Climate change mitigation potential of lignocellulosic succinic acid

Assessing feedstock supply and integrated land use options in a UK Wheat-Miscanthus bio-succinic acid-based bioplastics production system

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by

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Declaration of Originality

I hereby declare that this thesis, ‘Climate change mitigation potential of lignocellulosic succinic acid life cycle: Assessing feedstock supply and integrated land use options in a UK Wheat-*Miscanthus* bio-succinic acid-based bioplastics production system’, is entirely my own work. Information derived from others is clearly cited and referenced and/or with appropriate acknowledgement given.

-Yuanzhi Ni

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Abstract

This research addresses emergent societal concerns driving national policies that seek to replace or reduce the use of petro-based plastics. Whilst environmental pollution by plastics is the dominant contemporary driver, alternatives will also need to demonstrate wider environmental and social benefits, not least the reduction of Greenhouse Gas (GHG) emissions. Biodegradable plastics produced from bio-based Succinic Acid (SA) are evaluated as an alternative to petro-based plastics in the context of the transition to a post-petroleum era.

A case study-based methodology was adopted that uses a feedstock catchment area near Hull, England, to provide high spatial and temporal resolution bio-physical, agronomic and climatic data to parameterise quantitative models for crop growth, nitrogen and carbon turnover and life cycle assessment (LCA). The main research questions are: (1) how can the feedstock availability of lignocellulosic biomass (LCB) be optimized, and; (2) can the associated GHG emissions of the commercial scale production of LCB-derived SA be reduced by the using agricultural residues and/or perennial, LCB crops?

The results of this case study suggest that significant environmental benefits would result from the adoption of a mixed LCB resourcing strategy. Introducing the perennial grass crop *Miscanthus* into the arable landscape to replace winter wheat on selected low quality, and environmentally vulnerable soils (8% of the total area) is the main driver for the benefits. A ‘mixed production’ (MP) scenario, using *Miscanthus* and winter wheat, and a ‘winter wheat only’ single production (SP) scenario, were developed to investigate the productivity and the potential climate change mitigation impacts arising from the proposed land use change strategy i.e. a shift from the SP to MP scenarios.

LCAs were conducted to explore the climate mitigation potential of LCB-based SA production. Integrated feedstock provision strategies that include perennial-derived LCB are found to be crucial for the overall climate mitigation performance of bio-plastics. A significant bioeconomy and agricultural opportunity has been identified for the provision of LCB-derived bio-plastics from dedicated, perennial crops. Scenarios without the perennial crop resulted in GHG emission balances of bio-SA based plastics that were similar to grain and petro-based plastics. In the scenario of *Miscanthus* being cultivated on low-quality soils, the LCB-based SA life cycle results in a persistent net carbon sink being generated.

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Table of Contents

Table of Figures

Table of Tables

Abbreviations & Acronyms

1996 Guidelines	Revised 1996 Guidelines for National Greenhouse Gas Inventories
2000-GPG	2000 Good Practice Guidance and Uncertainty Management on National Greenhouse Gas Inventories
2006-AFOLU	Volume 4 Agriculture, Forestry and Other Land Use in the 2006 IPCC Guidelines for National Greenhouse Gas Inventories
ADMIT BioSuccInnovate	Adaptation and Mitigation through Bio-Succinate Innovation project (http://www.bio-succinnovate.com/)
AGB	Aboveground biomass
AHDB	Agriculture & Horticulture Development Board
ALCA	Attributional LCA
BC	Baseline climate
BDG	Biodegradation
BDO	1,4-butanediol
BEAT	Biomass Environmental Assessment Tool v2.1
BGB	Belowground biomass
CHP	Combined heat and power
CLCA	Consequential LCA
CMIP5	Coupled Model Intercomparison Project Phase 5
CV	calorific values
DEFRA	Department for Environment, Food and Rural Affairs
DM	Dry matter
DMY	Dry matter yield
DNDC	DeNitrification-DeComposition model
DPM	Decomposable plant material
DSP	Downstream processing
DW	Deadwood
EC	European Commission
EF	Emission factor
fb	Fully bio
GBS	Global Bioeconomy Summit
GHG	Greenhouse gas
GWP	Global warming potential
GPG-LULUCF	Good Practice Guidance for Land Use, Land-Use change and Forestry
Gt	Giga tonnes
HAC	High Activity Clay
HE	High emission
HI	Harvest Index
HPL	high purity lignin

IBERS	Institute of Biological, Environmental and Rural Sciences, Aberystwyth University
IPCC	Intergovernmental Panel on Climate change
ISO	International Organization for Standardization
kt	Kilo tonnes
LCA	Life cycle assessment
LCB	Lignocellulosic biomass
LCI	Life cycle inventory
LCIA	Life cycle impact assessment
MBE%	relative mean absolute bias error expressed as a percentage
MC	Moisture content
ME	Medium emission
MP	Mixed production
MPBC	Winter wheat and *Miscanthus* mixed production under baseline climate condition
MPHE	Winter wheat and *Miscanthus* mixed production under high emission (atmospheric CO_2) climate condition
MPME	Winter wheat and *Miscanthus* mixed production under medium emission (atmospheric CO_2) climate condition
MSWI	Municipal solid waste incineration
Mt	Million tonnes
NATMAP	UK National Soil Map (http://www.landis.org.uk/data/natmap.cfm)
NREU	Nonrenewable energy use
OS	Organosolv
PAS2050	Publicly Available Specification (PAS) 2050
pb	Partly bio
PBS	polybutylene succinate
PE	polyethylene
PET	polyethylene terephthalate
PP	polypropylene
R2	coefficient of determination
RED	Renewable energy directive
RMSE	Root mean square error
RPM	Resistant plant material
SA	Succinic acid
SCI	soil conditioning index
SDGs	Sustainable development goals
SE	Steam Explosion
SNS	Soil Nitrogen Supply
SOC	soil organic carbon
SP	Single production

SPBC	Winter wheat single crop production under baseline climate condition
SPHE	Winter wheat single crop production under high emission (atmospheric CO_2) climate condition
SPME	Winter wheat single crop production under medium emission (atmospheric CO_2) climate condition
SRC	short rotation coppice
STAMINA	'Stability and mitigation of arable systems in hilly landscapes' project/model
SUNLIBB	Sustainable Liquid Biofuels from Biomass Biorefining project
t	tonne
UKCP	UK Climate Projection model (http://ukclimateprojections-ukcp09.metoffice.gov.uk/)
UN	United Nations

Chapter 1. **Introduction**

1.1. Background

1.1.1. Bioeconomy strategy

With the world population estimated to reach approximately 9 billion by 2050, against a background of finite natural resources, renewable biological resources are needed not only for securing food and animal feed, but also for biofuels, biomaterials and other bio-based products. Decades of life-sciences research and the enormous progress made in biotechnology have brought the vision of a society with far less dependence on fossil fuels for energy and industrial raw materials closer than ever to becoming a reality. (European Commission 2012; White House 2012) In particular, the application of biotechnology for the sustainable processing and production of chemicals, materials and fuels from biomass creates an opportunity to significantly reduce our dependence on coal, oil and gas.

On 13 February 2012, the European Commission (EC) submitted its strategy and action plan for a sustainable bioeconomy in Europe, 'Innovating for Sustainable Growth: A Bioeconomy for Europe', to the European Parliament. (European Commission 2012) According to this strategy, a bioeconomy is defined as 'the production of renewable biological resources and the conversion of these resources and waste streams into value added products, such as food, feed, bio-based products [1] as well as bioenergy'. (European Commission 2012) The major aim of the strategy is to pave the way to a more innovative, resource-efficient and competitive society that reconciles food security with other sustainable use of biotic renewable resources, especially for industrial purposes, while minimising negative environmental impacts. Five key

[1] Note: Bio-based products are products that are wholly or partly derived from materials of biological origin, excluding materials embedded in geological formations and/or fossilised (CEN - Report on Mandate M/429". See also COM(2012) 60 final, p.3: SWD(2012) 11 final, p.5)

interlinked objectives were highlighted in the bioeconomy strategy, which are (1) ensuring food security, (2) managing natural resources sustainably, (3) reducing dependence on non-renewable resources, (4) mitigating and adapting to climate change, and (5) creating jobs and maintaining EU competitiveness. (European Commission 2012)

To accelerate the deployment of the bioeconomy strategy and maximise its contribution to a sustainable future, the 2012 strategy was updated in 2018, where the main priorities have been identified as: (1) strengthen and scale up the bio-based sectors, unlock investments and markets, (2) deploy local bioeconomies rapidly across Europe, and (3) understand the ecological boundaries of the bioeconomy. (European Commission 2018)

Bio-based products are central to the EC's bioeconomy strategy. This sector has been declared by the EU as a priority area with high potential for future growth, climate change mitigation, reindustrialisation and addressing societal challenges. An assessment by the EC indicated that bio-based products and biofuels represent approximately EUR 57 billion in annual revenue and involve 300,000 jobs. According to forecasts[2], the bio-based share of all chemical sales will rise to 12.3% by 2015 and to 22% by 2020, with a compounded annual growth rate (CAGR) of close to 20%.

The strategy and 2012 action plan highlighted the significance of major research and innovation focusing on sustainably addressing the supply side and increasing productivity, reducing losses and tapping into new biomass resources. (European Commission 2012) Moreover, the 2018 action plan further prioritises key action areas, including bio-based innovations in farming; developing new opportunities for bio-based-markets in rural and coastal areas with increased involvement and benefits for primary producers; and understanding the ecological boundaries of the bioeconomy, such as carbon sequestration capacity and sustainable biomass availability.

[2] Bio-based products, available at http://ec.europa.eu/growth/sectors/biotechnology/bio-based-products_en; accessed in 28 Nov 2018

In addition to the bioeconomy strategy, the bio-based products sector is also linked with other key EU policies, such as industrial policy, The Circular Economy Package, European Innovation Partnerships and the European Commission's Lead Market Initiative. In October 2018, the European Parliament voted to approve a complete ban on single-use plastic bags and cutlery, which have caused huge environmental problems, such as marine pollution. This might give rise to potential impacts such as behaviour change, increased use of paper- or wood-based alternatives and increased used of bio-based plastic products. In September 2018, the UK Department for Environment, Food and Rural Affairs announced the introduction of the Environmental Land Management scheme, under which farmers will receive subsidies based on the environmental benefits they provide. It will replace the £3 billion a year in subsidies that UK farmers currently receive under the EU Common Agricultural Policy, which is based on the area of the land being farmed.

1.1.2. Bio-based succinic acid and biomaterials

Succinic acid (SA) ($HOOC-CH_2-CH_2-COOH$, also known as amber acid and butanedioic acid) is an aliphatic, saturated C4 dicarboxylic acid. It has been recognised by the United States Department of Energy (DOE) as one of the 15 most promising biomass-derived chemicals as alternatives to oil-derived bulk chemicals. Its importance as a platform chemical has also been highlighted by Bechthold et al. (2008) and Peterson and Bozell (2010), as well as experts convened in the BREW project.(Patel et al. 2006)

The industrial potential of SA was recognised by Zeikus (1980) for the first time. Traditional applications of SA include food additives, detergents, cosmetics, pigments, toners, cement additives, soldering fluxes and pharmaceutical intermediates. (Zeikus et al. 1999) Apart from the aforementioned traditional markets, fermentation-derived bio-SA has the potential to become a large-volume commodity chemical. Being considered as a potential building block, SA is regarded as a promising "green" platform chemical

(Zeikus et al. 1999; Bechthol et al. 2008) that can be converted into several commodity or specialty chemicals owing to the versatility of its two carboxylic groups and its partial solubility in water. Additionally, components like diamines or diols, which are required in the production of polyamides (PA), polyesters and poly (ester amide)s, can also be obtained by chemical conversion of SA.(Bechthol et al. 2008)

According to the BREW report, SA was being produced in quantities of approximately 16 kilotons (kt) annually in 2006. The global market size for SA was estimated at around 47.5 kt in 2014[3]and 58.5 kt in 2015[4], while it is expected to grow at a CAGR of around 25% (24%[5] during the forecast period 2014-2020 and 27.2% from 2016 to 2021[3]). The major drivers for the growth of the SA market are the growing number of applications and the movement of the chemical industry towards bio-based sustainable chemicals.

Before the development of fermentation processes for its production, SA was exclusively derived from petroleum by catalytic hydrogenation of maleic anhydride. Since 2010, a number of companies and industrial consortia have been commercially producing first-generation bio-SA in various locations across the world, including Reverdia (Netherlands), Bio-Amber (Canada), and Myriant and Succinity (a joint venture between BASF and Corbion Purac, Germany).(Nghiem et al. 2017) Other stakeholders include Nippon Shokubai (Japan), Mitsubishi Chemical Holdings (Japan), Kawasaki Kasei Chemicals Ltd. (Japan) and several Chinese and Israeli companies[4].

As the main driver of the bio-based economy and its core component bio-based material, the global warming potential (GWP) reductions from using bio-SA as a platform chemical have been suggested by several life-cycle assessments (LCAs). Most of those

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[3] 'Succinic Acid Market Analysis By Application', available at https://www.grandviewresearch.com/industry-analysis/succinic-acid-market, accessed in 28 Nov 2018

[4] 'Succinic Acid Market by Type (Bio-based, Petro-based)', available at: https://www.marketsandmarkets.com/Market-Reports/succinic-acid-market-402.html, accessed in 28 Nov 2018

[5] 'Research and Markets', available at:http://news.bio-based.eu/research-and-markets-global-succinic-acid-and-bio-succinic-acid-market/

LCAs were conducted using conventional food crops as the feedstock, comparing with fossil fuel-based alternatives.

The choice of feedstock for bio-SA production is critical to both production costs and the environment. Although food-based biomass is currently the major feedstock and technology deployed in national bioeconomy strategies, concerns regarding competition for food, land-use change, loss of biodiversity and increased greenhouse gas (GHG) emissions have led to an increased focus on the utilisation of lignocellulosic biomass (LCB), resourced from agricultural and forestry residues and dedicated biomass crops. Nevertheless, despite a commercial willingness, production of second-generation bio-SA has yet to be realised, with one of the main barriers being the absence of a sustainable LCB supply supported by a concrete LCA demonstrating its real capacity and potential for GHG emission reduction. Feedstock availability and supply have been identified as the main limitations to the use of biomass as a resource for bioenergy and biomaterial production. (FitzPatrick et al. 2010)

1.1.3. ADMIT Bio-SuccInnovate Project

The Adaptation and Mitigation through Bio-Succinate Innovation (ADMIT Bio-SuccInnovate) project is funded by Climate KIC, one of three Knowledge and Innovation Communities (KICs) created in 2010 by the European Institute of Innovation and Technology (EIT). The aims of the ADMIT Bio-SuccInnovate project include:

- To demonstrate the production of second-generation bio-SA from lignocellulosic sugars;
- Determining the reduction of GHG emissions compared to current starch-based process;
- Determining the techno-economic feasibility;

- Demonstrating the applicability of the current biorefining process adopted by one of the project partners CIMV[6] and providing commercial uplift.

1.2. Conceptualising the research problem

One of the key sustainability strategies pursued in the Bio-SuccInnovate project is to produce fermentable sugars from sustainable LCB, including agricultural residue wheat straw and the dedicated perennial crop *Miscanthus*. However as indicated by O'Brien et al. (2017), the actual contribution of the bioeconomy to sustainability depends on how it is implemented. There are currently uncertainties regarding the actual GHG emission reduction potential of the lignocellulosic bio-SA production systems and the environmental impacts associated with the feedstock supply.

The major concerns are sustainability issues relating to feedstock production and availability; (Glithero et al. 2013; Hamelinck & Faaij 2006; Engel et al. 2005; Copeland & Turley 2008) the potential impacts on soil carbon of using agricultural residues and perennial crops;(Mann et al. 2002; Kim and Dale 2005) and GHG emissions associated with agricultural production activities and land-use change.

Preliminary estimates of potential life-cycle GHG emissions when using LCB feedstocks for the production of bio-SA suggest significant potential savings (60% to 80%) compared to non-renewable-based production pathways. (Patel et al. 2006; Patel et al. 2018) However, the actual reduction potential of specific production chains remains uncertain and depends on the specific production scenarios. (Don et al, 2012)

For agricultural residues, such as wheat straw and maize stover, concerns remain over the real availability of the agricultural residues, the impacts on other markets and the impacts on soil carbon change associated with their use for biofuel or biomaterial production. No LCA studies of bio-SA production have taken the impacts on soil

[6] Information available at: http://www.cimv.fr/cimv-technology/technology.html

carbon change into account when using agricultural residues as a feedstock. Dedicated energy crops are relatively less demanding during the cultivation stage in terms of energy input, fertiliser application, crop protection chemicals and land requirement. Their potential for increasing the soil carbon stock has been reported in several studies (Lugato et al. 2014; Davis et al. 2012) and makes them promising as feedstocks for biomaterial or biofuel production. Additionally, utilising arable land for perennial crop production might also alter the above-ground carbon stock. These factors should all be considered when conducting a LCA for bio-SA. However, current LCA studies of lignocellulosic bio-succinic have focused on the chemical conversion processes, only applying default values for feedstock supply. The real impacts on the GHG balances of utilising LCB as a feedstock for the bio-SA system needs further optimisation, investigation and demonstration.

As reflected by the recent view of EC 2012 bioeconomy strategy, (European Commision 2017) major findings and insights to date showed the complexity of a comprehensive biomass assessment facing significant data gaps, a diversity of supply, demand, policies and a large variety of sectors potentially affected. At the same time, data are lacking in some areas (waste, bio-based products) and, owing to the inherent complexity, limited progress has been made with regard to different supply and demand scenarios and their economic, social and environmental impacts.

1.3. Research questions, aims and objectives

This thesis aims at addressing the data and knowledge gaps regarding LCB feedstock supply capacity and GHG dynamics in the wider sustainably context; investigating and demonstrating the life-cycle GHG reduction potential of bio-SA produced from optimised LCB supply scenarios, using a series of liable modelling methodologies; ensuring feedstocks are delivered to a defined primary conversion centre with quantified and robust GHG reduction potential by optimising the carbon balance of the lignocellulosic bio-SA life-cycle.

Multiple research needs and knowledge gaps from various fields will be examined in this work, including agro-ecosystem modelling of LCB, sustainable lignocellulosic feedstock supply, climate change mitigation and the bio-SA life-cycle. The research questions are (1) how can the feedstock availability of lignocellulosic biomass be optimized, and; (2) can the associated GHG emissions of the commercial scale production of LCB-derived SA be reduced by the using agricultural residues and/or perennial, LCB crops? The overarching aim is to provide scientific evidence and an estimation of the availability and GHG emissions associated with different scenarios for biomass supply through crop modelling and LCA methodologies.

The expected original outcomes include:

1. Evaluation of current and future lignocellulosic feedstock production for a case study in England. This will be assessed by looking at the feedstock availability for two defined production scenarios (winter wheat only and winter wheat-*Miscanthus* mixed production) under current and future climate conditions.

2. LCA of LCB produced from two defined provision scenarios with traceable and case-specific figure inputs accounting for N_2O emissions resulting directly and indirectly from fertiliser application and carbon emissions from terrestrial carbon stock changes from major relevant carbon pools. Climate change impacts will be used as the main indicator and different level carbon stock-change accounting approaches will be applied and compared.

3. Ultimately, these results will be integrated into a ‘cradle to end-of-life’ LCA of bio-SA to investigate the influence of different feedstock provision scenarios on the overall GHG emission balances associated with the LCB-SA life-cycle, compared with starch-based and petro-based alternatives.

1.4. Thesis outline

This thesis consists of eight chapters. Whilst this first chapter provides the general introduction to the background of this research project from the bioeconomy strategy, the role of bio-based SA within the bioeconomy strategy and the ADMIT Bio-SuccInnovate project within which this PhD project was carried within.

Chapter 2 conducts the literature review on the LCB-based SA production, covering aspects of LCB feedstocks, SA production routes, the methodologies used to estimate the carbon balances associated with bio-SA life cycles and also a literature-based discussion on the sustainability, sustainable development and the bioeconomy strategy.

Chapter 3 describes the analytical framework, case study area and methodologies used in this study. Modelling-based methodologies were applied through this study, indulging LCA approaches, Tier 2 approach based on 2006 Intergovernmental Panel on Climate Change (IPCC) Guidelines for National Greenhouse Gas Inventories (Intergovernmental Panel on Climate Change 2006a) and process-based crop models deployed as a Tier 3 methods.

Chapter 4 presents the results regarding the LCB availability in the case study area for two land use scenarios under three climate conditions. These results were produced based on process-based model outputs and assumption regarding the current straw uses.

Chapter 5 presents the model estimated site-and management- specific N_2O and NO_3^- effluxes during the two production scenarios under baseline climate condition. The purpose was to test the N_2O emission reduction potential aroused by integrating *Miscanthus* into the wheat production system.

Chapter 6 presents the terrestrial carbon emissions estimated with two tiered approaches. The aim is to quantify the land use change related carbon emissions from the two defined feedstock production scenarios, exploring the land-based carbon sequestration potential associated with integrating *Miscanthus* into the wheat production system.

Chapter 7 conducted two LCAs with different system boundaries. One 'cradle to up-stream factory gate' was conducted to investigate the GHG emission reduction potential of the mixed production scenarios for delivered LCB feedstocks. The second, 'cradle to end-of-life' LCA was conducted to investigate the overall carbon balance of LCB-SA life cycle, demonstrating the climate change mitigation potential associated with different feedstock provision scenarios.

Chapter 8 begins with the integration of the results produced from Chapter 4 to Chapter 7, presenting the potential benefits of integrating *Miscanthus* into the wheat production system from aspects including availability whilst focusing on climate change mitigation potential. Main contributions, policy implications and recommendations for future works are also included as parts of the final conclusions.

Chapter 2. **Literature Review**

Part 1. Succinic acid and its feedstocks

This part of literature review aims to present the state-of-art of succinic acid production, especially through LCB feedstocks, current knowledge on straw production and *Miscanthus* cultivation. The concept 'sustainable feedstock supply' is also discussed from the environmental, social and economic perspectives, while a more systemic review of sustainable development will be included in the second part of literature review.

2.1. Succinic acid production

SA is a C4 dicarboxylic acid with the molecular formula of $C_4H_6O_4$. (Figure 2-1) It can be derived from renewable resources and has tremendous potential as a platform chemical for a number of other industrial chemicals. SA was isolated for the first time from microbial fermentation in 1546. (Song & Lee 2006)

2.1.1. Chemical synthesis

Traditionally, SA is produced by chemical synthesis from *n*-butane/butadiene via maleic anhydride, utilising the C4-fraction of naphtha (Figure 2-1), in quantities of about 15,000 t/yr with a price range of about 6–9 $/kg. (Bechthold et al. 2008; Patel et al. 2006) The production level was shown in Figure 2-2.

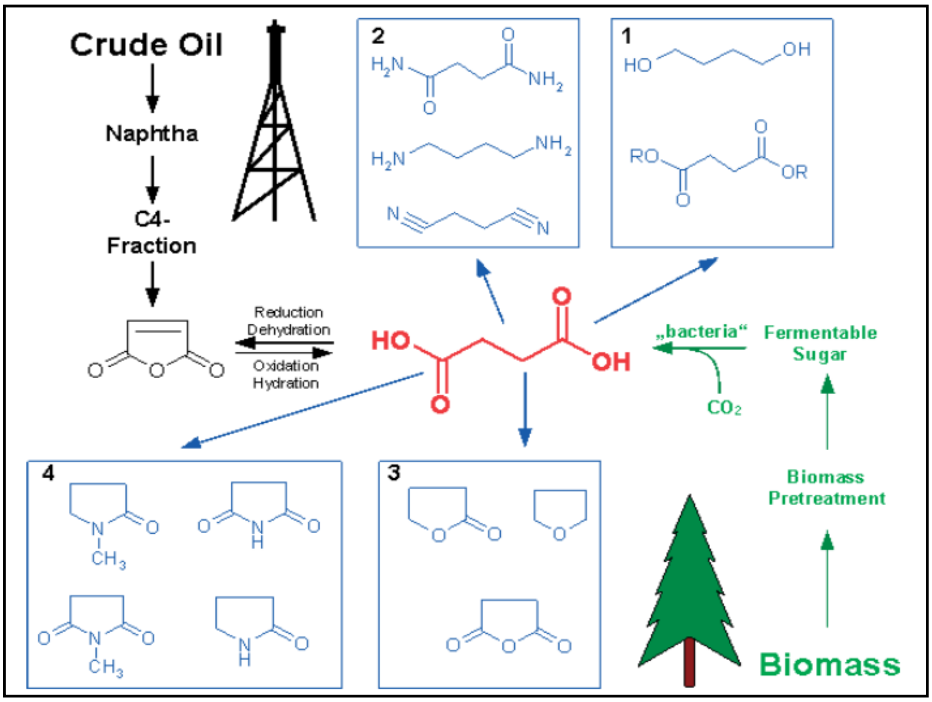

Figure 2-1Possible pathways for SA production and products derived by chemical conversions; 1) Acyclic O-containing, 2) acyclic O, N-containing, 3) cyclic O-containing, 4) cyclic O, N-containing (Bechthold et al. 2008)

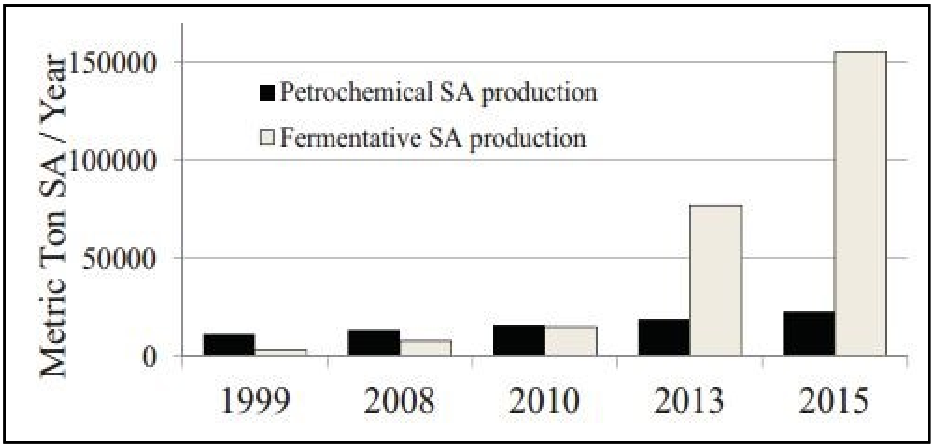

Figure 2-2 Evolution of worldwide SA production in metric tons per year (Pinazo et al. 2015).

2.1.2. Biological synthesis

Recently, academics and industries have started to investigate the production of SA from renewable feedstocks through microbial fermentation.(Chen & Patel 2011) Several microorganisms can be applied in SA fermentation, including gastrointestinal bacteria, rumen bacteria and *Lactobacillus* spp.. (Kaneuchi et al. 1988) Feedstocks that can be utilised include corn/wheat starch, corn steep liquor, whey, cane molasses, glycerol, lignocelluloses, cereals and straw hydrolysates. (Chen 2010) One of the best features of producing SA through fermentation is that carbon dioxide (CO_2) is needed by the microorganisms as a second substrate for SA production. Theoretically, SA production by fermentation consumes 1 mole of CO_2 and 0.5 mole of glucose per mole of SA produced.(Chen & Patel 2011) The chemical equation for this conversion is:

$$C_6H_{12}O_6 + 2CO_2 + 4\ \text{‘H’} \rightarrow 2C_4H_6O_4 + 2H_2O$$

Lignocellulosic bio-based SA production comprises the following main steps: pretreatment, hydrolysis of cellulose and hemicellulose, sugar fermentation, separation of lignin and downstream purification.

