, and hot/wet autumn.
```

```python

# ### First, The spin-up dataframe for the period 1970 to 2000, used to get average data to initialise the model
spinupdf = df2
spinupdf.head()

spinupdf = spinupdf.reset_index()

spinupdf = spinupdf.set_index(['time'])
spinupdf.head()

spinup = spinupdf.loc['1970-01-31':'2000-11-30'] #extract your years here
spinup.tail(n=100)

spinup = spinup.reset_index() #reindex the df so you should be able to append your data after this data
spinup.head()
spinup.tail()

#reset index for the coords of the netCDF file (NEEDS TO BE UNIQUE)
spinup.set_index(['latitude', 'longitude', 'time'], inplace=True)

#back to xarray dataset
spinup = spinup.to_xarray()
spinup

#comment this back in when you need it IF you want to save to NetCDF
#spinup.to_netcdf('E:/Path/ToFile/1970-2000.nc', engine='scipy') #save it as a NetCDF file

# ## Now generate your future run
# this blank dataframe will create annual or seasonal sequences - make sure you respect the seasonal sequence if doing individual seasons!
# Choose what you want your future scenario to be and ONLY choose the ones you actually want, for example if you want 10 hot years then just run the hotyear command with a 10 in it

future = [] #blank dataframe (should be the first argument in all following functions)

# 10 hot years
hotyear(future, 10)

# 10 normal years
normalyear(future, 10) #change number here for number of years

# 10 extreme years
extremeyear(future, 10) #change number here for number of years

#cold winter
futurewinter(future, extremecold, coldwinter)

#cold spring
futurespring(future, extremecold, coldspring)

#hot summer
futuresummer(future, extremehot, hotsummer)

#hot autumn
futureautumn(future, extremehot, hotautumn)

#concatenate the dataframe and print for inspection
future = pd.concat(future)
future.head()

# rename the columns
```

```
future = future.rename(columns={"time":"date"})

#write the future data to excel to use the EurasiaUtilsGUI which creates NetCDF files which function with GlobalECOSSE
futureXLS = future.to_excel('E:/Data/EObs/10VeryHotYears_Tg.xlsx') # write to Excel

# At this point use this excel file and the EurasiaUtilsGUI to generate future climate files


# ## ALTERNATIVE Creating Future Data without EurasiaUtilsGUI

# This section allows for the generation of a new NetCDF file from the spinup and future periods, by creating a dummy date variable from 2000-2010 for the future data, and joining this to the real data from 1970-1999

future = future.reset_index()
future.head()

# #### add new date variable from file
''''this excel file contains dates on a seasonal basis for each lat/lon combo
from 2000-2010 to allow for merging with the 1970-1999 EObs past data'''
df = pd.read_excel('E:/Vault/Dates2000-2010.xlsx')
df.head()

#add this to the future data as the 'time' column
future['time'] = df['date']
future.head()

# #### Join spinup and new df
#the spinup df goes to Nov 1999, the future df picks up in December 1999

spinup = spinupdf.loc['1970-01-31':'1999-11-30'] #extract your years here
spinup.tail(n=100)

#reset the index
spinup = spinup.reset_index()
spinup

#set the index so the xarray dataset has coordinates
spinup = spinup.set_index(['latitude', 'longitude', 'time'])
spinup.head()

future = future.reset_index()

#set the index so the xarray dataset has coordinates
future = future.set_index(['latitude', 'longitude', 'time'])
future.head()

#convert to xarray dataset
spinupds = spinup.to_xarray()

#convert to xarray dataset
futureds = future.to_xarray()

#merge the datasets using xarray merge command
merged = spinupds.merge(futureds)

#have a look at the new dataset
merged

#write the data to a netcdf file for running the model with
merged.to_netcdf('E:/Path/ToFile/10HotYears.nc')
```