Pretreatment is an important process. Although there are many pretreatment approaches available, they share a main objective, which is to alter or breakdown the lignin structure and disrupt the crystalline structure of cellulose in order to increase the enzyme's accessibility to the cellulose in the hydrolysis step and increase the yield of fermentable sugars. (Alvira et al. 2010; Mosier et al. 2005) Generally, pretreatment processes are classified into four categories, including physical, chemical, physico-chemical and biological. (FitzPatrick et al. 2010) As reviewed by FitzPatrick et al. (2010), physical pretreatment methods exhibit relatively lower yields but higher costs. Chemical pretreatment approaches could be used to process a wider range of feedstocks, while their relatively harsh reaction conditions might influence the downstream biological fermentations. (Mosier et al. 2005; FitzPatrick et al. 2010) Physico-chemical pretreatment is a combination of both physical and chemical conditions. Generally milder chemical conditions are used under more extreme operational conditions, such as higher pressures and temperatures. Biological pretreatments are considered as more promising and eco-friendly options, due to their lower chemical and energy requirements and milder operational conditions. (Mosier et al. 2005; Sindhu et al. 2016) The main barriers for the application of biological pretreatments are their long incubation time for effective delignification and are less controllable compared with other options. (FitzPatrick et al. 2010; Sindhu et al. 2016)

2.2. Lignocellulosic biomass supply

In general, lignocellulosic feedstocks can be divided into three groups: (1) agricultural residues, (2) forest residues and (3) dedicated energy crops. (Carriquiry et al. 2011)

2.2.1. Agricultural residues

For agricultural residues, the main crops considered are corn, sorghum, barley, wheat, rice and sugarcane. The major benefit of using agricultural residues is that, compared with dedicated energy crops, there is no additional land requirement. This minimises not only the (direct) impact on food prices, but also the GHG emissions related to direct or indirect land-use change. (Carriquiry et al. 2011; Searchinger et al. 2008) For some crops and some situations, removal of residues may be beneficial to crop production by helping to control pests and diseases, increasing the soil temperature in spring and increasing seed germination in colder climates. (Andrews 2006)

While there are also arguments that excessive removal of residues will have negative impacts on soil properties and crop production, for example, decreased yields in dry years owing to lower soil moisture or poorer germination and yield decreases with soil loss. (Aden & Heath 2009; Carriquiry et al. 2011; Williams & Inman 2009; Andrews 2006) Mann et al. (2002) reviewed the existing literature to evaluate the major environmental impacts potentially associated with stover harvest from reduced tillage maize production sites. The major concerns are erosion and the soil organic carbon (SOC) dynamic, with the latter of concern for both its role in soil quality and yield, and for global carbon cycle implications. They concluded that, although several research papers discussed the impacts of the residue harvest, few were focused on the impacts of maize stover harvest, and most discussions acknowledge potential trade-offs between positive and adverse effects. More researches and understandings were suggested on the following areas: erosion and water quality, especially pesticides and nitrates; rates of transformation of different forms of SOC; effects on soil biota and SOC dynamics in subsoil. (Mann et al. 2002)

The residue removal rate is a key parameter that needs to be taken in to account for agricultural residue utilization. The sustainable residue removal rate varies by system, according to factors such as management practice, crop species, crop yield, climate, topography and soil parameters. Tools such as RUSLE2, WEQ, and the soil conditioning index (SCI) are suggested by Andrews (2006) as the best way to predict safe removal rate.

It has been identified that the high ash content in cereal straw is one of the key challenges in its re-treatment processes for further biochemical utilisation, while the ash content in dedicated LCB crops such as Miscanthus were reported to be much smaller. (Adhikari et al. 2018; Swain et al.2019)

2.2.2. Forest residues

Forest residues include logging residues from commercial forests, fuel wood extracted from forestland, and primary and secondary wood processing mill residues. (Perlack et al. 2005; Williams & Inman 2009) Whittaker et al. (2011) argued that there are concerns about the long-term sustainability impacts resulting from removing large amounts of forest residues from forest sites, but it is still possible that a proportion of them could be extracted without adverse ecological impacts. As with agricultural residues, the sustainable residue removal rate is crucial, and system specific, so an Ecological Site

Classification Decision Support System is also recommended. For forest residues, the main components of the economic cost are collection and transportation. Additionally, there is an environmental concern regarding the potential decrease of recoverability in harvest areas. (Perlack et al. 2005; Carriquiry et al. 2011)

2.2.3. Dedicated energy crops

Dedicated energy crops are non-food biomass crops that could act as additional potential sources of feedstocks for biofuel or biomaterial production. Dedicated energy crops can be divided into perennial forage crops, for example, switch grass and *Miscanthus*, and woody energy crops, such as willow. According to Carriquiry et al.(2011), dedicated energy crops are generally less demanding in terms of inputs and they are considered to be able to reduce soil erosion, improve soil conditions and provide better habitats for wildlife than annual crops. Generally, a higher biomass productivity per unit of land can be achieved from dedicated energy crops compared with cereal crops.

Several studies have acknowledged the SOC sequestration potential of converting arable into grassland. Lugato et al.(2014) used the CENTURY model to assess six alternative management practice scenarios as alternatives to the business as usual situation (Lugato et al. 2014). The six scenarios consisted of the conversion of arable land to grassland (and vice versa), straw incorporation, reduced tillage, straw incorporation combined with reduced tillage, ley cropping system and cover crops. Conversion to grassland showed the highest SOC sequestration rates of between 0.4 and 0.8 tC/ha.yr, while the opposite scenario (100% grassland conversion into arable land) presented a SOC loss rate of 2 Gt C by 2100 (Lugato et al. 2014). However, dedicated energy crops still have the potential to compete with food production in terms of land use. For this reason, marginal land is suggested for the production of this type of feedstock. (Liska & Cassman 2008; Aden & Heath 2009; Carriquiry et al. 2011)

2.2.4. Sustainable feedstock supply

Increasing number of researches have recognised the importance of robust, reliable and sustainable biomass feedstock supply in delivering a competitive bio-based end-products to the end-user markets. (Awudu & Zhang 2012; Saavedra M. et al. 2018) Sustainable management is crucial in the agricultural system. It could be misleading that a resource such as crops is sustainable only because it is renewable or organic. On the contrary, sustainable could be contentious in the context of agricultural (Heaton et al. 2010). In some circumstances, crops used for human consumption could only renewable with a high level of resources, for example, fertiliser, soil conditioner, water resources, pesticides and labour inputs. (Lora et al. 2011) Moreover, bioenergy or biomaterial is not necessarily carbon-neural, considering the emissions of CO_2, CH_4 and N_2O during feedstock production may sometimes reduce or completely offset the CO_2 reduction of the substituted fossil fuels without appropriate farming practice. According to the UK national GHG Inventory, in the year 2017 agricultural production was responsible for 8.7% of the total national GHG emissions, increased from the year 1991 level of 6.1%, despite that the national net GHG emissions have been reduced by 40%. (Brown et al. 2019)

Moreover, it has been recognised that sustainability is much more than just environmental impacts (Finkbeiner et al. 2010) and other dimensions should be also taken into consideration. There have been multiple definitions of 'Sustainability'. The most widely adopted refers to the Brundtland report, which defines the sustainable development as 'development that meets the needs of the present generation without compromising the ability of future generations to meet their own needs'. (World Commission on Environment and Development 1987) Although there have been ongoing debated regarding not only the overarching definitions of 'sustainability' and 'sustainable development', but also the individual components of sustainability. (Rack 2017) The majority of definitions are based on three elements including environmental sustainability, social sustainability and economic sustainability. This is recognized by

Rack (2017) as one of the agreed fundamentals among the existing definitions of 'sustainability' and principles of 'sustainable development'.

Many works have suggested the potential environmental benefits of dedicated perineal crops compared with conventional food crops. These benefits include soil recuperation, increasing biodiversity and terrestrial carbon stocks enrichment. (Dale et al. 2010; Meijl et al. 2017). The main concern remains at the potential competition for land with food production. As clarified by O'Brien et al. (2017), the land competition concern can be viewed from two angles, (1) how much land can be used for production in an extensive sustainability context and (2) how much can be produced per hectare.

Regarding the first question, global land availability, two different views exists. Some resarches suggeseted potential land deficit phenomenon. (Alexander & Moran 2013) It was predicted that in 2030-2050 the global land deficit would be 200-300 million ha. (Lambin & Meyfroidt 2011) On the country, some researches argue that in global terms land availability might not be considered as a constraint, while a geographically uneven distribution of land availability exists. Souza et al. (2015) considers the availability was expect to be mainly concentrated in Latin America and sub-Saharan Africa and the agricultural area in Europe should remain stable. The current disagreement regarding future land availability estimation, predicted expansion of global population, especially middle class population, increasing requirements for food and non-food production together highlight the second question, 'how much can be produced per hectare?' and how to increase the productivity for per unit of land. This is also reflected in one of the merging research areas of bioeconomy that how to integrate dedicated energy crops into current arable landscape through high resolution land management to increase land productivity without negative impacts. (Costello & Ayoub 2019；Gopalakrishnan et al. 2011)

Another concern which has been widely discussed alongside with the EU bioeconomy evolution is the current high land footprints of the EU for both food and non-food purposes. According to O'Brien et al.(2017), cropland footprint for EU-27 is 0.29

ha/person in 2011, which is 40% higher than global average. For non-food cropland, Bruckner et al. (2018) analysed through modelling approach and illustrated that the EU was the main processer and the number one consumer region of non-food crops, despite being only the fifth largest producing region. Moreover, two thirds of the cropland required to satisfy EU non-food consumption are located outside the EU, which may results in a range of complex environmental and social issues, for instance, deforestation, carbon emissions, water security, and land access rights. (Bruckner et al. 2018)

From economic and social perspectives, it has been recognized that robust bioenergy or biomaterial markets with decent commodity prices could increase incomes and job opportunities in farming areas, especially in less developed countries or regions where a large percentage of population lives in rural area with land and agricultural as their main income. (Dale et al. 2010; Liu et al. 2011) While it was acclaimed that costs were the major barrier to commercial production of LCB-based bioenergy and biomaterial in the near to medium term. (Carriquiry et al. 2011)

2.2.5. Impacts of climate change on agricultural production

Climate change will affect the agro-ecological suitability of crops. (Fischer et al. 2002) A large number of studies analysed the climate change impacts on agricultural production for each individual countries, (Crost et al. 2018; Robertson et al. 2018; Lungarska & Chakir 2018; Wesseh Jr& Lin 2017) while some studies aimed at conducting a uniform assessment in the global level. (Fischer et al.2002; Asseng et al. 2014)

Climate change will influce global agro-ecological suitablity and agricultural production from three aspects. Firstly, it is considered that the elevated atmospheric CO_2 concentration will enhance plant photosynthesis and contribute to improved water-use efficiency, i.e. the CO_2 fertilization effect. (de Souza et al. 2013; Fischer et al. 2002; Lobell and Gourdji 2012). Field experiments with crops under 2050 CO_2 predicted levels increased the yield of rice, wheat and soybean by 15% in some regions, however effects are not globally uniform.(de Souza et al. 2013) Such potentially positive influence on crop production is mainly located regions at high latitudes in some developed nations, such as North America, North Europe and East Asia & Japan. (Fischer et al. 2002; Lungarska & Chakir 2018) On the other hand, the global warming will also increase the occurrences of extreme weather events, pest and disease infestations.(Fischer et al. 2002; Asseng et al. 2014) However this effects are considered being difficult to predict with current modelling approaches. (van Meijl et al. 2018) Thirdly, crop production may be jeopardized by drier condition and increased water stress in some regions, such as sub-Saharan Africa. Fischer et al. (2002) predicted that more than 60% of negative impacts occur in sub-Saharan Africa. Climate change scenario SRES B2 and A2 (Intergovernmental Panel on Climate Change, 2000a) will result in an expansion of arid land area by 5.4% and 8.5% in 2080s respectively compared with the reference climate (1961-1990). Other regions with predicted reduction in agricultural production include North Africa, South Asia, Central America and Latin America (Fischer et al. 2002; Crost et al. 2018; Altieri & Nicholls 2017)

As food production is considered as the core of agricultural production, most of the climate adaptation researches were conducted to understand the vulnerability of food supply under elevated atmospheric CO_2 conditions. de Souza et al. (2013) highlighted the importance and suggested further work should be conducted to understand and evaluate the response of dedicated perennial crops to climate change. de Souza et al. (2013) tested and proved the hypothesis that, as a C4 crop, the impacts of elevated atmospheric CO_2 concentration on its biomass production are minimum. However this study did not consider crops' response to the changes of other climatic parameters, such as increased rain fall level and warming temperature.

2.3. Wheat straw production and use in the UK

2.3.1 Wheat grain and straw production levels

The historical on-farm wheat grain yields in the UK are shown in Figure 2-3. The average winter wheat grain yield in the UK was 8.58 t/ha.yr in 2014, (FAO 2018) but it varies significantly between the regions. Figure 2-4 shows the variation of wheat yields across the UK regions. There were strong yields in all regions, with even the historically lower yielding North West and Merseyside showing 7.1 t/ha,(DEFRA 2015). The highest average yields were recorded in Yorkshire and the Humber region (9.4 t/ha) and the East Midlands (9.3 t/ha). (DEFRA 2015)

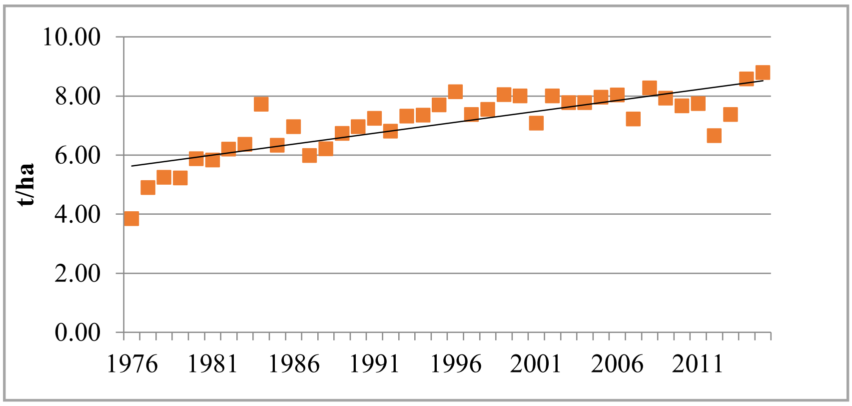

Figure 2-3 Commercial on-farm wheat grain yield in the UK from 1976 to 2015 (data source: FAO 2018).

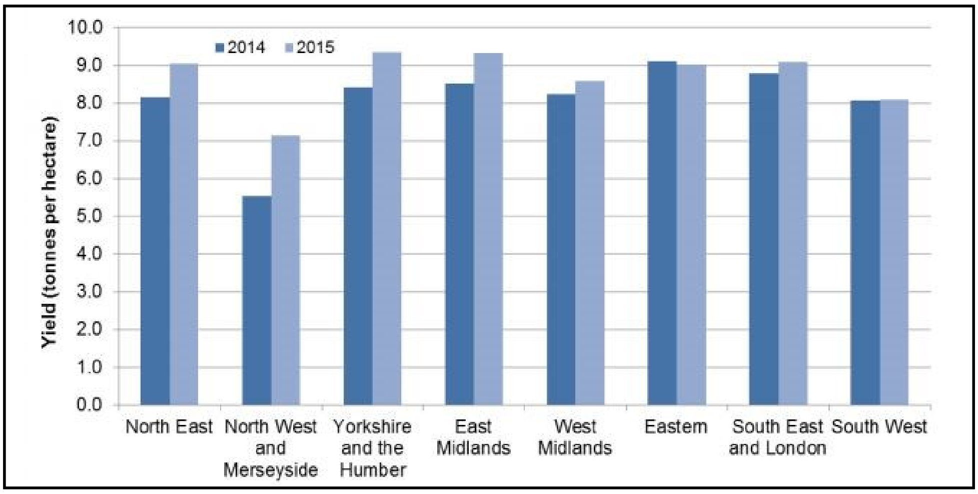

Figure 2-4 Wheat yield by English region 2014 to 2015(data source: DEFRA 2015)

2.3.1. Wheat straw production in the UK

Several studies have been conducted on straw production or straw yield in the US and UK. (Chad & Bill 2013; Donaldson et al. 2001; Glithero et al. 2013; Engel et al. 2005) According to Engel et al. (2005), most estimates of straw production levels were based on measurements of grain production and assumption of a strong relationship between grain and straw. For example, the USDA Natural Resources Conservation Service in Montana used grain yield and constant straw-to-grain ratios (1.33 and 1.67) to estimate the quantity of straw residues produced by spring wheat and winter wheat, respectively. Although the accuracy of the default values was acknowledged by Engel et al.(Engel et al. 2005), this method could only be used to estimate the total straw production levels, rather than the harvestable amounts. The harvestable straw yields are strongly influenced by the local proportion of total produced straw that are incorporate back to soil (straw-incorporated rate) due to its important role in maintaining soil structure and nutrient recovery.

An on-farm survey of 249 English farms (cereal, general cropping and mixed) was conducted and linked with farm business survey data to estimate current straw use and potential straw availability. (Glithero et al. 2013) The results showed no significant correlations between harvested wheat grain yield and straw yields. This was explained by the author as follows: ‘given the relatively low value of straw as an output from arable production, it is possible that inaccuracies could have occurred in the farmer’s recall of both number of bales produced and the percentage area from which straw was baled, leading to the low observed yields’.(Glithero et al. 2013) Another potential explanation for this could be that, to maintain the soil structure and soil nutrient level, the straw-incorporated rate should be a soil-type-specific value and might differ from farm to farm.

2.3.2. Current straw use in the UK

Straw is mainly used for animal bedding, horticulture and bioenergy, with some export potential in some years. (Nicholson et al., 2014; Brander et al., 2009) The average incorporation rate of wheat straw in the UK is reported to be from 32% (Glithero et al. 2013) to 39% (Brander et al., 2009). According to the Agriculture & Horticulture Development Board (AHDB) Straw Incorporation review (Nicholson et al. 2014), there are no official data available for straw usage in animal bedding, however estimates range between 5.8 Mt for the UK (Stoddart & Watts 2012) and 6.24 Mt for Great Britain (Copeland & Turley 2008) for all cereals (wheat, barley and oats) and oilseed rape straw. It is estimated that for Great Britain the straw usage across all livestock sectors and horticulture was over 8 Mt (68% of total production). (Copeland & Turley 2008) Brander et al. (2009) estimated that around 50% of all wheat straw was used for animal bedding. Regarding the proportion of straw used for bioenergy and biomaterial production, Brander et al. (2009) estimated that 200 Kt (3.13% of total production) of wheat straw was used for bioenergy/electricity generation in England. Stoddart and Watts (2012) reported that a total of 300 Mt of cereal and oilseed straw was used for bioenergy annually. In addition, the straw incorporated-rates for Yorkshire and the Humber and East Midlands are 17.96% and 35.34%, respectably. (Glithero et al. 2013) Based on the above information, the current uses and the proportion of each sectors were graphed in Figure 2-5.

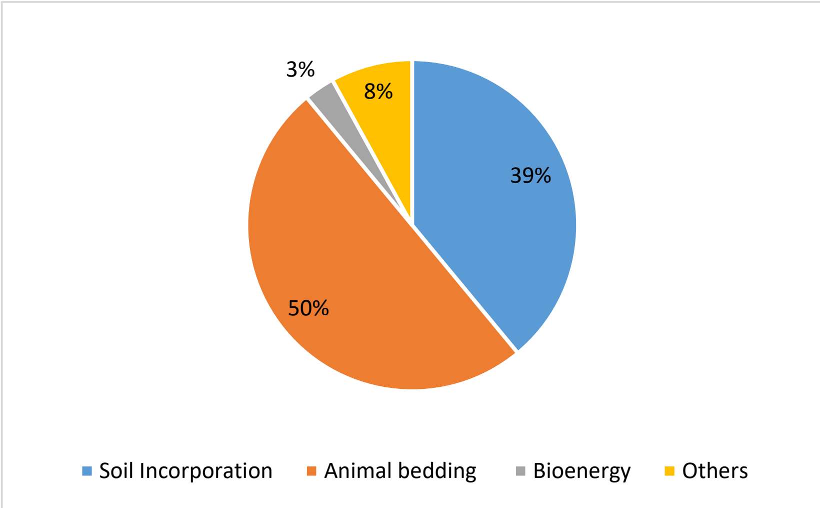

Figure 2-5 Current straw uses and the proportions in the UK.

It is worth mentioning that among the 8% 'other uses straw' (Figure 2-5), mushroom production is the main end use. (Nicholson et al. 2014) It has been recognised that mushroom cultivation from straw could effectively convert lignocellulosic residues into protein-rich food product, especially its economic value could be attributed to its low production cost and providing high yield and nutritious food source. (Petre et al. 2016)

2.4. An overview of *Miscanthus*

2.4.1. A high-yield crop and its production

Miscanthus is a genus involving 14 to 20 species of tall, perennial, rhizomatous grasses with a C4 photosynthetic pathway.(Heaton et al. 2010; Clifton-Brown et al. 2016; Lewandowski et al. 2000) Before it became popular as a bioenergy and biomaterial feedstock, it was mainly used for grazing and as a structural material in Asia. (Heaton et al. 2010)

Most reported trials of *Miscanthus* have used a vigorous sterile clone *Miscanthus* x *giganteus*.(Lewandowski et al. 2000; Clifton-brown et al. 2007; Clifton-Brown et al. 2016) Although a high growth rate is considered one of the best features of *Miscanthus*, its yields can vary significantly with different climate, temperature and soil conditions.

It could reach a yield of 40 t/ha.yr in Illinois, US (Heaton et al. 2008; Gopalakrishnan et al. 2012) and the autumn yield has been reported to exceed 30 t/ha.yr from irrigated trials in South Europe. In Europe, without irrigation, the autumn yield is expected to be around 10-25 t/ha.yr. (Lewandowski et al. 2000) In the UK, long-term average harvestable yields from a mature crop have exceeded 13 t/ha.yr at the most productive experimental sites.

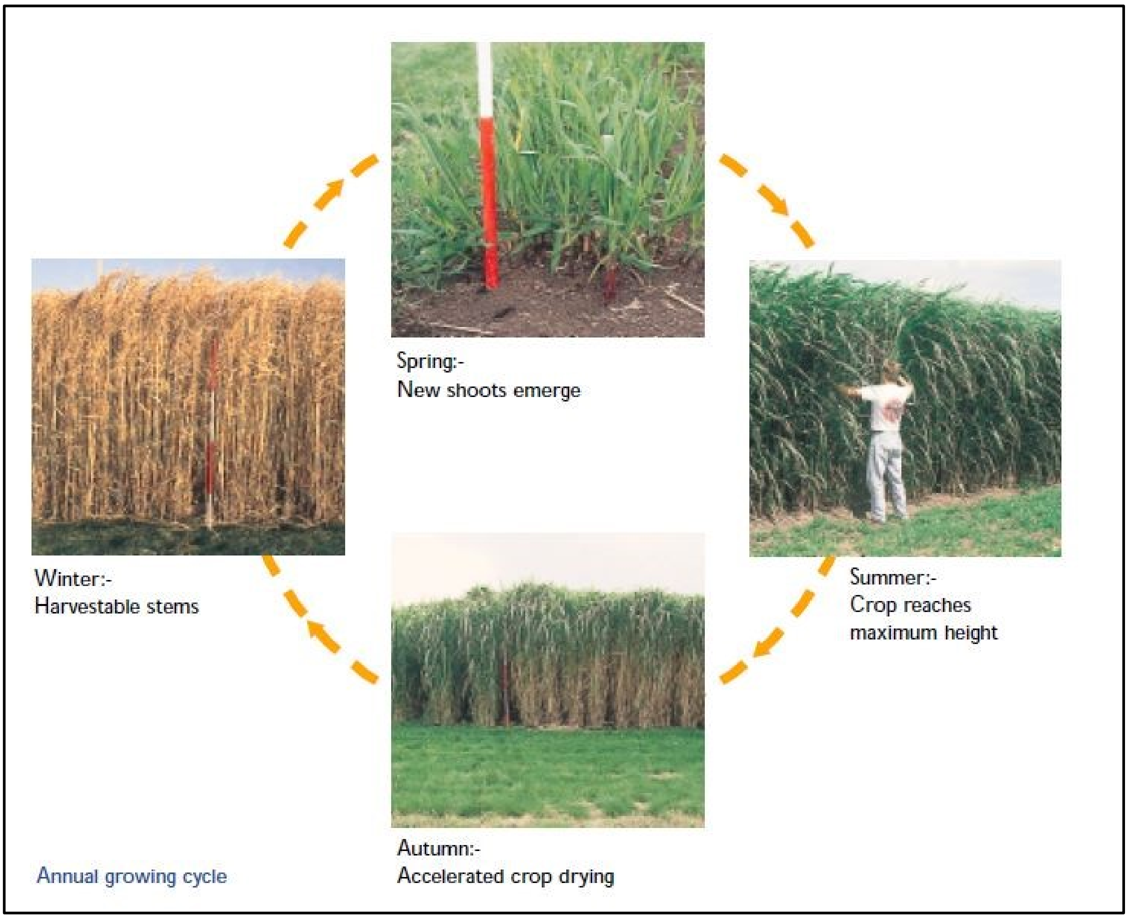

Figure 2-6 Annual growing cycle of Miscanthus (DEFRA 2001)

Miscanthus is established either by rhizome cutting or *in vitro* culture. (Lewandowski et al. 2000b) In the UK, it is usually planted in spring and the canes grown during the summer are harvested in winter when the stems have a relatively low moisture content (30–50%) (Figure 2-6).(DEFRA 2001) This growth pattern is repeated annually throughout *Miscanthus*' lifetime, which is at least 15 years, sometimes up to 20 years.

(Teagasc & AFBI 2010) Since the yields are relatively lower during the first season, the first harvest normally takes place in the second year of its establishment. Compared with short rotation coppice willow, another popular alternative biomass crop, *Miscanthus* is superior in the way that it gives an annual harvest and thus an annual income to the grower. (DEFRA 2001) All of the associated establishing, maintenance and harvest activities can be done with conventional farm machinery.

The net calorific value of *Miscanthus* is around 17 to 20 MJ/kg dry matter. (Axelsson et al. 2012; DEFRA 2001) Together with its relatively lower moisture and ash content, *Miscanthus* also represents a promising crop for both combustion and use in biomass-to-liquid conversion processes to produce biofuel and biochemicals.(Axelsson et al. 2012)

2.4.2. Environmental performance of *Miscanthus*

Miscanthus has long been acclaimed as environmentally benign compared with conventional annual crops. This is because of its relatively denser and continuous vegetative cover, which can protect the soil against erosion, potentially limit run-off and nutrient loss, provide carbon sequestration and increase biodiversity through improving wildlife habitats. Moreover, its high water-use efficiency and low requirements in terms of fertiliser inputs and pesticide application also enhance its sustainability performance from both environmental and economic perspectives. (Heaton et al. 2010; Lewandowski et al. 2000b; Agostini et al. 2015; McCalmont et al. 2017)

Numerous studies have indicated that *Miscanthus* growth does not respond to nitrogen fertiliser inputs, thus the annual fertiliser demands of *Miscanthus* are low. This high nutrient use efficiency is attributed to its capacity to internally recycle large amount of nutrients between above- and below-ground tissues during each individual growing season.(Heaton et al. 2010) It translocates nutrient to the shoot at the beginning of each growing season and then re-translocates them to the rhizomes in the later stages when the crop senesces.(Lewandowski et al. 2000) Its nutrient requirements during the following growing season could always be met by leaf litter decomposition, natural soil nutrient reserves, rhizome reserves and atmospheric depositions.(DEFRA 2001)

SOC enrichment associated with land converted to dedicated perennial crops is another aspect that contributes to *Miscanthus*' environmental performance. (Hansen et al. 2004; Dondini et al. 2009; Harris et al. 2015; Gregory et al. 2018) Lemus and Lal (2005) estimated that dedicated perennial crops cultivated on degraded land could potentially sequester C at rates ranging from 0.6 to 3.0 tC/ha.yr. McCalmont et al. (2017) reviewed and summarised nine experiment-based studies on land converted from both arable and grassland to *Miscanthus* cultivation. These studies consist of seven comparisons between *Miscanthus* land and grassland and 21 comparisons between *Miscanthus* lands and arable lands for periods of 3-19 years. The conclusion was drawn that previous arable land converted to *Miscanthus* cultivation was able to sequester soil carbon at annual rates of 0.42 to 3.8 tC/ha.yr.

For former grassland, the soil carbon change seems uncertain as three of the seven comparisons showed increases after converting to *Miscanthus* cultivation, while three showed decreases and one showed no change in soil carbon stock.(McCalmont et al. 2017)

Although the SOC sequestering ability of *Miscanthus* has been suggested by many studies (Poeplau & Don 2014; Richter et al. 2015; Zatta et al. 2014), there have always been concerns and uncertainties regarding the SOC equilibrium.(Agostini et al. 2015; Poeplau & Don 2014; Stockmann et al. 2013) The SOC equilibrium status has been determined from site measurements for crops with lower biomass carbon returns, such as winter wheat, (Novara et al. 2016) but not for *Miscanthus* cultivation.(Don et al. 2012; Poeplau & Don 2014) With regards to *Miscanthus*, such effects have been inferred by several model-based studies.(Pepper et al. 2005; Stockmann et al. 2013) Nevertheless, a 25-year field experiment revealed the possibility that when top soil layers reach saturation, carbon will be translocated to deeper soil layers and rapid SOC enrichment in deeper unsaturated layers could be observed. (Nicoloso et al. 2018)

It has also been recognised that GHG removal effects associated with *Miscanthus* cultivation involve not only SOC enrichment, but also carbon storage increases in above- and below-ground biomass (BGB) when planted in previous cereal fields owing to its relatively higher biomass productivity. (Dohleman et al. 2012) BGB of 7-year old *Miscanthus* was recorded as 27 t/ha in total for both the rhizome (21.5 t/ ha) and root biomass (5.6-5.9 t/ha) in Illinois, US, with a harvest yield of 38.1 t/ha. (Dohleman et al. 2012) A total BGB of 20.6 ± 4.6 t/ha was reported from a 15-year study in South Ireland with a harvest yield of only 13.4 ± 1.1 t/ha.(Clifton-brown et al. 2007) Richter et al. (2015) reported an accumulative BGB from a 15-year study established in a farm in Rothamsted, England as 33 t/ha for rhizomes and 12.88 t/ha to 14.69 t/ha for roots with a maximum yield of 15.9 t/ha. Robertson et al.（2017) reported an atmospheric GHG reduction potential of 24.5tCO_2eq/ha.yr for *Miscanthus* based on a ‘cradle to farm gate’ LCA, however in this study, no soil carbon enrichment was detected. It is also suggested by Robertson et al.(2017) that studies with high-resolution N_2O simulation would significantly increase the figure accuracy.

Nevertheless, it has been suggested that the extent to which these benefits are realised in practice depends on the specific management practices employed, previous land use and local environmental context. (Heaton et al. 2010; Agostini et al. 2015; McCalmont et al. 2017; Zang 2018) Case-specific investigations on the environmental impacts of *Miscanthus* across a wider range of environmental conditions where it might be cultivated are still lacking and are encouraged.

Part 2. Sustainability and eco-system model-life cycle assessment integrated approach

The definition of sustainability and the concept ‘sustainable feedstock supply’ have been briefly discussed in Section 2.2.4. This part of literature review aims to cover a more systematic review of substantiality, sustainable development goals (SDGs) and its assessments, while with focuses on the environmental component and terrestrial GHG simulations.

2.5. Sustainability

2.5.1. The origins and development of sustainability

The concepts of ‘sustainability’ and ‘sustainable development’ originated in response to the growing dissatisfaction regarding society’s development and associated lifestyles. (Rack 2017) It is considered not as an option, but an imperative to reach sustainable development and the sustainability concept has been firmly incorporated into political agendas for most countries. (Morrison-Saunders & Francois 2012; Rack 2017)

There are several important milestones through the origin and evolution of the ‘sustainable development’ concept. The 1972 United Nation (UN) Stockholm conference on Human Environmental is seen as the beginning of modern environmental diplomacy. (Grieger 2012) This conference first highlighted the concerns for preserving and enhancing the environment and its biodiversity to ensure human rights to a healthy and productive world. The issue of the 1987 Brundtland Report by the UN Commission on Environment and Development was seen as another important milestone in the development of sustainability concept. (World Commission on Environment and Development 1987) In Brundtland report, it is recognised that equity, growth and environmental maintenance are simultaneously possible, thus the whole society is capable of achieving its economic potential while enhancing the resources base. It also recognised the three key components to sustainable development, which are environmental, economic growth and social equity. The following 1992 Earth Summit in Rio de Janerio brought the world's governments to deliberate and negotiate an agenda for environment and development in the 21st century. It is seen as an important step which propelled the concept onto the global stage. (Morrison-Saunders & Retief 2012)

2.5.2. Sustainable development goals (SDGs) and the bioeconomy strategy

In 2015 the UN launched the Sustainable Development Goals, including 17 goals with 169 targets to be achieved by 2030. (UN 2015) (Figure 2-7) Pedersen (2018) considers the SDGs as a great gift to business, as these 17 SDGs represent a long tern political framework for business to contribute to sustainable development and outline wheat will be needed by the market long term.

Figure 2-7 The UN sustainable development goals (UN 2015)

O'Brien et al. (2017) highlighted that the actual contribution of the EU bioeconomy to sustainable development depends on the why how it is implemented. The high innovation potential of bioeconomy is accompanied by considerable risks, in particular regarding the exacerbation of global land use conflicts. Several studies criticized that as measures and strategies ensuring sustainability were missing in most of the bioeconomy documents, doubts remain regarding the actual relation between bioeconomy strategy and sustainable development. (Juerges & Hansjürgens 2016; Heimann 2019; Pfau et al. 2014；Ramcilovic-Suominen and Pülzl 2018) Pfau et al. (2014) argued that bioeconomy cannot be considered self-evidently sustainable, a range of risks and potential pitfalls have to be considered and avoided in the bio-economy deployment. He reviewed 87 relevant scientific articles and suggested the potential threatens from bioeconomy were mainly on land-based resources and competitions for food products. This land-based restoration is emphasized by the SDG 15 that ecosystems need to be restored, however it is outside the original focus of the bioeconomy documents. (Heimann 2019)

To ensure the robust contribution to sustainable development, the final report produced by the 2015 Global Bioeconomy Summit (GBS) distinguished between 'bioeconomy' and 'sustainable bioeconomy'.(GBS 2015) Heimann (2019) evaluated and compared the performance of bioeconomy and sustainable bioeconomy against the considered relevant SDGs, results indicated that bioeconomy scenario has positive as well as negative effects on the SDG targets, while a sustainable bioeconomy scenario outperforms the business as usual scenario against all tested individual SDGs (Figure 2-8). The 2015 GBS final report highlights that a sustainable bioeconomy could specifically contribute to achieving SDGs related to food-security and nutrition (SDG2), healthy lives (SDG3), water sanitation (SDG6), affordable and clean energy (SDG7), sustainable consumption and production (SDG12), climate change (SDG13), oceans, seas and marine resources (SDG14), and terrestrial eco-systems, forests, desertification, land degradation and biodiversity (SDG 15). (GBS 2015)

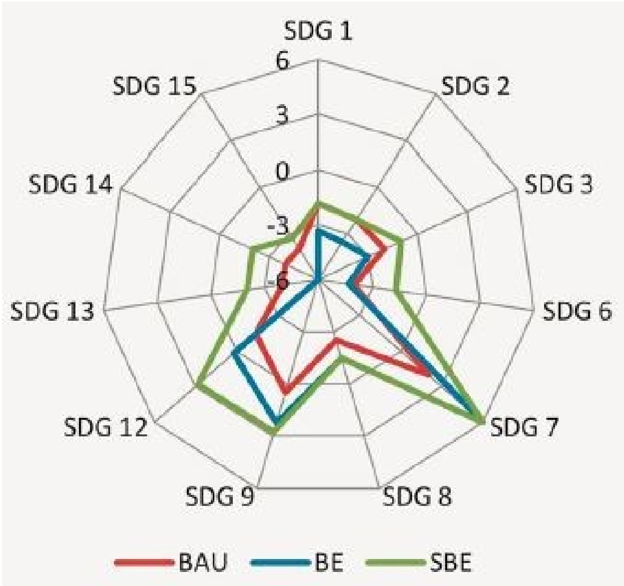

Figure 2-8 Scores of BAU, BE, SBE scenarios against SDGs, produced by Heimann (2019); BAU = business as usual; BE = bioeconomy; SBE = sustainable BE; SDGs = Sustainable Development Goals.

2.5.3. Sustainability assessment and life-cycle based approaches

Despite of the agreement on the three dimensions of sustainability (as discussed in Section 2.2.4) and numbers of works that attempted to establish a standardised assessment framework, knowledge is still evolving to find the appropriate and quantitative indicators for each dimension, especially for social sustainability component.(Popovic et al. 2018) Another great challenge in sustainability assessment, as recognised by Rack (2017) and Pope et al. (2004), is to interrelate different components of sustainability both within pillars (vertical integration, e.g. between different environmental impacts) and between pillars (horizontal integration), rather than just the simple sum of different and separate assessments. Sadler (1999) suggested that to help deal with the unavoidable trade-offs, a sustainability tool should include a minimum threshold for each component. Rack (2017) further indicated other potentially important features of a successful sustainability assessment tool, including transparency, subjectivity and flexibility.

Ness et al. (2007) reviewed and categorised the existing sustainability assessment tools into three main groups (1) indicators and indices, which could be further separated into non-integrated and integrated, (2) product related assessment tools, which focus on the material and/or energy flows of a product or service from a life cycle perspective, and (3) integrated assessment, which was a collection of tools usually focused on policy changes or project implementation. LCA is a representative life cycle based methodology and has been widely applied in product-focused micro-level analysis to quantify their environmental performance, or to assess under the environmental component within a sustainability assessment framework (Pedersen 2018; Rack 2017; Lundin & Morrision 2002) One of the key superiorities of LCA is that it is standardised by the International Organization for Standardization (ISO) series ISO14040-ISO14044. (ISO 1998; ISO 1999;ISO 2000; ISO 2006) Kloepffer (2008) considered LCA as the only internationally standardized environmental assessment method.

Regarding the weakness of LCA as a sustainability assessment tool under the environmental component, both Ness et al.(2007) and Rack (2017) considers that the lack of spatial scope and the incapability to reflect the localised impacts are the areas for improvement. However, integration of process-based ecosystem model generated results into the LCA framework has successfully reflected the impacts of locations on the LCA outputs, at least for agricultural products. (Guo et al. 2012) Holma et al. (2013) suggested other challenges of LCA, especially for soil quality and biodiversity, is that the impact category could not be comprehensively assessed with one or two indicators; instead, a set of indicators would be necessary.

Apart from LCA, the life cycle perspective is further reflected in other methodologies for social and economic sustainability assessments, the examples are Societal LCA (SLCA) and life cycle costing assessment (LCC), while their application were relatively limited. (Kloepffer 2008; Rack 2017)

2.6. Life-cycle assessment of biomaterials

As indicated in Section 2.5.3, due to this is a product-focused study, LCA has been selected as the main approach to quantify the GHG emissions associated with LCB-SA life cycle. As the most popular assessment approach of a product/service's environmental impacts, LCA has been widely used for bio-based chemicals/materials, especially on energy consumption and GHG emissions. Those chemicals/materials include both energy products, such as bioethanol, biodiesel and biogas, and non-energy materials, such as biochemicals. (Hillier et al. 2009; Kumar et al. 2012; Liang et al. 2013; Whitaker et al. 2012; Adler et al. 2007) The advantages and limitations of LCA as an environmental sustainability assessment method have been discussed in Section 2.5.3, this section aims to provide a systematic overview of the LCA methodology and previous LCA results on bio-SA studies.

2.6.1. LCA framework

LCA is standardised under the ISO series ISO-14040-ISO14044. According to the ISO standard, LCA comprises four phases: goal and scope definition, inventory analysis, impact assessment and interpretation. (ISO 2006)(Figure 2-9)

Goal and scope definition: This phase defines why and upon which system a LCA is conducted. System boundaries, the functional unit and what impacts will be taken into account in a study will be defined in this phase. This phase is important because it will influence the direction and depth of the study being conducted. The geographic extent and time horizon should also be addressed here. (ISO 1998)

Life-cycle inventory analysis (LCI): This phase involves the data collection and calculation procedures (ISO 1998), aiming at produce a compilation of the inputs (resources) and the outputs (emissions) from the product over its life-cycle in relation to the functional unit. (Finnveden et al. 2009)

Life-cycle impact assessment (LCIA): In this phase, based on the results of the LCI, the environmental impacts are examined using impact categories and category indicators (ISO 2000), aiming at understanding and evaluating the magnitude and significance of the potential environmental impacts of the studied system. (Finnveden et al. 2009) According to the ISO standard on LCA, LCIA includes two mandatory steps: selection of impact categories and classification, and characterisation, while another two steps of normalisation and weighting are optional. (ISO 2006) LCIA can be conducted at either midpoint or endpoint levels, which look at different stages in the cause–effect chain to calculate the impact. The endpoint method examines the impacts at the end of the cause–effect chain, while the midpoint method considers the impact before the endpoint is reached. (Chatzisymeon et al. 2017)

Life-cycle interpretation: Life-cycle interpretation is a systematic procedure that discusses and summarises the results of the second and third phases, LCI and LCIA, as a basis for conclusion, recommendation and decision-making according to the goal and scope defined in the first phase. (ISO 1999)

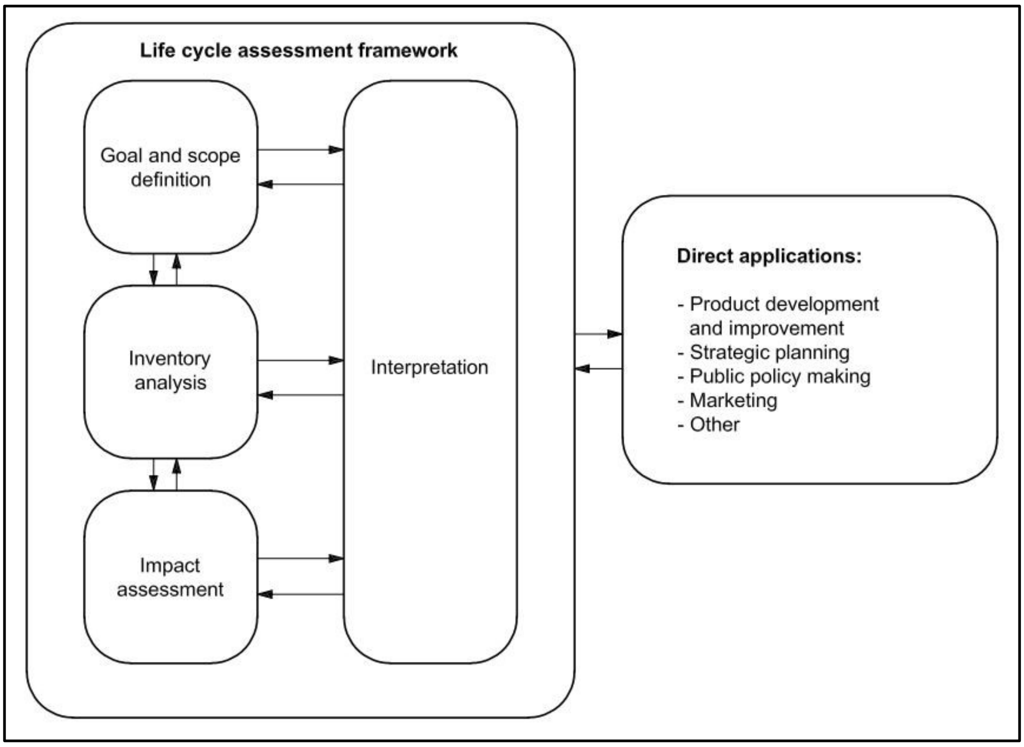

Figure 2-9 Stages of a life-cycle assessment (ISO 2006).

2.6.2. Consequential LCA and attributional LCA

Attributional LCA (ALCA) is a case-oriented, descriptive assessment, (Pawelzik et al. 2013) focusing on analysing the impacts of the processes used for production (and consumption and end-of-life management) of a product/service, but it does not consider the indirect effects that result from changes in the output of a product. (Thomassen et al. 2008; Brander & Tipper 2009) Consequential LCA (CLCA) has been described as an effect-oriented, prospective assessment. (Pawelzik et al. 2013) that aims to estimate how relevant physical flows within a system will change in response to a possible change in the output of the functional unit. (Thomassen et al. 2008; Brander & Tipper 2009) CLCA focus on the consequences of the changes in the output of a product.

However the current GHG LCA policies, such as the EU's Renewable Energy Directive (RED), the Renewable Fuel Standard in the US, and the UK's Renewable Transport Fuel Obligation (RTFO), do not distinguish between the use of these two methods (Brander & Tipper 2009), which may lead to the wrong application or combination in analysis, misinterpretation or unfair comparison of results obtained using different methods. (Brander & Tipper 2009; Finnveden et al. 2009)

The different outcomes resulting from choosing to apply either CLCA or ALCA were reflected in several studies. (Thomassen et al. 2008; Searchinger et al. 2008) Finnvenden et al. (2009) reviewed and discussed the differences between CLCA and ALCA. Arguments have been made as to what extent CLCA or ALCA are more suitable for decision-making. According to Finnvenden et al. (2009), the choice between CLCA and ALCA depends on the goal and scope definition of the individual study. Brander and Tipper (2009) summarised the different application situations applicable to CLCA and ALCA (Table 2-1). ACLA is suitable for quantifying the direct emissions from the production (and consumption and disposal) of a product, while CLCA is more useful when estimating and quantifying the total change in emissions arising from changes in the output level of a product/service. Since both direct and indirect changes are included in CLCA, CLCA is considered of greater relevance to policymakers than ALCA.

Table 2-1 Application difference between ALCA and CLCA(Brander & Tipper 2009)

	ACLA	CLCA
Appropriate situation	Quantifying and understanding emissions directly from the life-cycle of a product. Consumption-based emissions.	Informing consumers and policymakers about the changes in total emissions from purchasing or policy decisions.
Inappropriate situation	Quantifying the change in total emissions resulting from policies that change the output of a certain product.	Consumption-based emissions.

2.6.3. LCA of SA and biomaterials

Some LCA studies have been conducted to investigate the GHG emissions, non-renewable energy use (NREU) and land use of SA production from bio-based feedstocks.(Cok et al. 2014; Hermann et al. 2007; Patel et al. 2006) (Table 2-2) Cok et al. (2014) studied the NREU and GHG emissions of a corn-based SA production system. Three process routes were studied: (1) low-pH yeast fermentation with downstream processing (DSP) by direct crystallization, (2) anaerobic fermentation to succinate salt at neutral pH (pH 7) and subsequent DSP by electrodialysis, and (3) a similar process producing ammonium sulphate as a co-product in DSP. For comparison, three petrochemical production routes for maleic anhydride, SA and adipic acid were chosen as comparative systems. The results show that the first low-pH yeast fermentation route has the biggest potential in terms of GHG reduction and NREU saving.

2.3.3.1. **GHG Emissions**

GHG emissions are a key indicator for the sustainability assessment of bio-SA production systems, not only for the policy arena, but also for companies and the public. GHG emissions are normally calculated in CO_2 equivalents. It includes the GHG emissions from the system in the form of CO_2 and CH_4, as well as N_2O from the fertiliser application during the biomass production. (Hermann et al. 2007) As can be seen from Table 2-2, the GHG emissions for starch-based bio-SA are within the range of 0-5 kg CO_2eq/kg Bio-SA, while for lignocellulosic feedstock-based bio-SA production, much lower or even neutral GHG emissions can be achieved. (Hermann et al., 2007; BREW, 2006)

Table 2-2 Previous LCA studies conducted on bio-SA production systems

Study	Location	Feedstock	GHG emissions (kg CO_2 eq/kg Bio-SA)	NREU (MJ/kg Bio-SA)	Land use (ha/t Bio-SA)	SCOPE	Other environmental impact indicators (included or suggested)
Cok et al. 2014	Europe	Corn	0.88-1.47[1]	32.7 - 45.2[1]	0.22	Cradle to factory gate	NA
	Brazil	Sugarcane	-0.58 to -1.4[1]	NA[2]	NA		
	US	Corn starch	0.87–3.02[3]	NA	NA		
	China	Corn starch	2.85 to 4.95[1]	NA	NA		
Hermann et al. 2007	NA	Corn starch	2.3-4.6 (today) 1.8-2.9 (future)	27-67 (today) 28-47 (future)	0.25 (today) 0.14 (future)	Cradle to grave	Acidification, eutrophication, particulate emissions, human toxicity and environmental toxicity (suggested)
		Lignocellulosic	1.3-2.4 (future)	18-38 (future)	0.17-0.18 (future)		
BREW 2006	NA	Corn starch	3.1 (today)	27 (today)	0.25 (today)	Cradle to factory gate	NA
		Sugarcane	-0.2 (today)	5.4 (today)	0.26 (today)		
		Lignocellulosic	0.2 (today) 0.0 (future)	15 (today)	0.17 (today)		
Bio-Amber 2013	Canada	Corn starch	-0.18	NA	NA	Field to factory gate	NA
Myriant 2012	US	Multi-feedstock[4]	-0.41[5] 0.18	NA	NA	NA	NA
Reverdia 2012	Europe	Corn starch	0.88	32.7	NA	Cradle to factory gate	NA

1. for different synthesis routes;
2. NA= not applicable;
3. for different synthesis routes and national emission intensity for electricity production;
4. mainly are commercially available sugars;
5. With integrated heat and energy balance.

2.3.3.2. **NREU**

NREU is another crucial sustainability indicator. ‘Non-renewable energy' includes both nuclear and fossil energy use. NREU represents a straightforward and practical approach because many other environmental impacts are related to NREU. As shown in Table 2-2, for starch-based bio-SA production, the NREU is around 30–60 MJ/kg Bio-SA. (Cok et al., 2014; Hermann et al., 2007; BREW, 2006)

2.3.3.3. **Land Use**

In most of the studies reviewed, land use refers to agricultural land use only, while the amount of land used for industrial plants, transportation infrastructure and waste management is very small compared with agricultural land use. (Hermann et al. 2007)

2.6.4. Gaps and needs in LCA for biomaterials

Pawelzik et al. (Pawelzik et al. 2013) reviewed and summarised the critical methodological issues that are specifically relevant to bio-based materials but have not been properly guided in current approaches or fully addressed in most LCA studies for bio-based materials. The following issues were raised and discussed:

- The treatment of biogenic carbon storage is recommended, while product-specific life cycles and the likely time duration of carbon storage should be considered.
- Incorporating changes in SOC into LCA studies is recommended, although it is site-specific and can be complicated.
- The choice of allocation methods to attribute emissions and resource use among products is also a critical issue for life-cycle assessment.

2.7. Ecosystem modelling approach

2.7.1. The 2006 Agriculture, Forestry and Other Land Use Guidelines

Volume 4 Agriculture, Forestry and Other Land Use in the 2006 IPCC Guidelines for National Greenhouse Gas Inventories (2006-AFOLU) (Intergovernmental Panel on Climate Change 2006a) provides three tiered approaches for estimating GHG emissions from six land-use categories, including forest land, cropland, grassland, wetland, settlements and other land.

The IPCC guidelines for national GHG inventories have evolved through several stages. Since first being published in 1995, there have been the 1996 Revised Guidelines for National Greenhouse Gas Inventories, (1996 Guidelines)(Intergovernmental Panel on Climate Change 1996) the 2000 Good Practice Guidance and Uncertainty Management in National Greenhouse Gas Inventories (2000-GPG),(Intergovernmental Panel on Climate Change 2000b) Good Practice Guidance for Land Use, Land-Use change and Forestry (GPG-LULUCF)(Intergovernmental Panel on Climate Change 2003) and finally the 2006 IPCC Guidelines for National Greenhouse Gas Inventories. (Intergovernmental Panel on Climate Change 2006a). The underlying approach remains unchanged since the 1996 guidelines, while the 2006-AFOLU guidelines have made several improvements, such as clarifying that 'CO_2 emissions' are only the direct annual emissions of all carbon emitted as CO_2; and integrating the previously separate guidance for agriculture (Chapter 4) and land-use change and forestry (Chapter 5) of the 1996 Guidelines into one volume (the 2006-AFOLU) to avoid the chance of double accounting. (Intergovernmental Panel on Climate Change 2006a) This integration also recognises that all types of land can be involved in land-use change and associated GHG removals and emissions. The 2006-AFOLU has been identified as the latest guidelines with improved consistency and completeness, and with more and improved default data.

(Intergovernmental Panel on Climate Change 2006a) Thus, other IPCC guidelines were not considered in this work.

Chapter 5 in the 2006-AFOLU provides information on using Tier 1 and Tier 2 approaches to estimate carbon-related emissions from both 'crop land remaining as crop land use' and 'other land remaining as crop land' uses. Similarly, Chapter 6 provides guidelines on estimating carbon-related GHG emissions from 'grassland remaining grassland' and 'other land remaining grassland' uses. (Intergovernmental Panel on Climate Change 2006a) Additionally, Chapter 11 gives guidelines for using Tier 1 and Tier 2 approaches to estimate nitrogen-related GHG emissions from managed soils. (Intergovernmental Panel on Climate Change 2006a)

Conducting a higher tier approach improves the accuracy of the estimation and reduces the level of uncertainty, but the requirement for inputs is increased. 2006-AFOLU gives a detailed description and guidelines for a Tier 1 approach, which can also be applicable to Tier 2 methods, while the data on emissions and carbon stock changes provided under the Tier 2 approach are country- or region- specific. For Tier 3 methods, only good practices for application are given. The uses of process-based models fall into the Tier 3 methods category. (Intergovernmental Panel on Climate Change 2006a)

It is recognised in the 2006-AFOLU guidelines that land use converting to cropland from forest land, grassland and wetlands usually results in a net loss of carbon from biomass and soils, as well as N_2O being emitted to the atmosphere. However, when cropland is established on previously sparsely vegetated or highly disturbed lands (e.g., mined lands), it will act as a carbon sink for both biomass carbon and soil carbon.

2.7.2. DeNitrification-DeComposition Model

DeNitrification-DeComposition (DNDC) model was originally designed to simulate carbon and nitrogen biogeochemical cycles occurring in agricultural systems on regional scales in the US, (Giltrap et al. 2010) and was further expanded to cover a range of countries and regions, including China, Canada and Europe, (Abdalla et al. 2010; Kesik et al. 2006) and also other ecosystems, e.g. rice paddies, grazed pastures, forests and wetlands. Both land-use and land-management effects are taken into account in the DNDC model.(Giltrap et al. 2010)

As a process-based model, DNDC is now capable of predicting the soil fluxes of the main greenhouse gases, i.e. N_2O, CO_2, NO and CH_4, and other key environmental and economic indicators, including crop yields, ammonia(NH_3) volatilisation and nitrate(NO_3^-) leaching. (Giltrap et al. 2010; Li 2000)

2.3.2.1. **Model Description**

DNDC is constructed with two interacting components, containing six submodels (shown in Figure 2-10). The first component consists of three submodels for soil climate, plant growth and decomposition. This component calculates the status of the soil–plant system, such as soil chemical and physical status, vegetation growth and organic carbon mineralisation, (Leip et al. 2008) predicting soil temperature, moisture, pH, redox potential (Eh) and substrate concentration profiles (e.g., dissolved organic compounds, NH_4^+ and NO_3^-) based on ecological, environmental and anthropogenic factors. (Li 2000; Giltrap et al. 2010) The second component consists of nitrification, denitrification and fermentation submodels. It calculates the major processes involved in the exchange of GHGs with the atmosphere, (Leip et al. 2008) predicting NO, N_2O, NH_3 and CH_4 fluxes based on the soil environmental factors. (Li 2000; Li & Aber 2000; Giltrap et al. 2010)

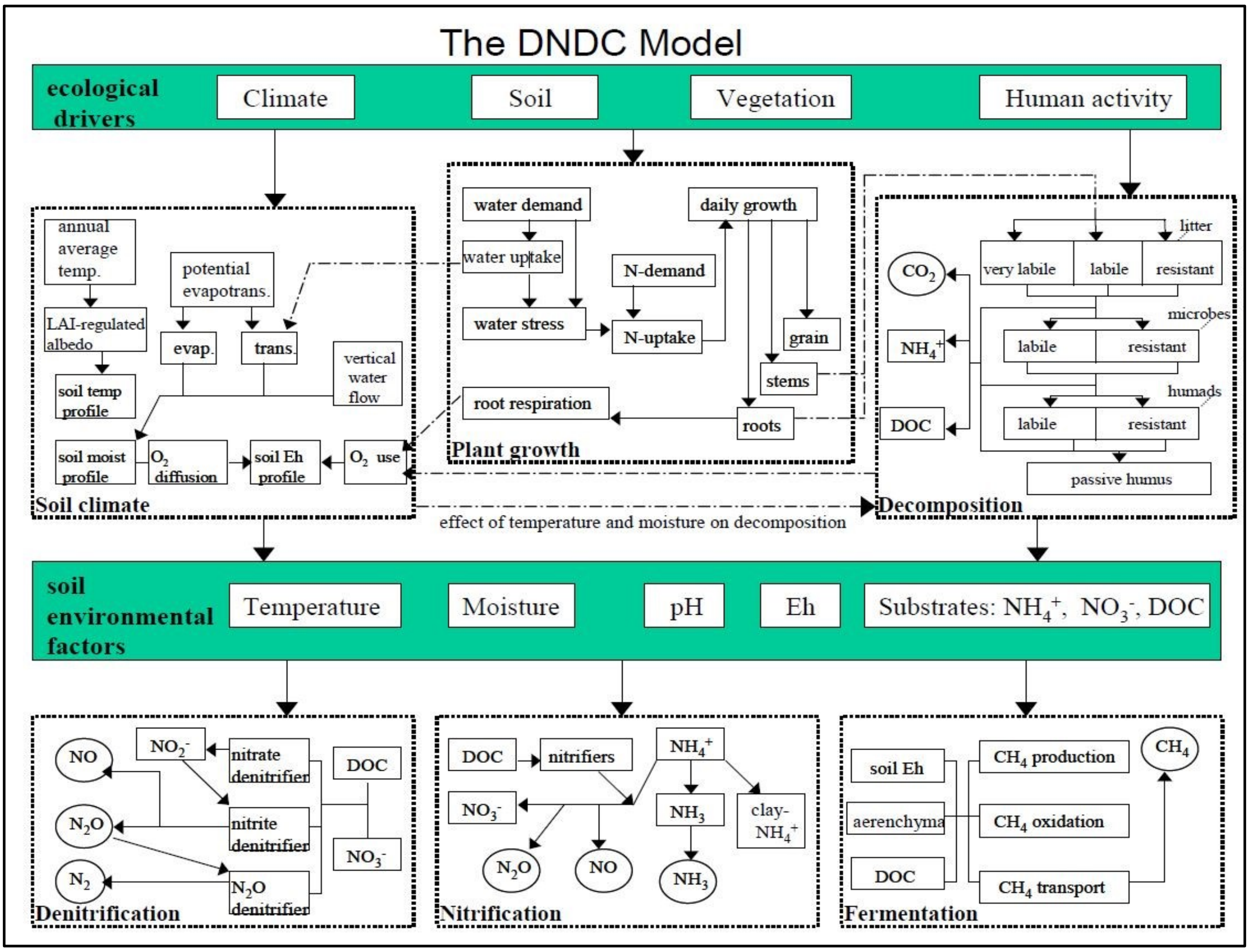

Figure 2-10 Schematic diagram of DNDC model structure (Li 2000).

2.3.2.2. **Plant Growth Model in DNDC**

In the plant growth submodel, it is possible to define a new crop. The crop parameters include maximum yield, biomass portioning, C/N ratio, season accumulative temperature, water demand and N fixation capacity. Crop growth is simulated by the driving factors, which include accumulative temperature, N uptake and water stress at a daily timestep. Crop demand for N is calculated based on the optimum daily growth and the plant C/N ratio. The limiting factors for the actual N uptake could include N or water availability during the growth season. (Li 2000)

Is it possible to analyse the sustainable removal rate using the DNDC model. According to the user guide, in the plant growth model, the model assumes that the root biomass is left in the soil profile after the harvest and a fraction of the above-ground crop residue remains as stubble in the field until next tilling application, and this fraction can be defined by the users. The crop residue remaining in the soil will be divided into three pools (very labile, labile and resistant litter pools) according to the C/N ratio. (Li 2000)

2.3.2.3. **Data Quality**

Specific reactions are parameterized by classical laws of physics, chemistry or biological or empirical equations generated from laboratory observations. (Li 2000) In the DNDC model, the empirical formulation of potential crop growth is highly temperature-driven, while water and nitrogen stress are formulated as limiting factors for the potential growth. Therefore, this model requires relatively less data inputs to assess of the impacts of crop growth and management on soil processes.(Kröbel et al. 2011) The DNDC model has been frequently used to simulate soil moisture (Tonitto et al. 2007; Kröbel et al. 2011), soil carbon (Wang et al. 2008), soil nitrogen(Li et al. 1994; Li et al. 1996; Giltrap et al. 2010) and GHG emissions (Li 2000; Li et al. 1996; Grant et al. 2004; Babu et al. 2006; Beheydt et al. 2007). The ability of DNDC to predict N_20 and SOC has been tested and proved against several field studies (Li et al. 1992; Li et al. 1994; Li et al. 1997; Frolking et al. 1998) and its ability to capture patterns and magnitudes of trace gas emissions NO, CH_4, NH_3 has been proved. (Li 2000)

2.3.2.4. **UK-DNDC**

UK-DNDC is a modified version for application in the UK, with the UK-specific input data already added in the database.(Brown et al. 2002) According to Gilhespy et al. (Gilhespy et al. 2014), the original UK-DNDC consists of four submodels based on work by Li et al. (1992) and Li and Aber (2000): the soil climate submodel, the crop growth submodel, the decomposition submodel and the denitrification submodel. However, the inconsistent development of DNDC and UK-DNDC led to different modelling performances between those two versions. Thus, a new version of UK-DNDC has been developed, which adopted most of the latest improvement and development in DNDC (Li & Aber 2000; Li 2000), namely: (1) crop growth, (2) farming management practices, (3) soil climate, (4) NH_3 volatilisation from soil, fertiliser and manure applications, (5) NO_3^- leaching loss, (6) gaseous N_2O emissions from nitrification and denitrification, and (7) CH_4 emissions from fermentation. (Gilhespy et al. 2014)

UK-DNDC can be run in both site and regional mode. In site mode, parameters such as soil characteristics, management and climate are input for a specified location. In regional mode, the county-level information is already in the database, so the estimation can be made at county scale or above. (Cardenas et al. 2013)

2.3.2.5. **DNDC-Europe**

DNDC-Europe combines the large-scale regionalised economic Common Agricultural Policy Regional Impact (CAPRI) model and the DNDC model to simulate GHG fluxes, carbon stock changes and nitrogen budgets of agricultural soils in Europe. It allows the *ex-ante* simulation of agricultural or agri-environmental policy impacts on a wide range of environmental factors, such as climate change, air pollution and groundwater pollution. (Leip et al. 2008)

2.7.3. 'Stability and Mitigation of Arable Systems in Hilly Landscapes' modelling system

The modelling system developed in the 'Stability and mitigation of arable systems in hilly landscapes' (STAMINA) project (Richter et al. 2006) simulates micro-meteorology, hydrology, crop development and growth in hilly terrain, integrating spatial information on soil and topography. (Richter et al. 2010; Hillier et al. 2009) Three interlinked physically based sub-models were included in the STAMINA modelling system. (Ferrara et al. 2010) These three submodels are the micro-meteorological model, based on Rana et al. (2007); the soil water balance submodel, which was based on the force-restore theory of the Interaction Soil Biosphere

Atmosphere (ISBA) approach; (Noilhan & Planton 1989) and the crop model, which was based on crop's net carbon assimilation as a balance of gross CO_2 assimilation and respiration. (Ferrara et al. 2010) The application of STAMINA model in wheat growth simulation have been published by Richter et al. (2010), Richter et al. (2006) and Ferrara et al. (2010), across sites in England and Italy.

2.7.4. RothC soil carbon model

The RothC model (Coleman & Jenkinson 1996) has been widely used for simulation soil carbon dynamics. (Smith et al. 2005; Coleman et al. 1997; Falloon & Smith 2006; Barancikova et al. 2010) It was originally developed and parameterised to simulate the organic C turnover in arable topsoils based on the Rothamsted long term field experiments.(Coleman et al. 1997) Its application covered a wide range of regions and vegetation types (e.g., cropland, grassland, and forests). (Francaviglia et al. 2012; Jiang et al. 2014; Hillier et al. 2009) RothC is the one of the most widely used models to simulate soil carbon dynamics for *Miscanthus* and other perianal energy crops, due to its relatively smaller data requirements and evaluated performance. (Agostini et al. 2015; Dondini et al. 2009; Zatta et al. 2014; Hillier et al. 2009; Poeplau & Don 2014) Hillier et al. (2009) conducted a modelling work for England and Wales, with the yield maps of four bioenergy crops with RothC to simulate the soil C turnover over a 20-year period. The crops in the study included *Miscanthus x giganteus*, winter wheat, short rotation coppice (SRC) poplar, and oilseed rape. The simulated terrestrial carbon emissions were then integrated with other life cycle emissions during crop cultivation. The GHG balances were estimated for each of the 12 land use change types associated with replacing arable, grassland, or forest land with each of the four crops. (Hillier et al. 2009) The results indicated that *Miscanthus* and SRC were most promising inters of soil carbon sequestration, while conventional food crops winter wheat and oilseed rape only presented with a net GHG balance or marginal benefits. (Hillier et al. 2009) This conclusion was close to other field experiments. (Richter et al. 2015; McCalmont et al. 2017)

Chapter 3. **Methodology**

3.1 Analysis framework

Lignocellulosic SA life cycle includes feedstock production, feedstock processing to sugars, polymer production, manufacture of product and end-of-life treatment. (Figure 3-1) This thesis focuses on the feedstock production stage, aiming to understandcatchment level LCB provision capacity from two provision scenarios and the GHG balances associated with their supply. Two provision scenarios include wheat straw from winter wheat single crop production (SP), and wheat straw and *Miscanthus* mixed supply from mixed production (MP) scenario. LCB availabilities are estimated based on winter wheat and *Miscanthus* yields generated by process-based crop model STAMINA, while assumptions regarding current and future use of winter wheat straw in case study area are made based on literature reported historical data. In the field to upstream factory gate LCA of LCB feedstocks, both carbon stock changes and nitrogen related emissions are taken into account, using outputs from process-based models. 2006-AFOLU Tier 2 approach was also included in carbon stock changes estimation. Following this, cradle to end-of-life LCA was conducted to compare overall carbon balance performance of bio-based end plastics produced from two feedstock provision scenarios. In the end, a system-level evaluation was conducted on SP an MP management scenarios, with quantified grain and bio-plastic product outputs and associated GHG emissions. GHG emissions from indirect land use changes in the MP scenario, i.e. GHG emissions aroused from the declined grain production were also included.

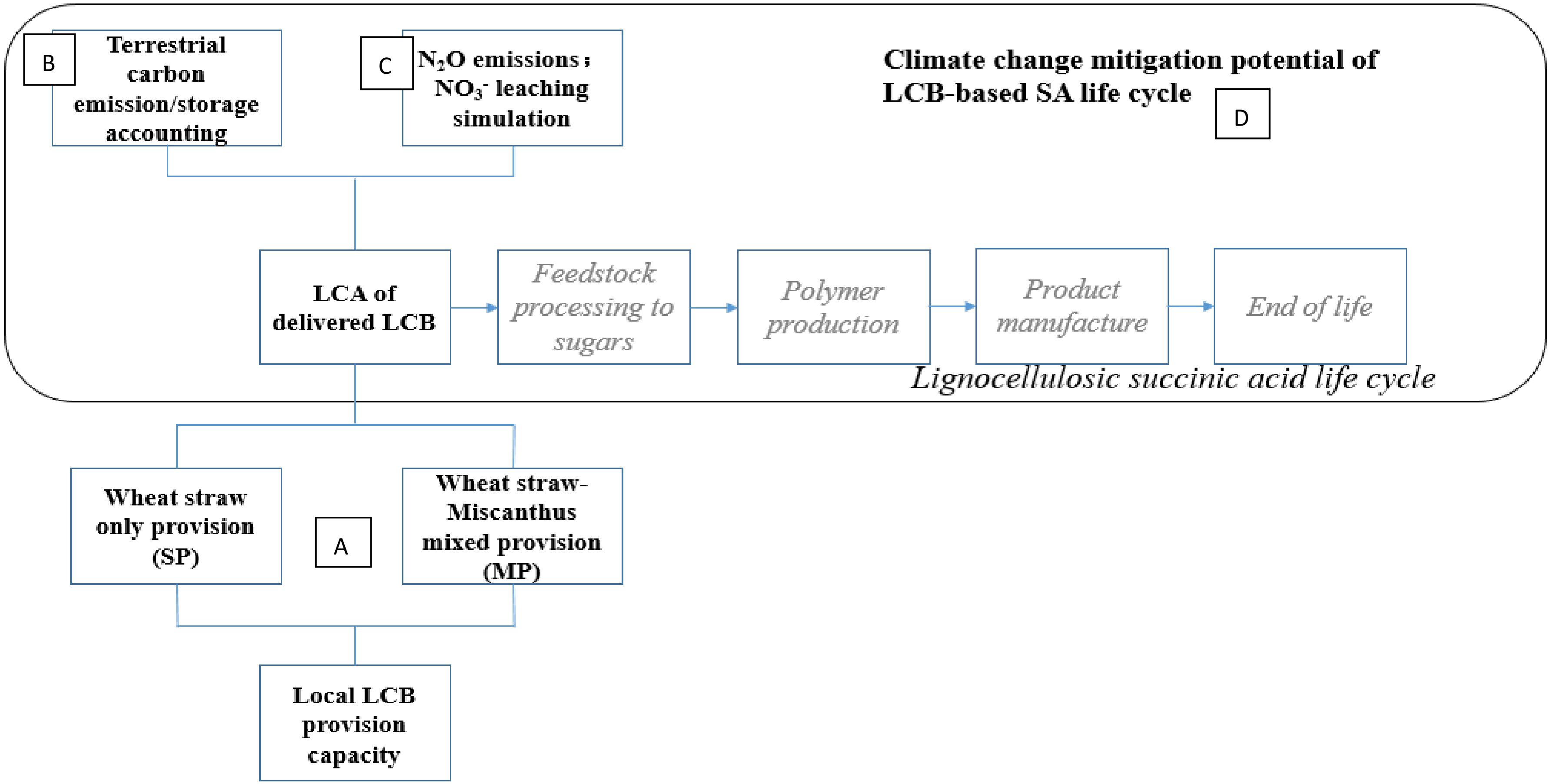

Figure 3-1 Analytical research framework

Table 3-1 Tasks, main methodologies and the result chapters for each research questions

Research Questions	Divided tasks	Chapter	Main methodology
How can the feedstock availability of LCB be optimized?	A. LCB provision from SP and MP scenarios	4	Literature based analysis on straw use; STAMINA model for future production estimation (details in Section 3.3)
Can the associated GHG emissions of the commercial scale production of LCB-derived SA be reduced by the using agricultural residues and/or perennial, LCB crops?	B. NO_3^- leaching simulation, direct and indirect N_2O emissions.	5	DNDC model (details in Section 3.4)
	C. Terrestrial carbon emission/storage accounting	6	IPCC 2006 AFOLU Tier 2 approach; RothC as Tier 3 approach (details in Section 3.5)
	D. Cradle to up-stream-factory gate LCA; cradle to end-of-life LCA	7	Integration of eco-system models into LCA framework (details in Section 3.6)

Figure 3-1 and Table 3-1 illustrate the main research tasks (A, B, C and D) addressed by this thesis. The interrelations between each element were reflected in Figure 3-1. Task A is designed to answer the first research question, how can the feedstock availability of lignocellulosic biomass be optimized? This is addressed by the literature based analysis regarding the current straw uses in UK and STAMINA model generated future LCB yields. The second question 'Can the associated GHG emissions of the commercial scale production of LCB-derived SA be reduced by the using agricultural residues and/or perennial, LCB crops?' is answered through the completion and integration of tasks B, C and D, using a range of modelling approaches.

3.2 Case study area

In accordance with Bio-SuccInnovate project, a catchment-level case study area was selected in this work to understand local feedstock provision capacity and to simulate GHG balances associated with the specified supply chains. This selected case study is a rural area nearby the city of Hull in England (max. 50 km as feedstock transport distance from farm to conversion plant) (Figure. 3-2). The 50 km farm to conversion plant radius was established based on work published in similar topic and research area

(Elliott et al. 2014; Littlewood 2013; Lewandowski et al. 1995; Gnansounou et al. 2009). This catchment area covers 5856 km^2 and comprised highly variable soil types taken from the UK National Soil Map (1 km grid). The catchment consists of parts of Yorkshire & Humber and East Midlands Regions which are the main wheat production areas in England. This area was also selected considering the allocation of the England's biggest operational wheat-based bioethanol plant, Vivergo Fuel Ltd.

Figure 3-2 Case-study area (50km radius from city of Hull, England)

3.3 Methodology for LCB availability estimation

3.3.1 Scenarios for LCB production simulation

As defined in Table 3-2, under SP scenarios winter wheat is assumed to be planted across the whole case study area, with winter wheat straw being the only LCB feedstocks for bio-SA production. In MP scenarios, it was assumed that winter wheat was remained as the dominating crop, while *Miscanthus* would be cultivated on the selected low-quality soils. Thus in MP, the LCB supply would be a mixed supply with *Miscanthus* and winter wheat straw. The low-quality soils were defined as the soils with highest NO_3^- leaching/wheat grain production ratio (kgN/t Grain). They were selected based on DNDC preliminary test results. Select low quality soils for *Miscanthus* cultivation in MP scenarios are CRANNYMOOR, EVERINGHAM, HOLME MOOR and KEXBY soils. Figures for NO_3^- leaching on those soils are presented in Chapter 5. Three climate change scenarios were used in the LCB production simulations, including baseline climate (BC), medium (ME) and high (HE) atmospheric GHG emissions scenarios. These three emissions scenarios enable an evaluation of the concurrent impacts of climate change on temperature, precipitations and CO_2 fertilization.

Table 3-2 Specifications on SP and MP LCB production and climate change scenarios BC, ME and HE; atmospheric carbon dioxide concentration [CO_2]

Scenario	**Description**	**Wheat cultivation allocation**	***Miscanthus* cultivation allocation**	**Climate change scenario**
SPBC	Single crop Production under Baseline Climate	On all arable soils	None	Baseline weather; [CO_2] 352 ppm
SPME	Single crop Production under Medium Emission climate change	On all arable soils	None	Medium Emission [CO_2] 447 ppm
SPHE	Single crop Production under High Emission climate change	On all arable soils	None	High Emission [CO_2] 449 ppm
MPBC	Mixed crop Production under Baseline Climate	Excluding selected low quality soils[1]	On Selected low quality soils	Baseline weather [CO_2] 352 ppm
MPME	Mixed crop Production under Medium Emission climate change	Excluding selected low quality soils	On Selected low quality soils	Medium Emission [CO_2] 447 ppm
MPHE	Mixed crop Production under High Emission climate change	Excluding selected low quality soils	On Selected low quality soils	High Emission [CO_2] 449 ppm

1. Low quality soils are those soils series with the highest NO_3^- leaching/wheat grain production ratio (kgN/t Grain) based on DNDC modelled results; and those soils are CRANNYMOOR, EVERINGHAM, HOLME MOOR and KEXBY

3.3.2 STAMINA model simulations

In this work, wheat straw availability was estimated based on simulated wheat grain yields. The approach used to convert grain yield to straw supply capacity will be described in Section 3.3.3. The yields for both winter wheat grain and *Miscanthus* were simulated with STAMINA model. For *Miscanthus*, the model simulated *Miscanthus* DMYs at harvest (1^{st} to 3^{rd} March) after two establishment years, for 13 years of harvest. 30-year average scenario yields (two 15-year growing cycles) were generated for each soil type to be used in the overall assessment.

Model performance for both two crops were evaluated with site measured yields data as shown in Table 3-3. The fitness of simulated and measured values were presented in the result chapter, Chapter 4. Three indicators, including coefficient of determination (R^2), root mean square error (RMSE) and relative mean absolute bias error expressed as a percentage (MBE%) were calculated to assess the goodness-of-fit between model simulated and measured yields of both crops.

Table 3-3 Datasets used for model calibration and evaluation for winter wheat and Miscanthus

Crop	Site	Years of Simulation
Winter wheat	Rosemaund (R)	1993-1996
	Gleadthorpe (G)	1991-1994
	Boxworth (B)	1993-1995
Miscanthus	Rothamsted 408 (408)	1997-2004

3.3.2.1 Soil inputs

In this work, the catchment region is represented as a matrix of $1km^2$ cells, within which all important variables of soil, climate, crop and crop management are assumed to be homogeneous. Key soil information includes soil texture, bulk density, and soil available water capacity within rooting depth, soil C and N levels. Those are derived from UK National Soil Map (Cranfield University 2016) on a $1km^2$ grid. The case study catchment area covers 5856 1 km^2 grid cells, which contain 67 different soil series.

However, among the 5856 cells, 1892 cells are excluded from model simulation and following calculation. These soil excluded series are 6 SALINE cells, 210 sea cells, 2 lake cells, 1456 cells with shallow layers (673 Andover soil series, 214 Beccles Cells, 65 Elmton, 128 Landbeach, 37 Longmoss, 170 Swaffham Prior, 33 Isleham, 18 Upton, 54 Aswarby, 50 Banbury, 12 Adventures, 1 Soham and 1 Sandwich) and another 218 cells with missing information. After excluding these cells, 47 soil series were used in the simulation which can be grouped in to nine soil texture classes shown in Figure 3-3.

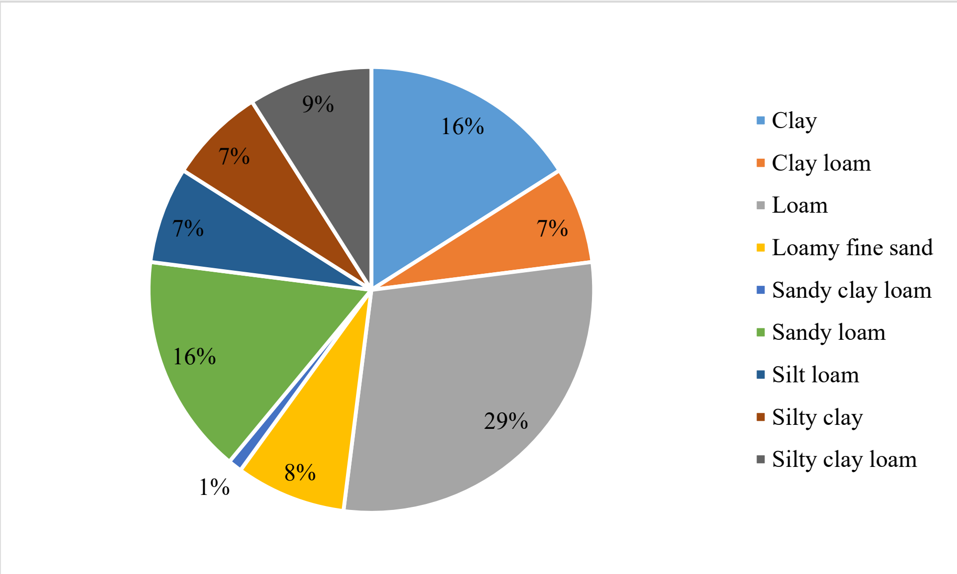

Figure 3-3 Proportion of each soil type in whole case study catchment area

3.3.2.2 Weather inputs

The impacts of climate change and atmospheric CO_2 concentration on crop productivity have been widely researched and reported, and process-based model has been the tool mainly applied to assess the impact of climate change on the crop yield in the future. (Jones et al., 2003) In this work, the simulation period was set as 30 years from 2021 to 2050. Three climate scenarios will be examined, i.e. baseline, medium and high CO_2

emission scenario. Hourly data collected from High Mowthorpe weather station from 1961-1990 are used as weather input to represent future baseline climate condition. Projected climate under climate change scenarios for medium CO_2 emission scenario and high CO_2 emission scenario are generated by UK Climate Projection (UKCP09) model. (Jenkins et al. 2009; Murphy et al. 2010)

The UK Climate Projections made in 2009 (UKCP09) gives projected changes for a number of climate variables, averaged over seven overlapping 30-year time periods, at 25 km^2 resolution for UK administrative regions and river basins. It gives greater spatial and temporal detail than other previous UK climate scenarios.(Murphy et al. 2010) The methodology designed by the Met Office Hadley Centre to provide probabilistic projections for UKCP09 is based on ensembles of climate model projections consisting of multiple variants of the Met Office climate model, together with other climate models from other centres. In the UKCP 09 model, CO_2 emissions under the three IPCC SRES scenarios A1FI, A1B1 and B1 (Intergovernmental Panel on Climate Change, 2000a) are used and labelled High, Medium and Low accordingly to how different emissions pathways affect future climate. The probabilities given by UKCP09 represent the relative degree to which each climate outcome is supported, based on the evidence currently available, taking into account current understanding of climate science and observations, and using expert judgement. There are three major sources of uncertainties in projecting future climate change: a) due to natural variability, b) due to incomplete understanding of climate system processes, and their imperfect representations in models and c) that due to uncertainty in future emissions. (Murphy et al. 2010)

The UKCP09 uses the Met Office regional climate model to downscale global climate projections to a 25 km^2 scale and all the climate variables are provided for a monthly means level. Thus the UKCP 09 Weather Generator (Jones et al., 2009) was used to provide weather variables on a daily or hourly basis to meet the input requirements of crop models. These variables are temperature, rainfall, humidity, shortwave radiation and sunshine amount. The Weather Generator works the same way as most of the other weather generators, where first a stochastic rainfall model simulates future rainfall sequences, and depending on whether the day is wet or dry, other weather variables (in the UKCP09 WG these are: mean daily temperature, diurnal temperature range, vapour pressure and sunshine) are determined by mathematical/statistical relationships with rainfall and values of the variables on the previous day.(Jones et al., 2009)

The UKCP 09 Weather Generator produces probabilistic projections as multiple (from 100 to 1000, which can be set before the model runs) statistically equivalent and stationary sets of hourly or daily climate data of 30 years in length. For the purpose of this work, the model is set to produce 100 sets of data. Among the 100 sets of data, 12 random sets were selected using a random number generator and used as climate input data for STAMINA model.

When the project was conducted in 2015, UKCP09 was the latest climate projection version. A next version UKCP18 will be launched in December 2018[7], while due to the timescale of this PhD project, the simulation could not be done using the most recent version UKCP18. However as suggested by Met Office[8], UKCP09 can still be treated as an appropriate tool and provides valid assessment of future UK climate over land. In its latest notes, it demonstrated that by comparing results generated by UKCP09 with resulted from Coupled Model Intercomparison Project Phase 5 (CMIP5), which is the most recent set of international models adopted by IPCC, they were consistent in future changes to summer temperatures, winter temperatures and winter rainfalls, while some difference in projected changes on summer rainfall (Met Office 2016). Both models projected that future summer rainfalls were more likely to decease than increase, while the projected reductions from CMIP5 are smaller than UKCP09.

[7] Information regarding the UKCP18 is available at http://ukclimateprojections.metoffice.gov.uk/, accessed in 28 Nov 2018

[8] Information regarding the capability of UKCP09 is available http://ukclimateprojections.metoffice.gov.uk/24127; accessed in 28 Nov 2018

3.3.3. From winter wheat grain yield to straw availability

Due to the limited availability of data on current straw production and use, we adopted a conservative estimation of winter wheat straw yield and potential availability for the case study area. Straw yield for per hectare field was estimated with Equation 1, basing on wheat grain production level, wheat grain harvest index (HI), harvestable straw incorporation and straw incorporation rate. In Equation 1, x represents the modelled grain yield (in t/ha, 14.5% moisture). Wheat grain HI is simulated by the STAMINA-winter wheat model, 30-year average value of 0.53 were used in case study scenarios. We assume that 50% of all the leaves and stems produced over the entire wheat growing season have been lost through decay and impossible for collect by the time of harvest. The remaining 50% of the residual biomass is harvested in the first two years, while in the third year it is left on the ground to maintain SOC content, thus a straw incorporation rate of 1/3 were used. Based on straw yield, the amount of total available straw was estimated by Equation 2, considering total cultivation area (396400 ha) and crop rotation, assuming 2/3 of total fields were under winter wheat cultivation.

Equation 1 $$Straw\ yield\ (t/ha) = \left(\frac{x}{0.53} - x\right) * 0.5 * \left(1 - \frac{1}{3}\right)$$

Equation 2 $$Total\ harvestable\ straw\ (t/year) = \left(\frac{x}{0.53} - x\right) * 0.5 * \left(1 - \frac{1}{3}\right) * 396400 * 2/3$$

3.3.4 Grain availability estimation

In MP scenario, as 8% of the low productivity sandy soils were allocated for *Miscanthus* production, a change in total grain production was foreseen. Thus the estimation and comparison of wheat grain production of the two provision strategies were necessary. This work was conducted based on STAMINA simulated wheat grain yields.

3.4. Estimating NO_3^- leaching and N_2O emissions

The carbon-nitrogen turnover model DNDC is used in this study to estimate NO_3^- leaching, direct and indirect N_2O emissions from soils for winner wheat and *Miscanthus* cultivation under baseline climate condition.

3.4.1. Parameters for winter wheat and *Miscanthus*

Winter wheat was parameterized for DNDC by using published values (Wattenbach et al. 2010) and site measured data as listed in Table 3-3. Although *Miscanthus* parameters were not included in the original DNDC model, they were parameterized and tested in 2011 (Gopalakrishnan et al. 2012)(values shown in Table 3-4), in which the parameters were estimated based on literature data and the calibration and valuation were conducted using observed yields within four years at a site in Urbana, Illinois, USA. To demonstrate the ability of DNDC model for simulating *Miscanthus* under the UK conditions, we evaluated the model performance with the datasets shown in Table 3-3 as well. Those parameters and model goodness performance were then evaluated by the same dataset as for STAMINA model, using the same indicators (i.e. R^2, RMSE and MBE%) Comparison between modelled and measured yields will be given in Chapter 5.

Table 3-4 Parameters used in DNDC for Miscanthus simulation, based on Gopalakrishnan et al. (2012)

Parameter	Values
Leaf+Stem fraction of total Biomass	0.7
C/N ratio for leaf and stem	110
C/N ratio for root	70
N fixation index	1.2
Water requirement (kg water per kg dry matter of biomass)	300
Optimum Temperature	15
Thermal degree days	1200

3.4.2. Input climate, soil and crop management information

GHG flux is modelled using 9-year weather data from 1986 to1994, with the CO_2 concentration of 360 ppm. While apart from weather information, DNDC model also requires some other background parameters, which are

1) Background N concentration (i.e. Rainfall N concentration and Atmospheric NH_3 concentration)

Rainfall N concentration are derived from UK Eutrophying and Acidifying Network[9] (UKEAP): Precip-Net. Within the EAP PrecipNet, 38 sites were established to measure the chemical composition of precipitation (i.e. rainwater) the network allows estimates of wet deposition of sulphur and nitrogen chemicals. Measured rainfall NH_4^+-N and NO_3^--N concentration at Thorganby station from 2009 to 2014, which was within our case study catchment area is shown in Figure 3-4. Since the data recoded on 23/04/2014 was too high compared with the general level, so it was excluded from the average value calculation. The calculated mean N value was 1.27ppm and applied in this study.

Atmospheric NH_3 concentration was obtained from UKEAP-National Ammonia Monitoring Network[10], which was established in 1996 and the objectives of the network are to quantify temporal and spatial changes in air concentrations and deposition in NH_3 and NH_4^+(included since 1999) on a long term basis. Measured Atmospheric NH_3 concentration at Easingwold station from 2009 to 2014 is shown in Figure 3-5. The six-year average value 2.54 µgN/m3 and applied in this study.

[9] Information and access to UKEAP:Precip-Net are available at https://uk-air.defra.gov.uk/networks/network-info?view=precipnet; accessed in 28Nov2018

[10] Information about UKEAP-National Ammonia Monitoring network is available at: https://uk-air.defra.gov.uk/networks/network-info?view=nh3; accessed in 28Nov2018

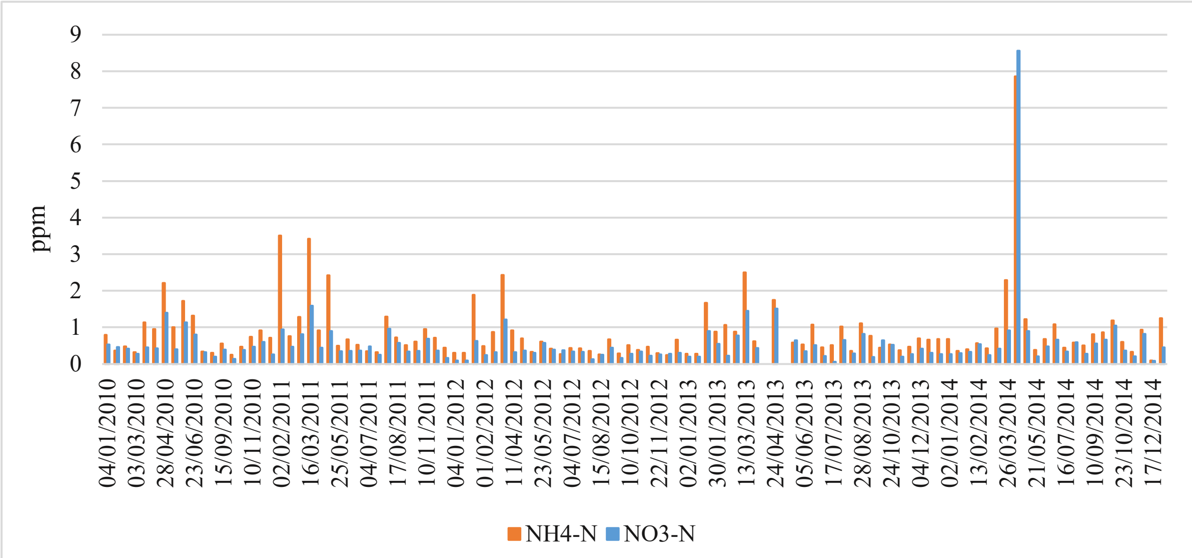

Figure 3-4 Measured rainfall NH_4^+-N and NO_3^--N concentration at Thorganby station (Data source: UKEAP: Precip-Net)

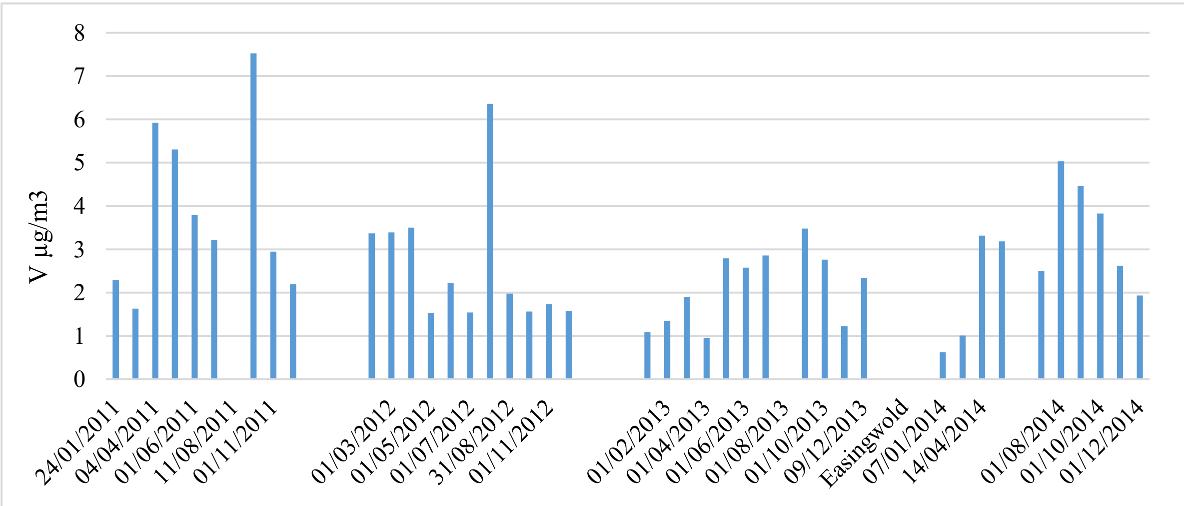

Figure 3-5 Daily and Multi-day air quality monitoring data (NH_3) at Easingwold station (Data source: UKEAP-National Ammonia Monitoring Network)

2) Nitrogen fertiliser inputs for winter wheat production

Fertilize inputs level was calculated based on Department for Environment, Food and Rural Affairs (DEFRA)'s fertiliser manual (RB209).(DEFRA 2010) The RB209 manual aims to help farmers and land managers better assess the fertiliser requirement for the range of crops they plan to grow to achieve on-farm optimum economic crop yields of marketable quality with minimum adverse environmental impact. (DEFRA

2010) The recommended nitrogen fertiliser input level is influenced by the factors including,

- The amount of nitrogen from all sources, including the soil, which must be available to achieve the optimum on-farm economic yield.
- The amount of nitrogen that the soil can supply for crop uptake.
- The cost of nitrogen fertiliser and the likely value of the crop.
- Any particular crop quality requirements, for example grain protein in bread making wheat or in malting barley (DEFRA 2010)

In the RB209 fertiliser manual,(DEFRA 2010) the nitrogen fertiliser input level is determined using Soil Nitrogen Supply (SNS) index system. Generally, SNS index is first determined by field specific information including previous cropping, fertiliser use, soil type and rainfall. Then the recommended nitrogen fertiliser application level can be obtained by referring to the appropriate crop table. (DEFRA 2010)

The nitrogen fertiliser input value for each soil series is shown in Figure 3-6, ranging from 160 to 220 kgN/ha.yr, assuming previous crops were winter wheat. The overall weighted average annual N input was 205 kgN/ha.yr.

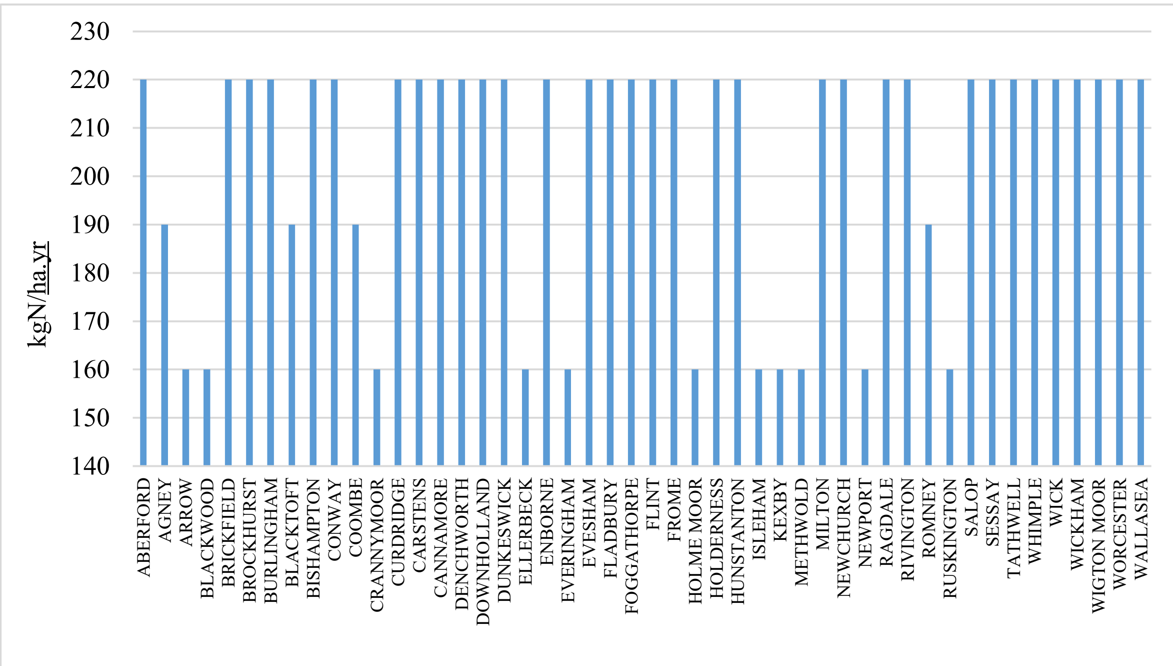

Figure 3-6 N fertiliser inputs for all the soil series used in this study

3) Nitrogen fertiliser inputs for *Miscanthus* cultivation

The nitrogen fertiliser input level for *Miscanthus* cultivation was also derived from RB209 guide. (Agriculture and Horticulture Development Board 2017) In RB209, it is stated an annual nitrogen fertiliser application amount of 60-80 kgN/ha.yr input for all the soil series should be sufficient for *Miscanthu*s cultivation under the UK conditions, mainly to replace the nitrogen removed in the harvested biomass. An application level in the lower side (60 kgN/ha.yr) was applied as the inputs information for *Miscanthus* simulation, considering that a number of researches stated that no observations were found regarding the *Miscanthu*s' responses to increased nitrogen fertiliser application and increased nitrogen fertiliser inputs would lead to the increase of NO_3^- leaching and N_2O emissions during *Miscanthus* cultivation. (Christian & Riche 1998; Behnke et al. 2012)

3.5. Methodology for Carbon stock changes accounting

3.5.1. General structure of carbon stock accounting

Carbon stock change accounting is conducted in both SPBC and MPBC scenarios with Tier 2 and Tier 3 approaches.(Intergovernmental Panel on Climate Change, 2006a) Starting from 2021, four simulation periods (30-year, 50-year, 100-year and 150-year) were modelled. Five carbon pools are considered in this work, according to the general structure provided by 2006-AFOLU guidelines (Table 3-5). Carbon stock change in litter were excluded in the estimation. This is on consideration of its relatively smaller quantity compared with aboveground biomass (AGB), belowground biomass (BGB) and soil organic carbon (SOC) pools;(Richter, Agostini, Redmile-Gordon, White & Keith W T Goulding 2015) secondly, in arable systems biomass turnover are generally fast, thus eventually litter are decomposed and carbon will be transfer to SOC pools and atmosphere. (Clifton-brown et al. 2007) Carbon stored in deadwood is not accounted in this study either, due to its relatively small amount in winter wheat and *Miscanthus* fields. Thus the total annual carbon stock changes in this cases study area is estimated by Equation 3 for both tiered approaches.

$$\textit{Equation 3} \qquad \Delta C_{CS} = \Delta C_{AGB} + \Delta C_{BGB} + \Delta C_{SOC} + \Delta C_{LI} + \Delta C_{DW}$$

where ΔC_{CS} is annual terrestrial carbon stock change in casestudy area (tC/year); other subscripts denote the following carbon pools: AGB= above-ground biomass, BGB=below-ground biomass, SOC=soil organic carbon; LI=litter, and DW=deadwood; ΔC_{LI} and ΔC_{DW} are assumed to be zero in this study for both Tier 2 and Tier 3 approaches.

'Stock-Difference Method' (Intergovernmental Panel on Climate Change, 2006a) approach was used in estimating carbon stock change in each pools. With this method, carbon stocks in relevant pools are measured at two points in time to assess carbon stock change (Equation 4). The main difference between the two tired approaches lies on the different methods used to estimate the carbon stock levels at the two measured points for each carbon pools.

$$\textit{Equation 4} \qquad \Delta C_{PL} = \frac{(CPL_0 - CPL_{(0-T)})}{T}$$

Where ΔC_{PL} =annual carbon stock change (tC/ year) in each carbon pool; CPL_0 = carbon stock in the last year of the defined timeframe in this carbon pool (tC); $CPL_{(0-T)}$= soil organic carbon sock at the beginning of the defined timeframe in this carbon pool (tC); T is the defined timeframe. In this study four timescales were accounted for, i.e. 30 years, 50 years.150 years and 150 years.

Carbon stock change accounting requires first defining previous land use and future land use type. It is assumed in this study that in all the casestudy areas previous land used are crop land producing winter wheat. Regarding future land use, SPBC scenario assumes all the soils remaining as winter wheat fields; MPBC assumes *Miscanthus* being cultivated in selected four soil series and winter wheat in the other fields.

Table 3-5 Five carbon pools defined in 2006-AFOLU and the accounting approached used in this study

Defined Carbon pools		Methodology
Biomass	Aboveground biomass (AGB)	Considered and accounted with Tier 2 and STAMINA-based Tier 3 approach
	Belowground biomass (BGB)	Considered and accounted with Tier 2 and Literature data
Dead organic matter	Deadwood	Not considered
	Litter	Not considered
Soils	Soil organic carbon (SOC)	Considered and accounted with Tier 2 and Roth_C-based Tier 3 approach

3.5.2 AGB carbon pool

3.5.2.1 Tier 2 approach

According to the definition of 'cropland' given in 2006-AFOLU, the cropland category includes arable land, tillable land, rice fields, agroforestry system in which the vegetation structure falls below the thresholds used for the Forestland category and is not expected to exceed those threshold at a longer period. (Intergovernmental Panel on Climate Change 2006a) In other words, all the crops considered in this study (winner wheat and *Miscanthus*) fall into this category. Thus when Tier 2 approach is used, the land use regime is 'cropland remaining cropland' for both SPBC and MPBC scenarios.

According to Tier 2 guidelines, the change in biomass is only accounted for in perennial woody crops, thus if Tier 2 approach is applied, carbon stock change in AGB in zero for both SPBC and MPBC scenarios. (Intergovernmental Panel on Climate Change, 2006a)

3.5.2.2 Tier 3 approach

In SPBC scenario, as winter wheat is assumed to be cultivated in whole casestudy area through all the simulation periods, thus no potential land use change is detected. In MPBC scenario, *Miscanthus* is assumed to replace winter wheat on the selected areas, thus on those areas more biomass carbon will be stored in (or lost from) AGB pool due to the yield difference between *Miscanthus* and winter wheat. Additionally, excluding selected soils from winter wheat cultivation also changed the weighted average yield of winter wheat in MP scenario, thus carbon stock in winter wheat AGB is also changed accordingly. Another assumption was made that winter wheat yields prior to the simulation begins are same as STAMINA simulated average 30-years winter wheat yields under baseline climate condition. Thus, the carbon stock changes in AGB pool were simulated with Equation 5. As modelled outputs are in unit of kg DMY/ha, a factor 0.475 is used to convert DMY to C content.

Equation 5

$$\text{Annual carbon stock change in AGB (kg C/ha. yr)} = \frac{\text{Future crop biomass (kg DMY/ha)} - \text{ Previous crop biomass(kg DMY/ha)} * 0.475}{\text{simulation timeframe (years)}}$$

3.5.3 BGB carbon pool

3.5.3.1 Tier 2 approach

Similar to the estimation for AGB, carbon stock changes in this pool only accounted for in perennial woody crops, thus the carbon stock change in SPBC and MPBC are assumed to be zero.

3.5.3.2 Literature data

The estimation structure of carbon stock change in BGB pools are similar to the AGB pools. In SPBC scenario, winter wheat production is assumed to remain the same as the conditions prior to simulation begins, thus BGB carbon stock in SPBC is nil. While in MPBC, due to that parts of the soils were allocated to *Miscanthus* cultivation, not only BGB carbon stock changes in the *Miscanthus* fields, but also the weighted average value of biomass productivity in the rest wheat fields changed correspondingly. The estimation involves both *Miscanthus* BGB and winter wheat BGB.

BGB of Miscanthus crop: In this work, literature data from two European studies were considered to define the potential BGB change of *Miscanthus* cultivation. Both of the two 15- year's studies reported with close climate regimes and harvested *Miscanthus* yields to this work. One experiment was established in South Ireland and a total cumulative BGB of 20.6 ±4.6 t/ha was measured and reported with average annual harvest yield of 13.4±1.1 t/ha. (Clifton-brown et al. 2007) Another experiment was established in Rothamsted farm, England and the recorded cumulative BGB was 33 t/ha for rhizomes and 12.88 t/ha to 14.69 t/ha for roots with the max yield of 15.9 t/ha. (Richter, Agostini, Redmile-Gordon, White & Keith W T Goulding 2015) An average value of the reported BGB (combining both rhizomes and roots biomass) was used in this study. It is worth mentioning that, although BGB is not harvest every year (maybe never been harvest) and it is possible that cumulative BGB will increase beyond 15 years when the crop age getting older. This study assumed that the 15-year level will be the threshold of the BGB for all the simulation periods. This is considering that, the *Miscanthus* life cycle in this study is also assumed to be 15 years and after 15 years the whole crop will be removed and a new *Miscanthus* crop will be established on the same field. Consequently, the BGB from first *Miscanthus* crop will be either removed or left in the soil. If removed, the stored carbon will leave this farming system and if retained in the soil, it will be decomposed and carbon will transfer to either SOC pool or atmosphere.

BGB of winter wheat crop: as root being the only belowground organ for winter wheat crop, thus the carbon storage in winter wheat BGB is based on STAMINA simulated winter wheat yields and the shoot/root ratio reported by Bolinder et al (1997). The adopted shoot/root ratio is 4.33. This is calculated from a winter wheat species of which the grain yield (7.45 t/ha) and HI (0.49) are close to the winter wheat simulated in this study. (Bolinder et al. 1997)

3.5.4 SOC pool

Estimate of carbon stock change in SOC pool also followed 'the stock-difference method' (Intergovernmental Panel on Climate Change, 2006a) and the following Equation 6 is used,

Equation 6

$$\Delta C_{SOC} = \frac{(SOC_0 - SOC_{(0-T)})}{T}$$

Where ΔC_{SOC} =annual carbon stock change (tC/yr) in SOC; SOC_0 = soil organic carbon stock in the last year of the defined timeframe (tC); $SOC_{(0-T)}$= soil organic carbon sock at the beginning of the defined timeframe (tC); T is the defined timeframe.

Tier 3 approach outperformed Tier 2 in the way that Tier 3 using process-based models to define SOC at each time point, while Tier 2 used default parameters given by the 2006-AFOLU guidelines.

3.5.4.1 Tier 2 approach

Tier 2 approach estimates the SOC level at each time point with the following Equation 7,

Equation 7

$$SOC = \sum_{c,s,i} \left(SOC_{REF_{c,s,i}} \times F_{LU_{c,s,i}} \times F_{MG_{c,s,i}} \times F_{I_{c,s,i}} \times A_{c,s,i} \right)$$

Where c represents the clime zones, s represents the soil types and i represents the specific management system; $SOC_{REF_{c,s,i}}$ is the reference carbon stock (tC), of which the default value is provided by 2006-AFOLU guidelines considering climate, soil and management conditions; F_{LU}, F_{MG} and F_I refer to carbon stock change factors for land use, management and input of organic matter respectively; A is the land area estimated.

The climate classifications of the casestudy area is defined as cold temperate, moist climate (based on Annex 3A.5, AFOLU); (Intergovernmental Panel on Climate Change, 2006a) Soil classifications are decided according to USDA Taxonomy. (Soil Survey Staff 1999) and shown in Table 3-6; values for F_{LU}, F_{MG} and F_I are listed in Table 3-7.

Table 3-6 Soil classifications of casestudy area and corresponding SOC_{REF}

Soil classification	Area (ha)	Area proportion	SOC_{REF}
Sandy soil	30200	7.62%	71
High Activity Clay (HAC)	366200	92.38%	95

Table 3-7 Defined factor value type and 2006-AFOLU default factors for F_{LU}, F_{MG} and FI for winter wheat and Miscanthus fields

Cultivated Crop	Land Use level	F_{LU}	Tillage level	F_{MG}	Organic Matter Input level	F_I
Winter wheat	Long term cultivated	0.69	Reduced	1.08	Low	0.92
Miscanthus	Perennial	1	No-till	1.15	High without manure	1.11

3.5.4.2 Tier 3 approach

RothC model was used in this study as the Tier 3 approach to estimate carbon stock changes in SOC pool.

1) Input data specification

Apart from Tier 2 approach basing on land use type, climate condition etc., RothC model was also applied in this study to achieve higher resolution simulated results on carbon stock changes in SOC pool. This approach accounts for the effects of soil type, temperature, moisture content and plant cover on the soil carbon turnover process. RothC uses a monthly time step to calculate total organic carbon (t/ha), microbial biomass carbon (t/ha) and Δ14C on a years to centuries timescale. (Jenkinson et al. 1987; Jenkinson, 1990; Jenkinson et al. 1991; Jenkinson et al. 1992; Jenkinson and Coleman, 1994) Similar to other process-based models, inputs data needed to be prepared and their resources are listed as following:

- Monthly rainfall (mm) and air temperature (°C) were calculated basing on 30 years data recorded in High Mowthorpe weather station (Appendix A);
- Monthly open pan evaporation(mm) were calculated using Equation 8, according to RothC user guide (Coleman & Jenkinson 2005). Mean potential evaporation was from Muller's (1982) collection of meteorological data for station in Kingston-Upon-Hull, England (53°45'N/0°16'W) (Muller 1982);

Equation 8

$$\text{Open\_pan evaporation} = \text{Mean potential evaporation}/0.75$$

- Clay content of the soil is obtained from NATMAP data (same as data used in DNDC and STAMINA simulations in this work) and depths of soil layers were set as 30cm;
- An estimate of the decomposability of the incoming plant material (decomposable plant material(DPM)/resistant plant material(RPM) ratio); the DPM/RPM ratio used for winter wheat was set as 1.44 which has been widely used in slimier works; (Wang et al. 2016; Jenkinson 1990; Coleman et al. 1997) for *Miscanthus*, a lower DPM/RPM ratio of 0.66 was used to reflect the slower decomposition rate of *Miscanthus* compared with winter wheat; (Richards et al. 2016)

- Soil cover status for individual month: for *Miscanthus*, as it is a perennial crop, soil were set as covered (vegetated) in all the months; for winter wheat, soil was set as covered (vegetated) from October, November, December, January, February, March, April, May, June, July; and bare in August and September;
- Monthly input of the plant residue (t C/ha): monthly inputs were calculated based on STAMINA simulated crop annual yield and equations for 'plant inputs to the soil'. The same equations were used as the work of Hiller et al. (Hillier et al. 2009), which adapted the characterization as a function of yield as employed in SUNDIAL.(Smith et al. 1996; Smith et al. 2005) The Equation 9 and Equation 10 were applied for winter wheat land and *Miscanthus* respectively.

Equation 9

$$C_{input}(t\ ha^{-1}yr^{-1}) = 1.346(1.23 + 1.4(1 - e^{-0.24\times Yield(t\ ha^{-1}}))$$

Equation 10

$$C_{input}(t\ ha^{-1}yr^{-1}) = 6.85(0.5 + 0.5(1 - e^{-0.23\times Yield}))$$

2) Simulation procedures

Simulation were conducted for SPBC and MPBC scenarios following the procedures below,

Step 1. Current SOC content in top 30 layer were calculated with soil bulk density (g/cm3) and soil organic carbon content (%) from NATMAP database for each soil series.

Step 2. The previous land use was assumed as agricultural land with RPM/DPM ratio of 1.44. Preliminary run was conducted with RothC model to estimate monthly carbon inputs with to the soil to reach the target (current soil carbon content) for each soil series. This output is regarded as the carbon inputs prior to the land used for LCB feedstock production.

Step 3. For SPBC scenario, RothC was first run to match the equilibrium, with the estimated monthly carbon inputs from Step 2 and a RPM/DPM ratio of 1.44 for each soil. After equilibrium the model was set to run 150 years with predicted organic carbon input calculated based on STAMINA winter wheat simulation and RPM/DPM ratio remaining as 1.44.

In MPBC scenario, for soil series CRANNYMOOR, EVERINGHAM, HOLME MOOR and KEXBY, RothC was first run to match the equilibrium with the outputs from Step 2 and a RPM/DPM ratio of 1.44 for each soil. After equilibrium the model was set to run 150 years with carbon input calculated with Equation 10 and RPM/DPM ratio of 0.66; for other soil series, the model was set to run with the same condition as SPBC scenario.

3.6. LCAs

As one of the most widely applied approaches for estimating GWP and other environmental impacts, a field to upstream factory gate LCA of delivered LCB feedstocks was conducted to assess the GHG emissions related to the two proposed production scenarios SPBC and MPBC.

Additionally, the GHG emission figures associated with LCB feedstocks supply were further integrated into a ‘field to end-of- life’ analysis of Lignocellulosic succinic acid LCA in order to understand the impacts of agricultural production phase on whole succinic acid production from lignocellulosic feedstock.

3.6.1. LCA for LCB feedstocks

3.6.1.1. Goal and scope definition

Aiming to achieve site- and supply-chain specific GWP figures for delivered LCB feedstocks within 30-years' timeframe, whilst exploring the GHG emissions reduction potential associated with lignocellulosic feedstock supply, the system boundary was set as 'field to up-stream factory gate' (Figure 3-7), with function unit of 'per kg LCB delivered'. The LCA covered the emissions associated with the feedstock cultivation, preparation of the feedstock for transport, transport to storage and transport to feedstock processing plant in the defined case study area (Figure 3-2). Farm machinery manufacture and maintenance was excluded in this analysis as it was considered to be outside the systems boundary. Within the cultivation phase, the emissions were considered from upstream production of materials and raw material extraction, fuel inputs required for on-farm cultivation, nitrogen related GHGs from fertilizer application as well as carbon storage and removals associated with potential land use change. LCA were conducted for both SPBC and MPBC provision scenarios. SPBC was set as the reference system to investigate the reduction potential on climate change impacts of integrating *Miscanthus* into wheat production system. The timescale was set as 30 years.

[redacted]

Figure 3-7 'Cradle to up-stream factory gate' LCA of delivered LCB feedstocks

3.6.1.2. Allocation procedures

As wheat crops consists of both wheat grain and wheat straw with grin being the main product, most of the production data gathered are either for the whole wheat crop (with unit of 'per ha') or for the wheat grain (with unit of 'per kg grain produced'). Therefore, allocation procedure needed to be applied in order to apportion the associated impacts between the grain and straw. Three allocation approach choice were considered and used in this work.

- *Economic allocation:* following the Publicly Available Specification 2008:2050 (PAS2050) the activities and associated GHG emissions are allocated between the co-products according to their economic values. Three years historical data from June 2015 to June 2018 on UK wheat grain and straw prices were downloaded from

AHDB website[11] (Appendix B). Three years average values (127£/t for grain and 49£/t for straw) are used in this work.

- *RED_allocation:* this allocation method follows the Renewable Energy Directive (RED) where suggests that straw shall be considered to have zero life-cycle greenhouse gas emissions up to the process of collection of those materials. (RED, 2009)
- *Energy_allocaiton*: in this revised energy allocation method, the emissions were attributed based on the real calorific values (CV) of wheat grain and straw. The calorific values for wheat grain and straw are 16.5 MJ/kg and 17.6 MJ/kg respectively. (BSI 2010)

3.6.1.3. Assumptions and background data for Life cycle inventory (LCI)

LCI phase considers a compilation of all the inputs (resources) and the outputs (emissions) of a product over its life-cycle in relation to its functional unit.(Finnveden et al. 2009) In this case, all the inputs and emissions associated with LCB supply were gathered per kg LCB delivered covering all the processes from the field to the upstream factory gate. All the background data for LCI development are listed in Appendix C.

For winter wheat, most cultivation data was taken from the Biomass Environmental Assessment Tool (BEAT) v2.1 database, which derives its data from the Farm Management Pocketbook (NIX 2008), except for activities with specific values to the case-study region.

These activities include, ammonium nitrite application levels generated based on RB 209 for each soil series in consistency with DNDC simulation and a weighted average value were used in LCA; direct N_2O emission, NO_3- leaching and indirect N_2O were generated based on DNDC outputs; figures of AGB and SOC carbon storage changes

[11] 'Farm expenses' available at https://dairy.ahdb.org.uk/

were generated by either RothC or STAMINA models; literature data were used for BGB carbon stock changes; and data for allocation procedures as described in section 3.6.1.2.

Miscanthus cultivation data has been compiled from the Sustainable Liquid Biofuels from Biomass Biorefining (SUNLIBB) project database (Mortimer et al., 2014) which has been developed for Europe from primarily UK data. The cultivation data has also been verified by IBERS (Institute of Biological, Environmental and Rural Sciences, Aberystwyth University).(IBERS 2016 private communication) Ammonium nitrite application level was assumed as 60kgN/ha.yr, in accordance with DNDC simulation. Same as winter wheat, direct N_2O emission, NO_3^- leaching and indirect N_2O are generated based on DNDC outputs; figures of AGB and SOC carbon storage changes were generated with Tier 3 process-based models; BGB carbon stock changes were produced based on literature data.

For both crops, upstream data related to production of the inputs wass taken from Ecoinvent v3.1 (Wernet et al. 2016). The combustion of diesel in agricultural equipment for various tasks (e.g. fertiliser application, harvesting and baling) was taken from IPCC (2006) and Kubica et al., (2009). Transport distance from farm to storage and from storage to conversion plant are all assumed to be 50km. Transport methods were selected as 'Transport, freight, lorry>32 metric ton, EURO3' from Ecoinvent database. (Wernet et al. 2016)

3.6.1.4. Life Cycle Impact Assessment (LCIA)

In this work the two mandatory steps, selection of impact categories and classification, and characterisation are included. The optional steps normalisation and weighting is not conducted. In maintaining consistency with the goal of this study, the impact category Climate change is selected. The results on climate change impacts were generated using the ReCiPe Midpoint (H) LCA impact assessment methodology from SimaPro 8 database using the LCI described in section 3.6.1.3.

3.6.2. 'Cradle to end-of-life' LCA for lignocellulosic SA life cycle

As part of the Bio-SuccInnovate project, the estimated GHG balances associated with LCB provision were further integrated with climate changes impacts from the following stages of lignocellulosic succinic acid life cycle. These processes were modelled by project partner University of Geneva, covered from LCB feedstock pretreatments, succinic acid production, polymer production, product production to end-of-life treatment. A brief description regarding the main processes and data sources are given in this section. It is worth mentioning that results of this analysis have now been published by Patel et al. (Patel et al. 2018).

3.6.2.1 Goal and Scope definition

This is a 'cradle to end-of-life' LCA based on (Patel et al. 2018). The aim of this work is to further investigate the climate-change impacts of the plastic end products derived from the lignocellulosic succinic acid-based polymer polybutylene succinate (PBS) with detailed and site-specific figures associated with LCB supply. Their climate change mitigation potentials were compared with two reference systems, conventional starch-based PBS and the petro-based alternatives. The second objective is to explore and demonstrate the influence of different LCB provision scenarios on the overall GHG balance of succinic acid life cycle. The function unit was CO_2eq per kg product.

Two plastic end products were considered, plastic trays for food packaging and agricultural mulch films (Patel et al. 2018). For film, end-of-life waste treatment was assumed as degradation on the fields; and for plastic trays, two end-of-life treatments were assumed, energy recovery in a municipal solid waste incineration (MSWI) plant or industrial composting (Figure 3-8).

LCB-based PBS trays and films were both compared with starch-based PBS trays and films produced from maize grain, with the same end-of-life treatments incineration or composting. Besides, petro-based plastic products were also used as reference materials in this study. LCB-based PBS-trays were compared with petro-based polypropylene (PP) trays and petro-based polyethylene terephthalate (PET) trays. LCB-based PBS-films was compared with petro-based polyethylene (PE) films. Petro-based reference products were all treated with MSWI after uses.

Biogenic carbon embedded in the products were considered for both starch-based and LCB-based products. For consistency, the CO_2 emissions from embedded carbon during end-of-life treatment were also reflected in this work.

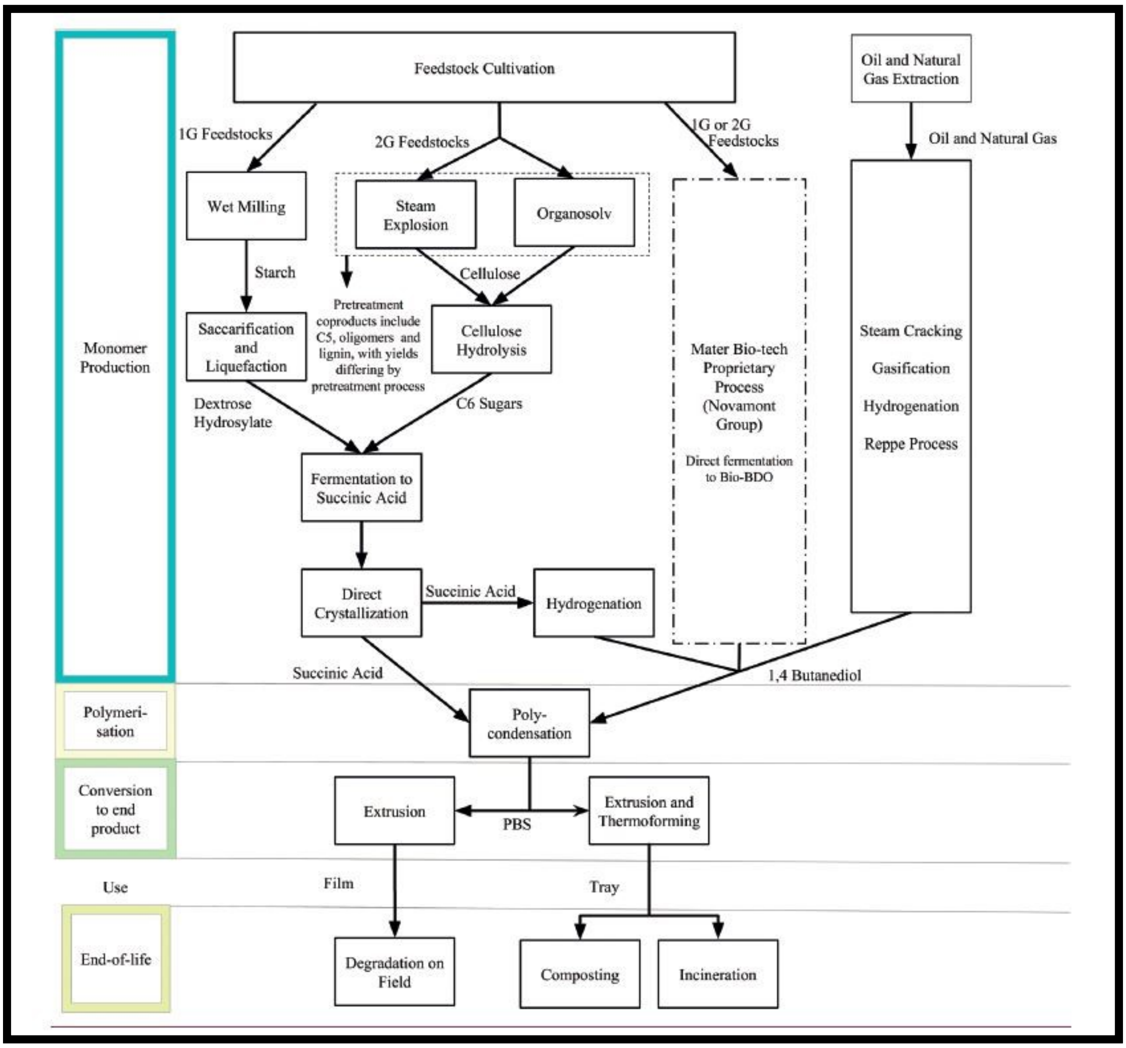

Figure 3-8 Life cycle of lignocellulosic (refers to the 2G in the figure) succinic acid succinic acid, covering monomer production, polymerisation, conversion to end products, use, and end-of-life waste management options (Patel et al. 2018).

3.6.2.2 Allocations

Maize starch-based PBS trays and films were selected as reference products in this study. Allocation is necessary to attribute the impacts among maize grain and maize strove. The production figure for maize grain is adapted from Cok et al. (2014) which was produced with a black-box economic allocation.

For LCB feedstock, in consistency with ‘cradle to up-stream factory gate’ LCA, three allocation approaches and the corresponding factors were also used here, i.e. economic allocation, energy content allocation and RED allocation.

Allocation was also required in when Organosolv (OS) pretreatment was applied. The outputs of OS included not only C6 sugars which would be processed into fermentation stage to produce succinic acid, but also high purity lignin (HPL). Economic allocation was applied to attribute the impacts among HPL and C6 sugars. The assumed economic values are 1.00€ per kg HPL and 0.36 € per kg C6. (Patel et al. 2018)

3.6.2.3 Assumptions and background data for LCI

LCI for LCB feedstocks were described in Section 3.6.1.3. This section presents a brief description regarding some key assumptions been made, covering from LCB pretreatments to the end-of-life treatments. Detailed information can also be found in Patel et al (2018). A full set of applied data resources is included in Appendix D.

a. Pretreatment, fermentation and polymerization and plastics end-products processes

Two pretreatment processes converting LCB feedstocks to C6 sugars (and co-products) were considered, i.e. Organosolv (OS) and Steam Explosion (SE). The simplified flowcharts are shown in Figure 3-9. Both pretreatment processes produce C6 sugars and C5 sugars. Additionally, OS process also produce high purity lignin. (Patel et al. 2018)

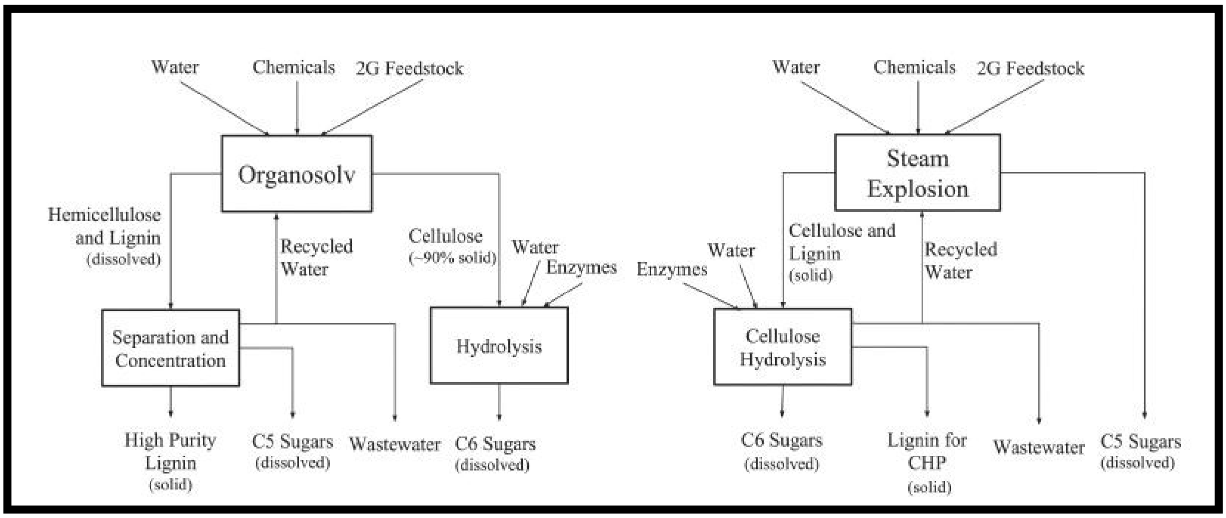

Figure 3-9 Flowcharts of two considered pretreatment methods of LCB feedstocks (refer to 2G feedstock in the flowcharts) (Patel et al. 2018).

The fermentation process converting C6 sugars to succinic acid is amused to be integrated in the same plant of LCB pretreatments. As a consequence, the excessed heat from pretreatment processes could be utilized during SA production. This also saved the concentration of C6 sugars and transport between pretreatments and SA production. Bio-BDO production was also assumed to be integrated in the same site (details within BDO production were given below).

As indicated in Figure 3-8, co-products produced from pretreatments include C5 sugars, oligomers and lignin. Only when HPL was produced from OS pretreatment, economic allocation was applied to attribute the impacts among HPL and C6 sugars. For all the other co-products from OS and all the co-products from SE, it was assumed that they were utilized in on-site biogas production with combined heat and power (CHP) facility to provide heat and electivity. If the produced natural gas or electricity were not sufficient, these were supplemented by purchasing from the grid. In the case of excess biogas being produced, a credit was obtained with the biogas being injected into the natural gas grid

As illustrated in Figure 3-8 that bio-based PBS can only be produced from SA with 1,4-butanediol (BDO), with the mass ratio 57:43 of SA vs BDO. Three pathways were considered for BDO production, including petro-based pathways, hydrogenation of LCB-based SA and fermentation of C6 sugars. In other words, PBS can be produced fully based on biomass or partly biomass (with bio-based SA and petro-based BDO). Fully bio(fb)-based PBS and partly bio(pb)-based PBS were both considered for starch-based bio-plastics and LCB-based bio-plastics systems.

In simulation for the production of PBS trays, two-step process 'extrusion and thermoforming 'were assumed (Patel et al. 2018), with material efficiency of 95.3%. For PBS films, the process extrusion was assumed (Patel et al. 2018) with material efficiency of 97.7%.

Due to confidentiality concern, some of the data regarding of bio-SA and plastics production are not present in this thesis, while the data sources and considered processes are included in Appendix D.

b. Production of reference products

Climate change impacts associated with maize grain production was adapted from Cok et al. (2014), 2.58kg CO_2 eq/kg SA. This figure did not include the biogenic carbon stored in SA. Figures regarding PP, PET and PE production were from EcoInvent 3.(Wernet et al. 2016)

c. Estimates of biogenic carbon embedded in bio-based plastics, biogenic CO_2 emissions and fossil-based CO_2 emissions from end-of-life waste managements

The amounts of biogenic carbon embedded in bio-based products were calculated based on the molar masses of PBS and CO_2. In the production of PBS, the reaction molar ratio of SA vs BDO is 1:1. Thus biogenic carbon embedded in fb and pb PBS products were calculated with Equation 11 and Equation 12.

Equation 11

$$Biogenic\ carbon\ in\ fb\ PBS(kg\frac{CO_2}{kg}PBS) = \frac{1}{Molar\ mass\ (PBS)} \times 8 \times Molar\ mass\ (CO_2)$$

Equation 12

$$Biogenic\ carbon\ in\ pb\ PBS\left(kg\frac{CO_2}{kg}PBS\right) = \frac{1}{2} \times \frac{1}{Molar\ mass\ (PBS)} \times 8 \times Molar\ mass\ (CO_2)$$

Biogenic CO_2 emissions from bio-based plastics differ from end-of-life treatment options. The values were calculated based on the embedded carbon amounts and the proportions of carbon released to atmosphere. The latter were derived from literature by Yeung et al. (Yeung et al. unpublished) and is included in Appendix E.

For PP, PE, PET based products, emissions during end-of-life treatments were derived from EcoInvent 3. (Wernet et al., cited in Patel et al. 2018)

b. Transportation

Same as LCA for LCB, two road transport stages of 50km was assumed for 'farm to storage and drying' and 'storage to plant'. As the pre-treatment was assumed to be integrated with fermentation plant, no transportation was assumed in this phase. For maize starch-based SA, transportation prior to down-stream fermentation plant gate was assumed to be included in the figure generated by Cok et al. 2014. In maintaining consistency with Patel et al. (2018), another 1000km road transportation was assumed after bio-SA has been produced from LCB or starch feedstocks, covering all the other transportations needed from down-stream factory gate of bio-SA to end-of-life treatment sites. Transport method was selected as 'Transport, freight, lorry>32 metric ton, EURO3' from Ecoinvent v3.1 database. (Wernet et al. 2016)

e. End-of-life treatments

Three end-of-life treatments were considered in this study, Incineration, Composting and field degradation. For petro-based products incineration with energy recovery were assumed as the only option. For PBS-based tray products, incineration and composting were considered. For PBS-based agricultural films, only field biodegradation BDG) was considered as end-of-life option. The same figures were used as Patel et al. 2018, which were adapted from Yeung et al. (unpublished) and included in Appendix E.

3.6.2.4 LCIA

The ReCiPe Midpoint (H) LCA impact assessment methodology from SimaPro 8 database was used to generate results from the LCI based on the climate change impact category.

Chapter 4. **Current and future LCB feedstock provision capacity in case study area**

4.1. Introduction

Although LCB has been considered as a superior feedstock option compared with conventional food crop in terms of climate change impacts, (Patel et al. 2018) land and energy efficiency, (Black et al. 2011) food security, ecological and social issues etc.,(Intergovernmental Panel on Climate Change 2011) there are still considerable concerns regarding the actual provision capacity of LCB, especially for agricultural residues such as wheat straw. It is also identified that high production cost has been a major barriers for the commercial production of LCB-based biomaterials (Carriquiry et al. 2011) and sufficient LCB supply could potentially reduce the overall production cost. Although there have been many attempts to calculate this potential, (Chad & Bill 2013; Donaldson et al. 2001; Glithero et al. 2013; Engel et al. 2005; Copeland & Turley 2008) it remains uncertain to quantify. (Rosillo-Calle et al. 2007) Most of the estimation of straw production level was based on measurements of grain production and the assumption of a constant relationship between grain and straw yield, without considering current straw use demands.

In this chapter, we adopted a process-based model STAMINA to estimate the LCB provision capacity from wheat only and wheat-*Miscanthus* mixed production systems. In the mixed production system, *Miscanthus* is assumed to be planted on selected four soil series with Loamy fine sand soil (detailed reasons will be justified in following chapter). Winter wheat straw availability was estimated considering the wheat grain production level, wheat planted area, wheat grain harvest index, harvestable straw fraction, incorporation rate and competition in demand of other uses. Climate change scenarios were also considered in this study, aiming to quantify their potential impacts on LCB supply capacity.

4.2. STAMINA model evaluation

According to 2006-AFOLU, when process-based model was used in biomass production estimation, it is crucial to evaluate the model's performance with field measured data. (Intergovernmental Panel on Climate Change, 2006a) As mentioned in Section 3.3.2, three indicators were used to evaluate the model's performance. The RMSE between measured and simulated winter wheat yields is 1.36 t/ha and MBE % is 12% (Figure 4-1). The RMSE between measured and simulated *Miscanthus* yields was 1.58 t/ha and MBE% is 12%.

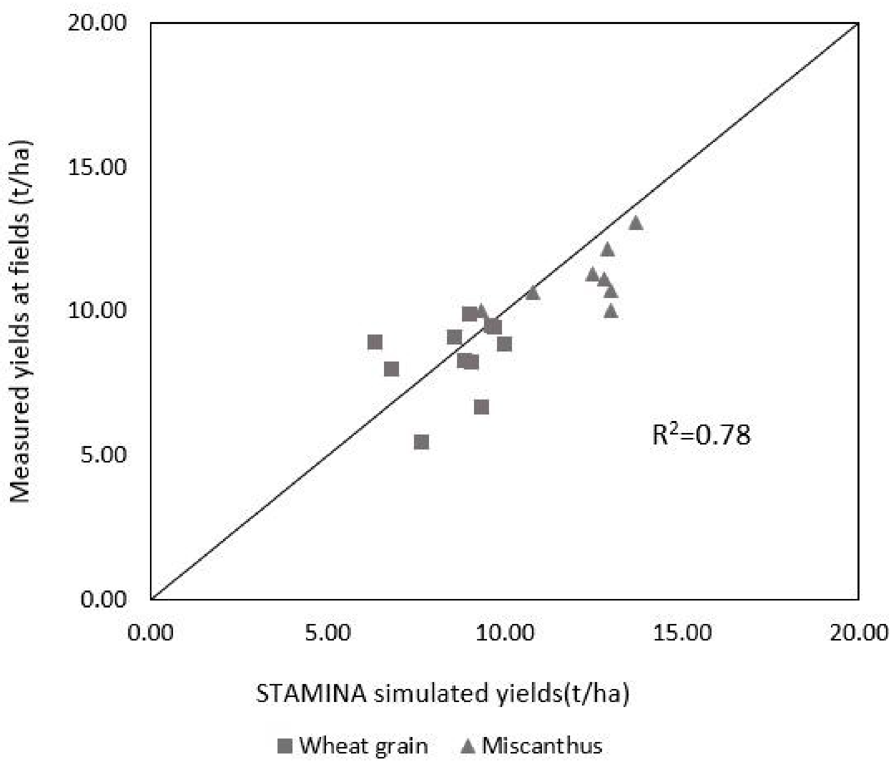

Figure 4-1 STAMINA simulated vs site-measured DMY for wheat grain and Miscanthus

4.3. Simulated winter wheat and *Miscanthus* yield in case study area

4.3.1. Simulated wheat grain yields

In STAMINA-winter wheat model, direct modelled output are grain yields (in 100% dry matter (DM)) for each soil series. Figure 4-2 shows the grain yields under BC when moisture content (MC) is adjusted to 14.5% (All the reported yields will be in 14.5% in moisture in Chapter if no special notice is given.) Modelled 30-year average wheat grain yields for all the soil series ranged from 7.23 to 8.35t/ha.yr under BC, depending on variable soil available water contents (AWC)s. The overall weighted average yield in the region was 7.73 t/ha.yr.

Modelled yields under ME and HE scenarios for all the soil series were graphed in Figure 4-3 and Figure 4-4 respectively. For ME scenario, the 30-years average yield was around 8.38 to 8.88 t/ha.yr. Similar to the BC results, soils with higher soil water holding capacity tend to achieve higher yields. The overall weighted average yield for ME was 7.32 t/ha.yr (DM) and was equivalent to 8.56 t/ha.yr when MC is adjusted to be 14.5%. For HE scenario, the 30-years average yield was around 8.59 to 9.09 t/ha.yr [1]. The overall weighted average yield is 7.46 t/ha.yr (DM), and was equivalent 8.73 t/ha.yr when MC was adjusted to 14.5%. Unlike the yields under BC condition, variations of 30-year averaged yields of each soil series appeared much smaller among ME and HE climate conditions. Comparing simulated grain yields in future climate change scenarios with BC (Figure 4-5), it indicated that the annual wheat yields in the region would be likely to increase in yields and decrease in variation.

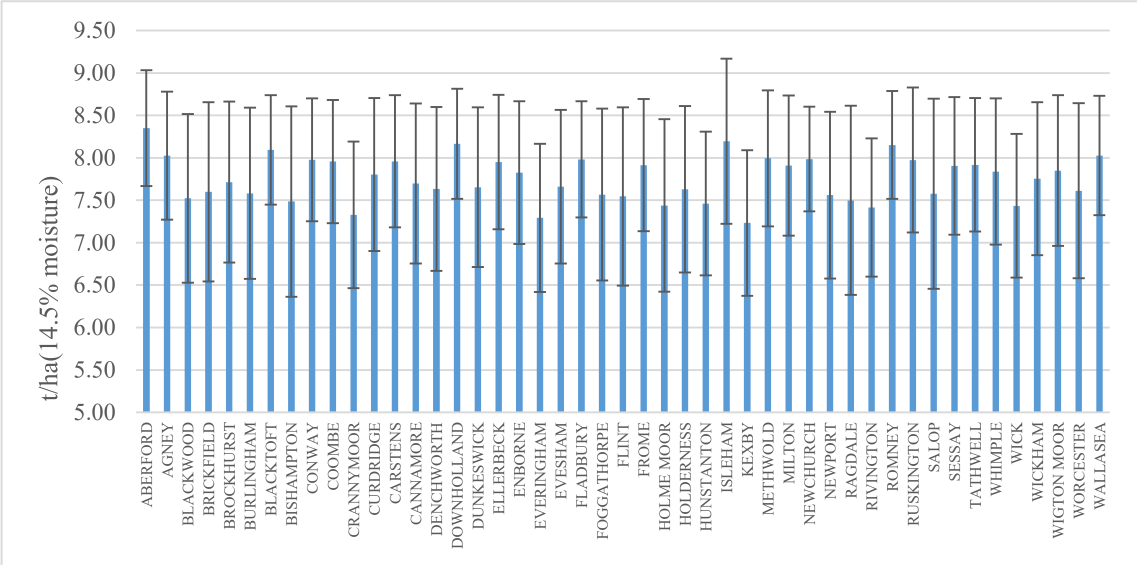

Figure 4-2 Simulated winter wheat grain yields of all the 47 soil series under BC (average value of 30 years)

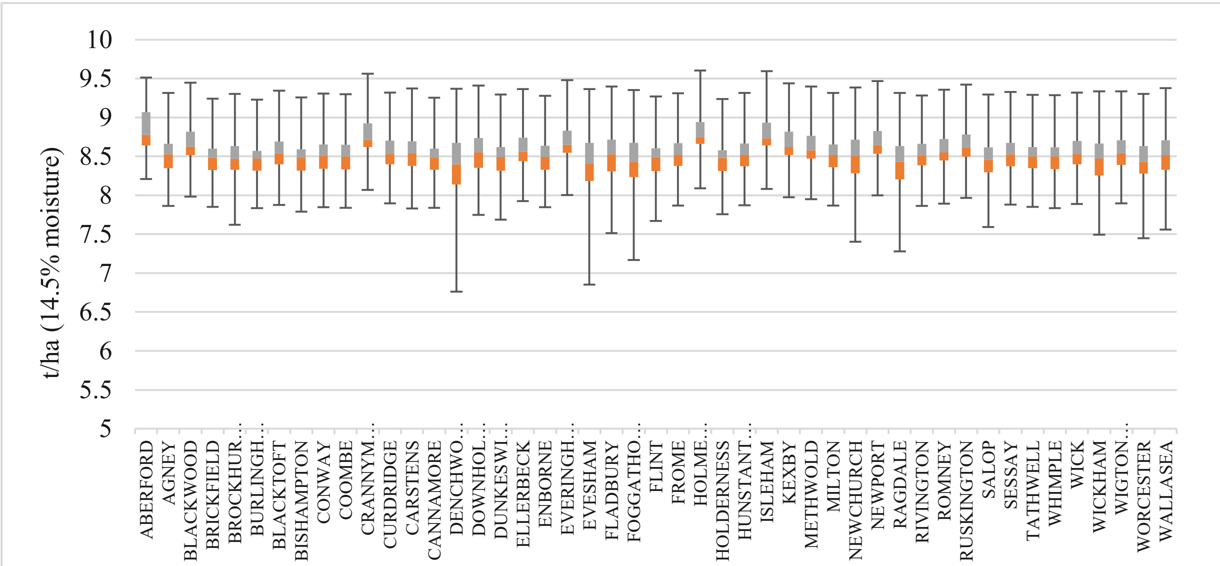

Figure 4-3 Simulated winter wheat grain yields under ME scenario; the central mark in the box is the Median, the edges of the boxes are 25th and 75th percentages, the whisker extend to the smallest and highest figure

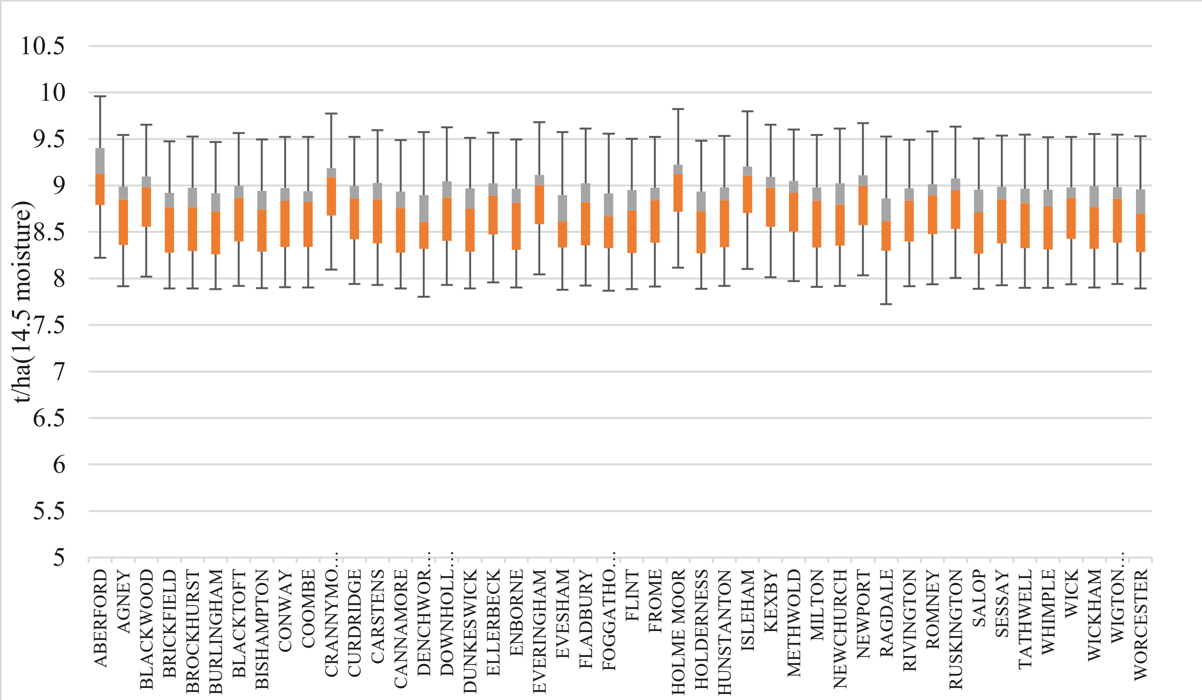

Figure 4-4 Simulated winter wheat grain yields under HE scenario; the central mark in the box is the Median, the edges of the boxes are 25th and 75th percentages, the whisker extend to the smallest and highest figure

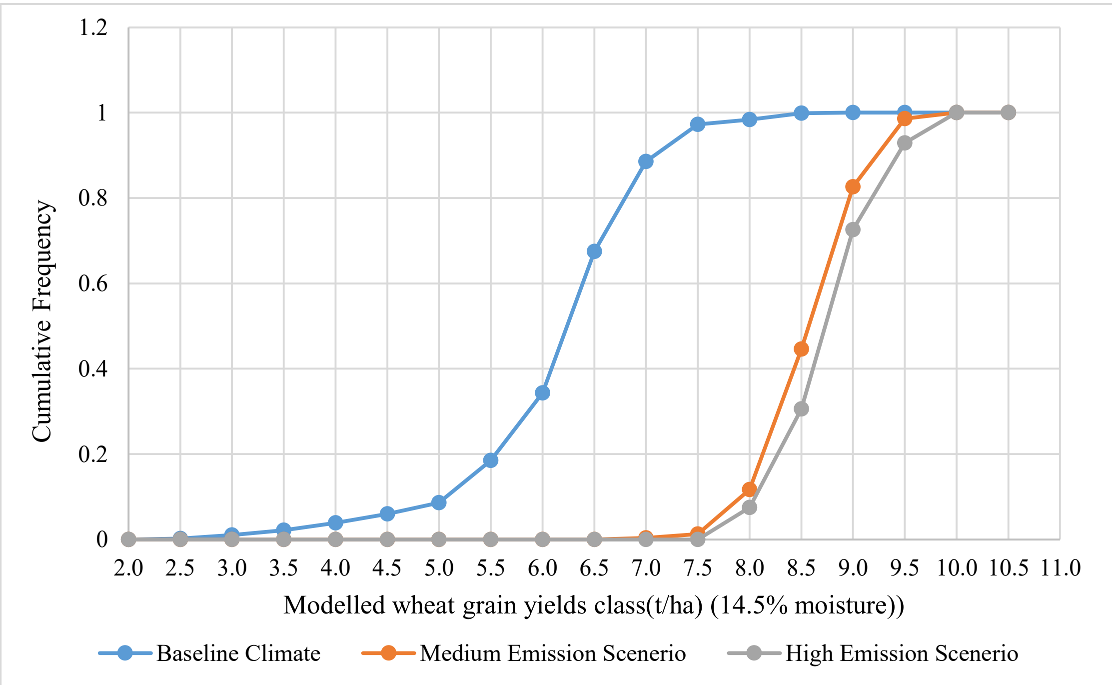

Figure 4-5 Cumulative frequency of modelled wheat grain yield under BC, ME and HE scenarios

4.3.2. Simulated *Miscanthus* yields

STAMINA simulated *Miscanthus* yields under BC, ME and HE were graphed in Figure 4-6, Figure 4-7 and Figure 4-8 respectively. As stated in methodology part, in this work, *Miscanthus* was modelled for two growing cycles. Each growing cycle consists of 15 years. *Miscanthus* is planted in the first year and reaches its full harvest yield at the third year and can be harvest once every year ever since. Under BC, *Miscanthus* yields range from 8.07 to 13.15 t/ha.yr depending on different soil series. An obvious increase on *Miscanthus* yields was also predicted by STAMINA model when atmospheric CO_2 concentration rises. The yields range from 9.15 to18.4 t/ha.yr for ME scenario and 9.71 to 18.95 t/ha.yr for HE scenario.

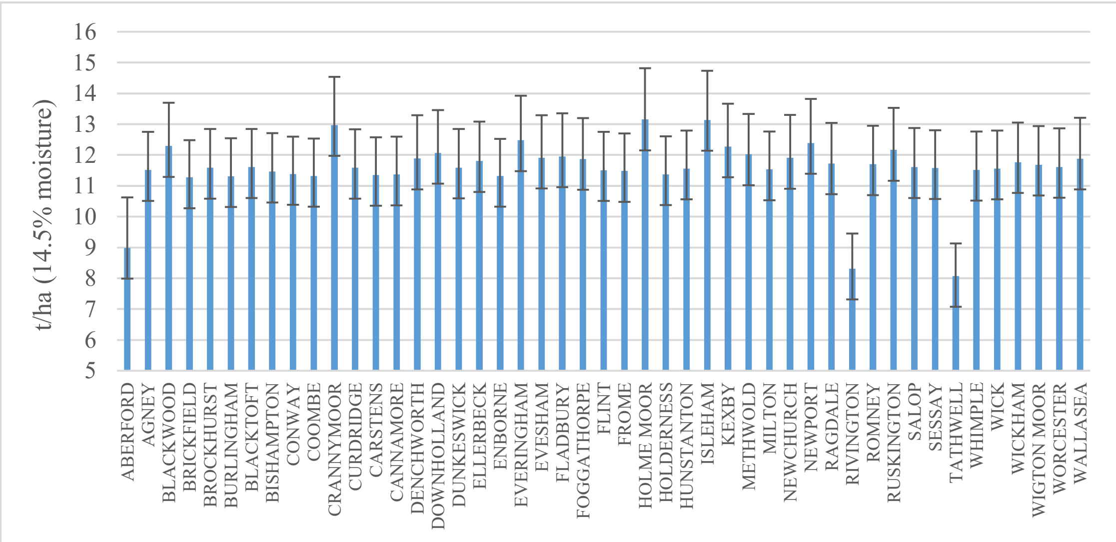

Figure 4-6 Simulated Miscanthus yields of all the 47 soil series under BC (averaged value of 30 years)

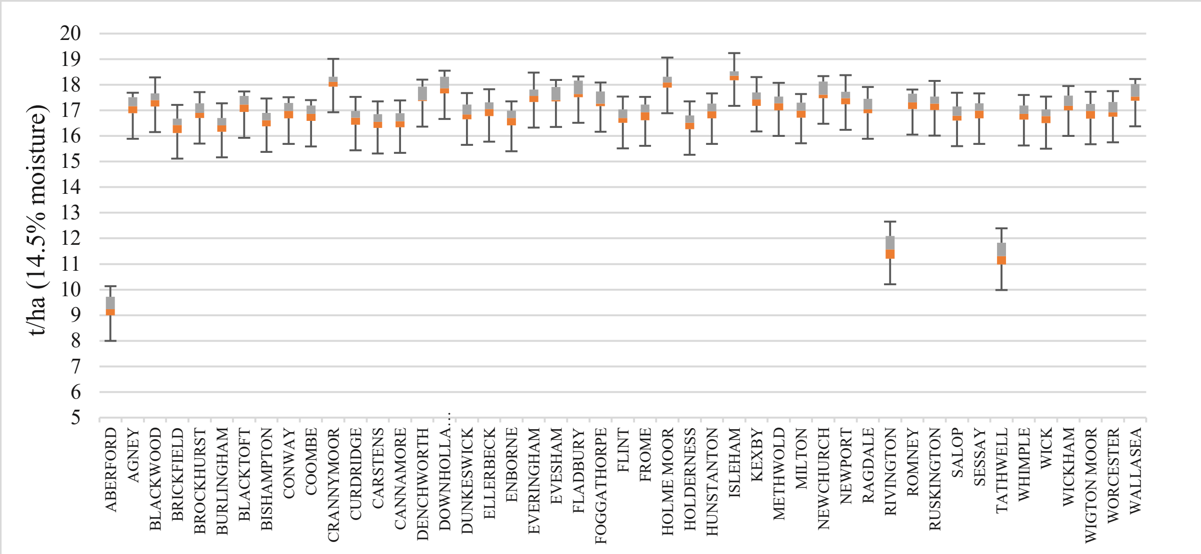

Figure 4-7 STAMINA simulated Miscanthus yields under ME scenario; the central mark in the box is the Median, the edges of the boxes are 25th and 75th percentages, the whisker extend to the smallest and highest figure.

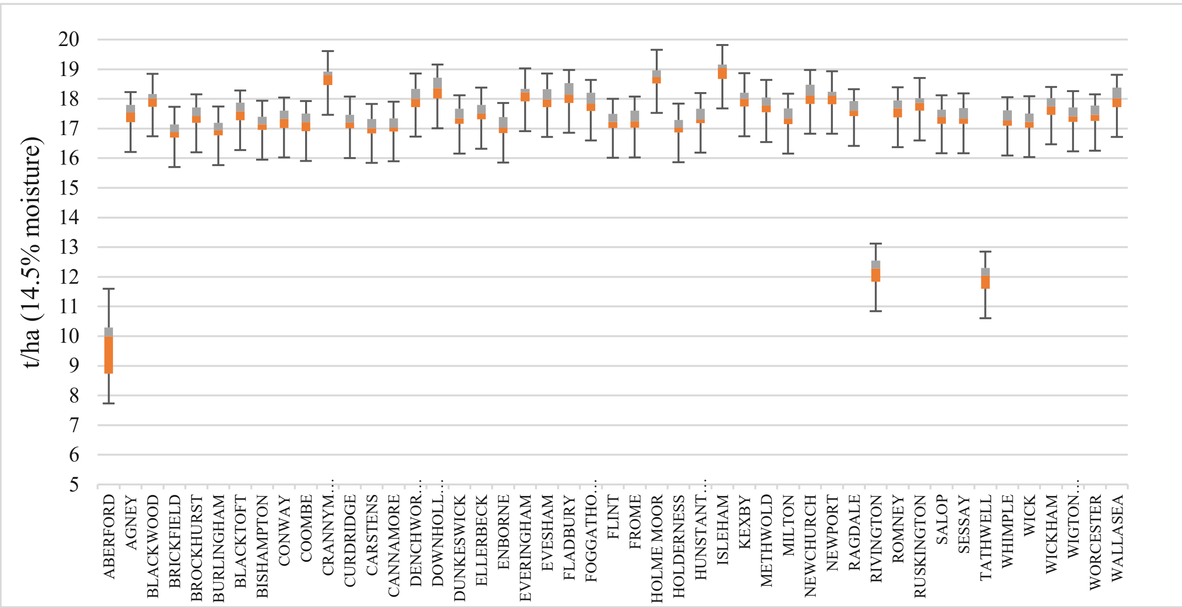

Figure 4-8 STAMINA simulated Miscanthus yields under HE scenario; the central mark in the box is the Median, the edges of the boxes are 25th and 75th percentages, the whisker extend to the smallest and highest figure

4.4. LCB provision capacities of SP and MP scenarios

4.4.1. LCB provision capacity of SP scenario

Annual straw yields calculated using Equation 1 were around 2.28 to 2.58 t/ha.yr depending on different climate scenarios. This was close to previous estimations (Glithero et al. 2013). Amounts of total harvestable straw under each provision and climate scenarios were estimated using Equation 2 and were listed in Table 4-1. This approach takes into consideration of the wheat grain production on case study area, total wheat planted area, wheat grain HI, harvestable straw fraction, straw incorporation rate and crop rotation. Total available straw which could be used as feedstock for succinic acid production were estimated by subtracting the straw demands of other uses from the total harvestable straw.

Table 4-1 Weighted average (and standard deviation) of grain and straw in catchment area

	SPBC	SPME	SPHE
Grain yield (t/ha.yr 14.5% moisture)	7.73 (0.39)	8.56 (0.12)	8.73 (0.11)
Straw yield (t/ha.yr 14.5% moisture)	2.28	2.53	2.58
Grain production (t/ha.yr 14.5% moisture)	2042.78	2262.12	2307.05
Total collectable straw (kt/yr 14.5% moisture)	603.74	668.77	681.63
Total available straw (kt/yr 14.5% moisture)	18.11	83.14	96.00

Weighted average yields calculated basing on the proportion of each soil series in total area were listed in Table 4-1. Total amount of harvestable wheat straw are estimated with Equation 1. Total collectable straw were estimated to be 603.74, 668.77 and 681.63 kt/yr for the whole case study area under baseline, medium and high emission scenarios, respectively. About 97% of the current wheat straw currently has been demanded by other users (Nelson 2002; Copeland & Turley 2008), which is 586.63 kt/yr, leaving only 18.11 kt/yr straw would be available for bio-succinic acid production. Under medium and high emission scenarios, assuming the annual demands from other uses remain stable, then the total amounts available straw would rise to 83.14 and 96.00 kt/yr respectively. It is clears that even under increased atmospheric CO_2 conditions, it would be impossible for single production scenario by winter wheat only to produce sufficient LCB feedstock, supporting commercial scale Lignocellulosic succinic acid production plant which normally requires 350kt LCB feedstock per year.

4.4.2. LCB provision capacity of Mixed Production scenario

In the MP scenario, *Miscanthus* was assumed to be planted on all those soils with loamy fine sand texture, including Crannymoor, Everingham, Holme Moor and Kexby soils. Yields for these four soil series are shown in Table 4-2. On these soil series, *Miscanthus* produces about 12 to13 t/ha.yr under baseline climate, compared to only 1.5 to 2.0 t/ha.yr of winter wheat straw becoming available. Compared with the SPBC scenario, total available LCB increases from 18.11 kt/yr to 363.37 kt/yr under MPBC. (Figure 4-9) Under the medium and higher emission climate change scenarios, *Miscanthus* annual yields on targeted soils increase to 17.86 t/ha.yr and 18.40 t/ha.yr. Consequently, the differences of total available LCB between SP and MP increase from 345.26 kt/yr (under BC) to 487.09 kt/yr (under ME) and 502.65 kt/yr (under HE) respectively (Figure 4-9).

Table 4-2 Simulated Miscanthus yield (and standard deviation) on selected loamy fine sand soils

	Total area (ha)	Yield under BC (t /ha.yr) [1]	Yield under ME (t /ha.yr) [1]	Yield under HE (t /ha.yr) [1]
CRANNYMOOR	4700	12.97	18.17	18.72
EVERINGHAM	14300	12.48	17.64	18.15
HOLME MOOR	9200	13.15	18.11	18.73
KEXBY	2000	12.28	17.52	17.99
Weighted average yield	NA	12.75	17.86	18.40
Weighted SD	NA	0.19	0.15	0.17

1. yields are in 14.5% moisture

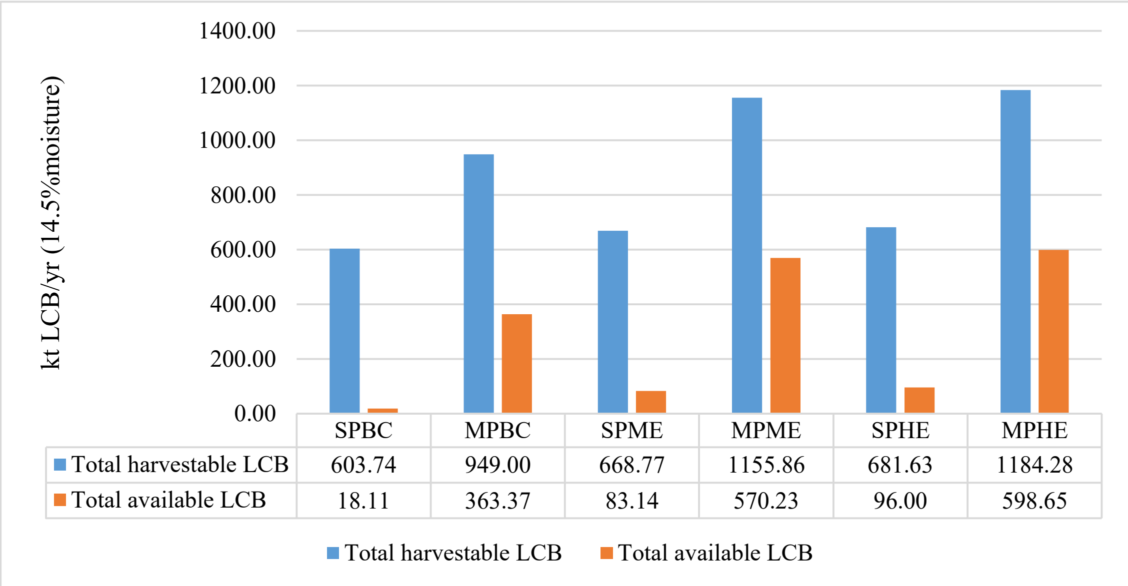

Figure 4-9 Total LCB provisions of SP and MP scenarios

4.5. Grain production of SP and MP scenarios

As MP scenarios assumed that *Miscanthus* was planted on the selected soils, reduction of grain production in MP scenarios was estimated based on the wheat grain yields simulated by STAMINA model (Table 4-3). Annual reduction of wheat grain production remained stable among the three climate conditions, approximate 115kt DM/year and accounted for 6% to 8% of the total production in SP scenarios. It is possible that the grain reduction could be compensated by enhanced effect of CO_2

fertilization and improved breeding technologies. Moreover, growing *Miscanthus* on the less productive soils for wheat cultivation might also allow better management on the rest of wheat cultivation area and increase overall grain production. While a simplified estimation on the indirect clime change impacts associated with reduced grain was included in the study and presented in in the final discussions (Chapter 8).

Table 4-3 Grain production in SP and MP scenarios

	BC	ME	HE
SP (kt/yr)(DM)	1746.28	1934.37	1971.57
MP (kt/yr)(DM)	1631.38	1783.32	1817.98
Reduction in MP (kt/yr)(DM)	114.91	151.05	153.59
Reduction percentage	6.6%	7.8%	7.8%

4.6. Summary and Discussion

4.6.1. LCB production in the context of climate change

In this work, medium and high atmospheric CO_2 climate scenarios (ME and HE) were modelled for winter wheat and *Miscanthus* growth, however both STAMINA model and UKCP only examine the impacts of altered atmospheric factors (CO_2 concentration, rainfall, temperature etc.) on winter wheat and *Miscanthus* growth, and ignoring altered pest and diseases incidence.

The impacts of climate change on agricultural production have been widely tested and considered as geographically uneven. For instance, it is predicted that CO_2 fertilisation effects would benefit food production in some of the developed countries, while the elevated temperature, water stress and expansion of arid land may severely jeopardize the agro-ecological suitablity in most of the African and South American regions. (Fischer et al. 2002) It is important to conduct regional studies with site-specific data to understand the local agricultural vulnerability under climate change conditions.

Based on simulations of projected CO_2 concentration and corresponding weather information from the UKCP, no negative impacts on wheat and *Miscanthus* yields have been seen. On the contrary, the simulation in this study predicted yields increase of 10.78% and 12.89% for wheat grain under ME and HE climate conditions restrictively. The model also predicted 40.09% and 44.36% increases for *Miscanthus* yields under ME and HE, compared with yields under BC (on target soil series).

Simulated increases on wheat productivity in this study were in accordance with most of the current researches that C3 crops show yield increases in response to rising CO_2 concentration through increased photosynthesis. (de Souza et al. 2013; Röder et al. 2014) Unlike C3 crops, the impacts of elevated CO_2 concentration on C4 crops growth remains uncertain. (de Souza et al. 2013) In theory, the increase of biomass from elevated atmospheric CO_2 concentration on C4 crops should be limited or even none. (de Souza et al. 2013) However our simulation witnessed a significant increase in *Miscanthus* biomass production under tested climate change scenarios. This can be explained by the increased temperature (48.71% and 46.67% higher average hourly temperature), higher average humidity (13.91% and 14.21% higher humidity) and slightly higher annual precipitation level (2.51% and 2.56% higher annual rainfall) projected by UKCP compared with the BC. It has been well discussed that *Miscanthus* growth in Northern Europe is mainly constrained by the cold temperature from reaching its potential yields. (Kandel et al. 2016; Lewandowski et al. 2000)

However the differences between ME and HE for both wheat grain and *Miscanthus* production were not significant. A yield increase of 1.99% was predicted compering wheat grain yields under SPHE with SPME, while for *Miscanthus* this figure was 3.0%. It is probably due to that for the prediction period, the increase of atmospheric CO_2 concentration from ME to HE was quite small (2ppm), thus the impacts of elevated atmospheric CO_2 concentration and other altered correlative climate parameters on crop growth were limited.

4.6.2. Summary

This chapter presented the availably assessment results of LCB and wheat grain production in both SP and MP production scenarios. It is impossible for the establishment of the hypothetical LCB-based SA plant in the case study area with under SP scenarios, even under HE climate condition, when the available LCB as estimated to be 83.14 kt/yr. While with the 8% selected fine sandy loam soils converted from wheat production to *Miscanthus* cultivation, available LCB supply was estimated to be 363.37 kt/yr under MPBC, 570.23 kt/yr under MPME and 598.65 kt/yr under MPHE, which are expected to be sufficient to support one to two commercial scale lignocellulosic biofuel or biomaterial plants.

Comparing the estimated total available LCB of SP and MP under different climate change scenarios, it is clear that although both LCB increase as the CO_2 concentration elevated and the other climate factors altered correspondingly, the proposed MP scenarios benefits significantly more than SP scenarios. The strong CO_2 fertilisation effect on LCB production predicted in this casestudy area, especially on *Miscanthus* growth further indicates the potential opportunity of introducing *Miscanthus* into the current arable landscape to increase LCB provision on per hectare land. As recognised by Fischer et al. (2002) that response to climate change is not only about measuring and reducing the impacts and risks, but also requires strategies to maximise the possible benefits and opportunities of climate change.

Due to the lack of information on current straw production and uses, a conservative estimation of winter wheat straw provision potential was adopted in this work. Although it has been suggested that straw which was used for animal bedding could be used locally for soil incorporation after (serving as farmyard manure), then the amount of the incorporated straw could be reduced substantially and more straw could become available for bioenergy and material production. However, this is considered less possible based on current records that the large volume of straw used for animal bedding was moved from the eastern counties of England to the south west of Wales or Scotland to meet the market demands of the livestock sector, (Copeland & Turley 2008) rather than being used in locally.

Chapter 5. NO_3^- leaching and N_2O emissions under SPBC and MPBC production scenarios

5.1. Introduction

Actuate estimates of GHG emissions and resource efficiency are important in understanding and determining the sustainability of production of bioenergy and bio-based chemicals. LCA of bio-refinery production chains are often constrained by the lack of information on pre-harvest GHG balance related to agricultural management, especially on fertiliser application related N_2O emission and carbon storage change.

In this chapter, process-based model generated results on nitrogen emission and NO_3^- leaching are presented and discussed.

N_2O is emitted from agricultural systems to atmosphere through both direct and indirect pathways. Direct N_2O refers to N_2O emitted through microbial nitrification and denitrification of fertiliser and manure nitrogen that remains in agricultural soils. Indirect N_2O is produced from nitrogen that is removed from agricultural soils via volatilization, leaching, runoff, or harvest of crop biomass. Same as their direct counterparts, the long-term fate of agricultural nitrogen also eventually provides substrate for microbial nitrification and denitrification, with associated N_2O production. Both direct and indirect N_2O are taken into account in this work.

5.2. N_2O emissions from SP and MP production

5.2.1. DNDC model calibration and evaluation

In DNDC, N_2O emissions were determined based on denitrification and nitrification pathways as a function of climate, crop growth and soil environmental factors. DNDC has been parameterized for winter wheat under UK condition already by Wattenbach et al. in 2010. (Wattenbach et al. 2010) In this study, its performance for simulation winter wheat under UK conditions were further evaluated using site specific data across England as described in Chapter3. Comparison between modelled and measured yields is shown in Figure 5-1. Modelled yields compare quite well with observations, considering the average values (8.64 and 8.65 t/ha respectively) and statistics (RMSE of 1.02 t/ha and MBE% of 12%).

Miscanthus parameters in the DNDC model have been parameterized and tested earlier in 2011.(Gopalakrishnan et al. 2012) This study evaluated these parameters using measured *Miscanthus* DMYs from 1997 to 2004 in the Rothamsted 408 trial (Richter et al. 2008), for the model to be used under UK condition confidently. The simulated and observed DMYs are graphed in Figure 5-1, with RMSE of 1.57 t/ha, and MBE % of 11%.

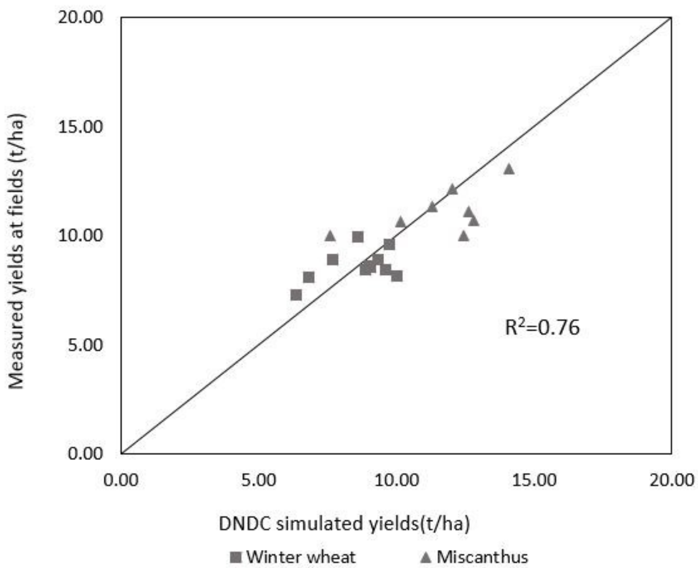

Figure 5-1 DNDC model evaluation results for winter wheat and Miscanthus

5.2.2. Nitrogen dynamics of winter wheat production

This section presents the DNDC simulated results for winter wheat production in whole case study area from 1986-1994, assuming straw were left on soil once every three years to maintain soil quality as a reflection of the reality. Results (Table 5-1) suggest significant variation in gas (Figure 5-3) and liquid (Figure 5-4) efflux from different soil types.

As shown in Figure 5-2, DNDC model simulates nitrogen cycles by several submodels, including, Soil Climate, Plant Growth, Decomposition, Denitrification and nitrification submodels. Nitrogen inputs include fertiliser (synthetic nitrogen fertilisers and manure) application, atmospheric deposition and decomposition of soil organic matter. Losses from the ecosystem are by leaching and runoff of dissolved nitrogen, erosional loss, gaseous losses from ammonia volatilization and both nitrification and denitrification, and removal of nitrogen in plant tissues at harvest. (Li et al. 2001)

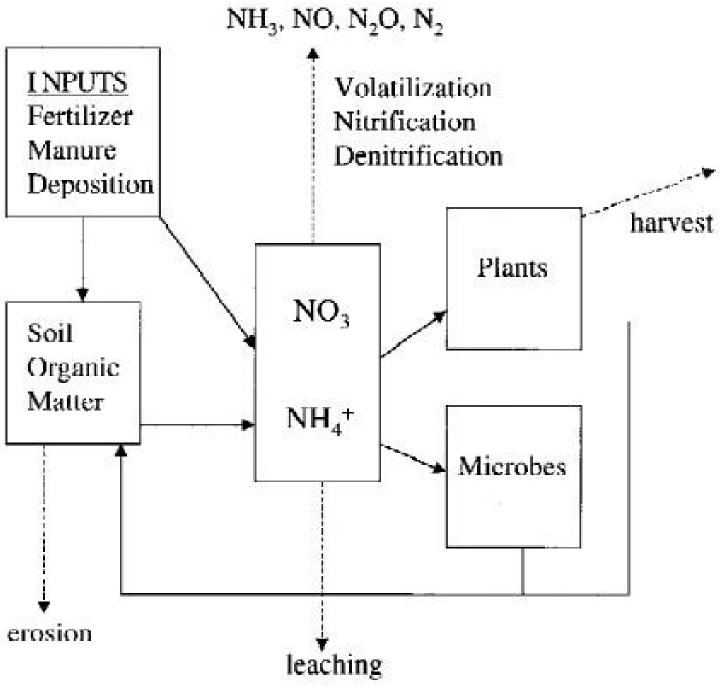

Figure 5-2 A schematic representation of the nitrogen cycle in agro-ecosystem as captured in DNDC (Li et al. 2001)

Table 5-1 8-year average nitrogen dynamics of winter wheat cultivation of each soil type and whole case study area; most soil types contain more than one soil series, thus weighted average values and weighted SD were reported, according to area size; figures for whole area were weighted average figures generated with area sizes of each soil series；indirect N_2O *emission are estimated based on* NO_3^- *leaching amount and EF5 in 2006-AFOLU , Emission Factor for Nitrogen leaching and runoff;*

		Clay	**Clay loam**	**Loam**	**Loamy fine sandy**	**Sandy clay loam**	**Sandy loam**	**Silt loam**	**Silty clay**	**Silty clay loam**	**Whole area**
Direct N_2O	kgN/ha.yr	1.36	0.96	0.68	0.45	0.72	0.37	0.27	0.99	0.53	0.71
	SD	0.22	0.23	0.12	0.12	0.00	0.06	0.05	0.17	0.20	0.08
NO	kgN/ha.yr	0.87	0.80	0.69	0.37	0.65	0.41	0.40	0.72	0.53	0.62
	SD	0.13	0.14	0.07	0.05	0.00	0.04	0.04	0.13	0.13	0.04
N_2	kgN/ha.yr	0.03	0.01	0.00	0.05	0.00	0.02	0.04	0.04	0.02	0.02
	SD	0.01	0.00	0.00	0.01	0.00	0.00	0.01	0.01	0.01	0.00
NH_3	kgN/ha.yr	0.10	0.06	0.03	0.02	0.03	0.02	0.13	0.13	0.23	0.07
	SD	0.07	0.03	0.01	0.01	0.00	0.01	0.02	0.03	0.06	0.02
NO_3^-	kgN/ha.yr	19.90	58.66	71.88	131.03	109.03	95.69	73.00	23.10	39.77	66.03
	SD	5.36	3.38	1.94	8.57	0.00	3.20	0.69	0.88	3.17	5.97
Indirect N_2O	kgN/ha.yr	0.15	0.44	0.54	0.98	0.82	0.72	0.55	0.17	0.30	0.50
	SD	0.04	0.03	0.01	0.06	0.00	0.02	0.01	0.01	0.02	0.04
Leaching rate	$kgNO_3^-/kgN$ input	9.05%	26.66%	32.67%	81.89%	49.56%	54.14%	37.51%	10.50%	20.01%	34.01%
	SD	2.43E-02	1.54E-02	8.80E-03	5.36E-02	0.00E+00	4.41E-02	1.33E-02	3.98E-03	1.78E-02	3.79E-02
Direct N_2O	kgN/kg grain (DMY)	1.57E-04	1.25E-04	9.91E-05	1.32E-04	1.07E-04	8.86E-05	4.54E-05	1.16E-04	6.87E-05	1.05E-04
	SD	2.57E-05	2.96E-05	1.72E-05	3.34E-05	0.00E+00	1.30E-05	1.60E-05	4.20E-05	2.52E-05	8.98E-06
NO_3^-	kgN/kg grain (DMY)	2.31E-03	7.88E-03	1.07E-02	3.97E-02	1.69E-02	2.45E-02	1.33E-02	2.71E-03	5.35E-03	1.30E-02
	SD	6.33E-04	5.06E-04	2.55E-04	2.01E-03	0.00E+00	2.63E-03	9.24E-04	2.16E-04	4.21E-04	1.98E-03
Indirect N_2O	kgN/kg grain (DMY)	1.73E-05	5.91E-05	8.00E-05	2.98E-04	1.27E-04	1.84E-04	9.97E-05	2.04E-05	4.01E-05	9.77E-05
	SD	4.75E-06	3.80E-06	1.91E-06	1.51E-05	0.00E+00	1.98E-05	6.93E-06	1.62E-06	3.16E-06	1.49E-05

a. All the SD for Sandy clay loam soil is 0 is due to that there is only one soils series falls into this soil category.

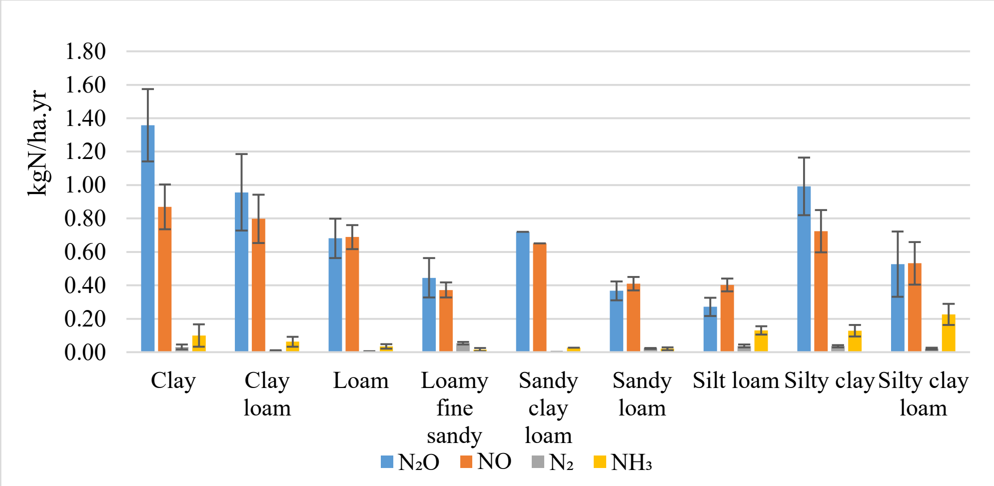

Figure 5-3 Average NH_3, NO, direct N_2O, N_2 emissions from winter wheat cultivation per hectare during 1986 to 1994, grouped by soil types.

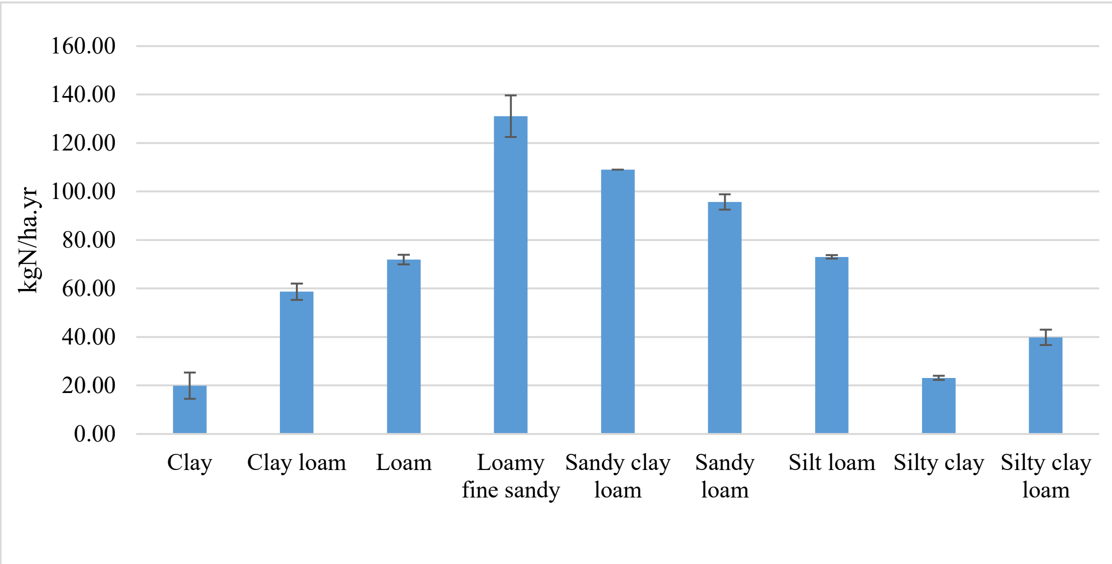

Figure 5-4 Average NO_3^- leaching from winter wheat cultivation per hectare during 1986 to 1994, grouped by soil types

Figure 5-3 and Figure 5-4 give an overview of nitrogen losses of through NH_3, NO, direct N_2O, N_2 emissions and NO_3^- leaching of winter wheat cultivation. It can be also seen from Table 5-1, NO_3^- leaching and N_2O emissions are the two dominating sources of nitrogen losses. Although nitrogen can also be lost through NH_3, NO and N_2, their volumes are relatively small and are not considered as GHGs, thus the dynamics related to NH_3, NO and N_2 are not reported or discussed in this work.

5.2.2.1 NO_3^- leaching of winter wheat cultivation

NO_3^- leaching amount is important to N fertiliser use efficiency and a caused of indirect N_2O emissions. Depending on soil types, the 8-year average NO_3^- leaching amount is between 19 to 131 kgN/ha.yr (Table 5-1). Average NO_3^- leaching rates (NO_3^- leaching amount/N fertiliser input) for different soil types range between 3.89% and 90.61%; weighted average figures by soil types are shown in Table 5−1. In whole case study area, weighted average leaching amount is 66.03 kgN/ha and the corresponding leaching rate is 34.01%. This result is in accordance with the 2006-AFOLU Tier 1 empirical methodology for FracLEACH-(H) [N losses by leaching/runoff for regions], where suggests the rate of nitrogen loss by leaching/run off as 30%, with an uncertainty range of 10% to 80%. (Intergovernmental Panel on Climate Change 2006b)

Although NO_3^- leaching amount varies highly among different soil types, NO_3^-leaching event is always sensitive to the timing of rainfall and nitrogen fertiliser application. Daily NO_3^- leaching flux over the winter wheat crop cycle of year 1986 to 1987 was selected as an example and graphed in Figure 5-5. The red arrows are the day of nitrogen fertiliser application. Figure 5-6 shows the annual NO_3^- leaching level and accumulative annual precipitation amounts from year 1987 to 1994. It can be seen that the largest leaching always occurs soon after fertiliser application events.

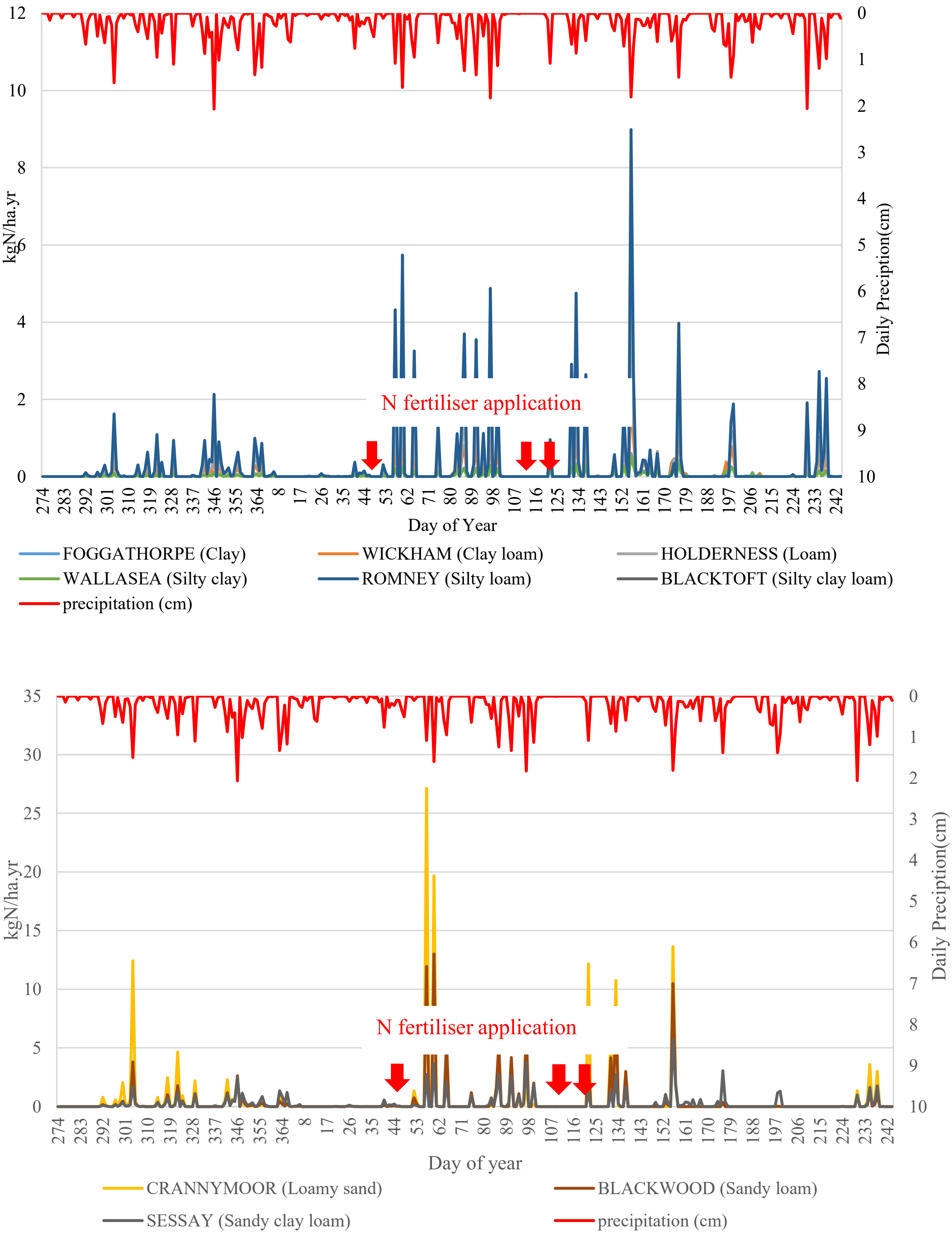

Figure 5-5 Daily NO_3^- leaching flux over winter wheat crop cycle (1986-1987) for different soil types; blank control values were not excluded in these two figures

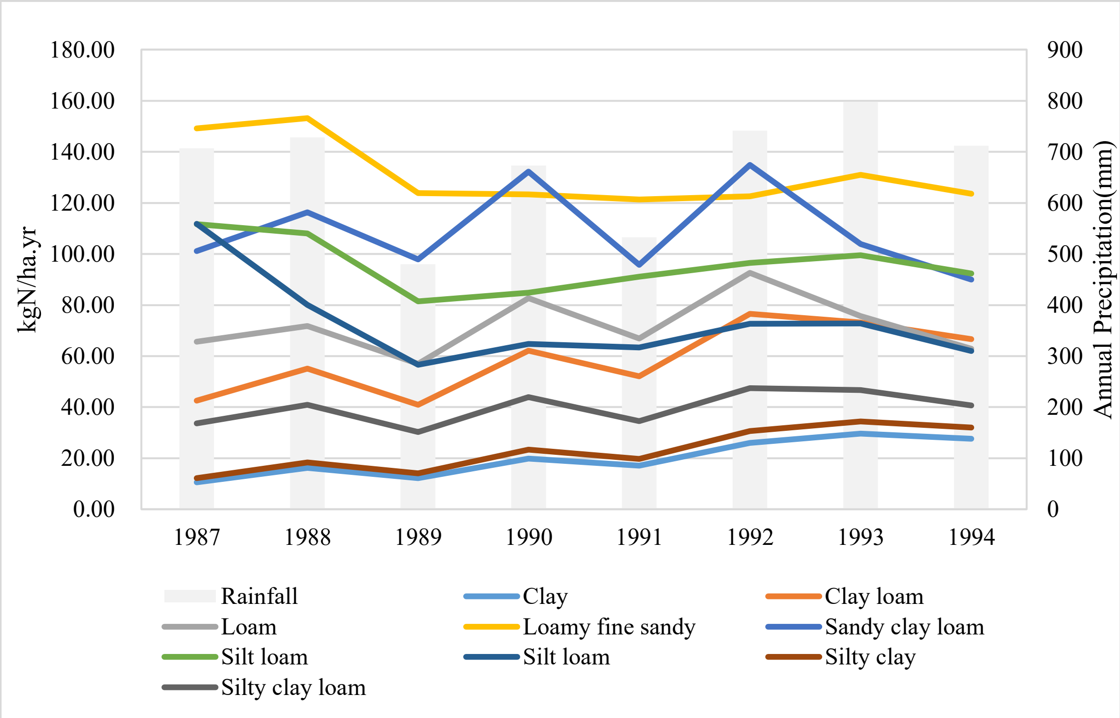

Figure 5-6 Annual N leaching and annual precipitation level from 1986 to 1994, grouped by soil types

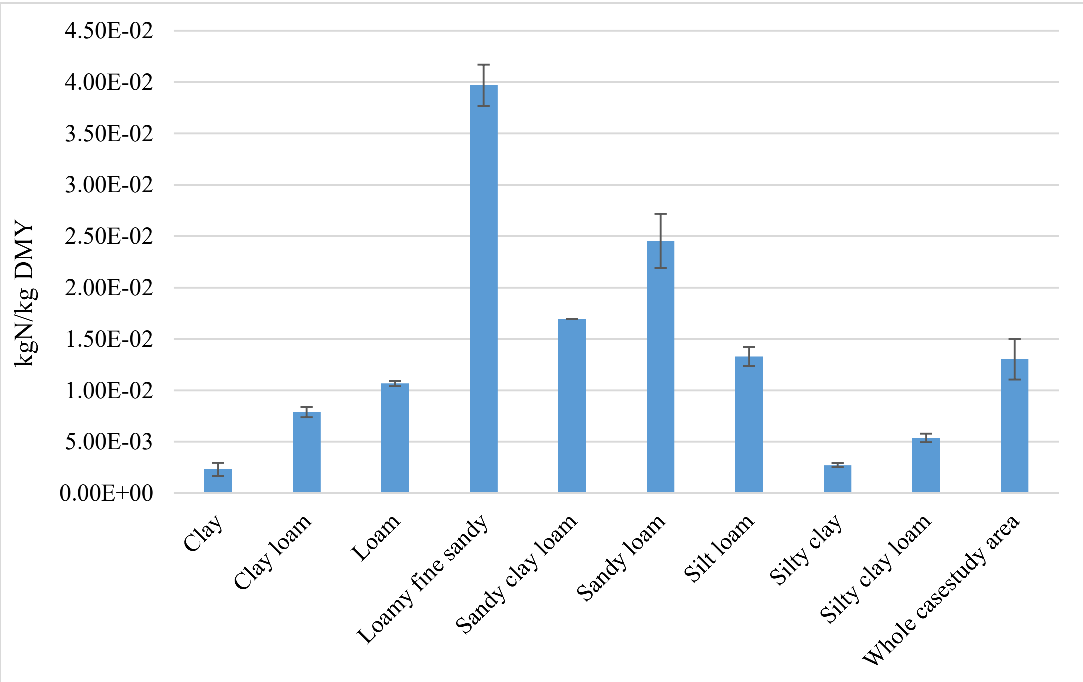

Figure 5-7 NO_3^- leaching for per kg DMY grain produced (kgN/kg grain) for each soil types and across whole case study area

Direct outputs of DNDC model are for per hectare field, figures for NO_3^- leaching, direct N_2O and indirect N_2O for per kg winter wheat grain were produced for different soil types and for the whole case study area as well, based on modelled DMY (Table 5-1). Those figures were grouped by soil types (Table 5-1) and graphed in Figure 5-7. Weighted average value for NO_3^- leaching for the whole case study area is 0.0013kgN/kg grain.

Among all the soil types, wheat cultivation on loamy fine sandy soils results in the highest NO_3^- loss for per unit grain produced, as a combined result of both high NO_3^- leaching amount (131.03 kgN/ha.yr) and low grain yields (weighted average value of 3366 kg/ha.yr, SD = 66.58 kg/ha.yr). There are four soil series fall into the loamy fine sand soil category, including Crannymoor, Everingham, Holme Moor and Kexby. Those four soil series cover a total area of 302km^2, 7.6% of whole case study area. NO_3^- leaching on those soils accounts for 16% of total NO_3^- loss, while only produce 2.4% of total wheat grain.

5.2.2.2 N_2O emission of winter wheat cultivation

Direct N_2O is one of the main outputs simulated by DNDC model. It is emitted from agricultural soils as a result of nitrification and denitrification processes arises predominantly from nitrogen fertilisers applied to the field. N_2O efflux is subject to rainfall, irrigation and nitrogen fertiliser application. Similar to NO_3^- leaching, daily direct N_2O effluxes are graphed in Figure 5-8, indicating that the peaks in N_2O emission effluxes are highly related to the nitrogen fertiliser application events. Figure 5-9 graphs the annual precipitation level and N_2O emissions of differenced soil types, showing that direct 2O losses are highly influenced by annual precipitation; in those years with higher rainfall, direct N_2O emissions are always higher.

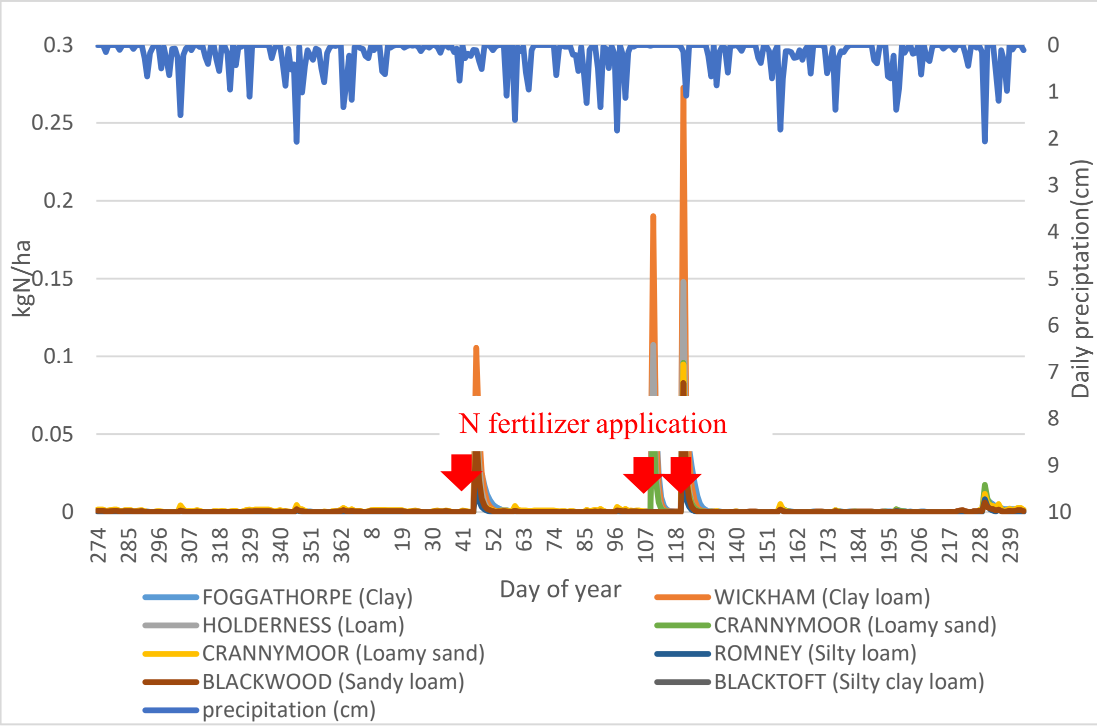

Figure 5-8 Daily N_2O Flux and precipitation over winter wheat crop cycle (1986-1987)

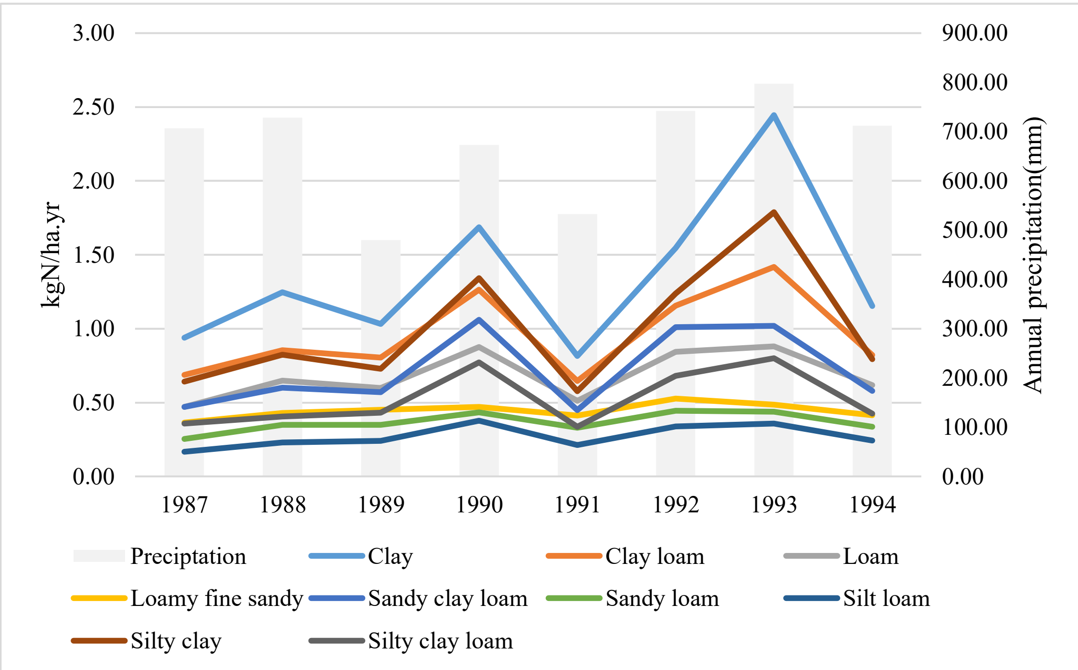

Figure 5-9 Annual N_2O emission and annual precipitation level from 1987 to 1994

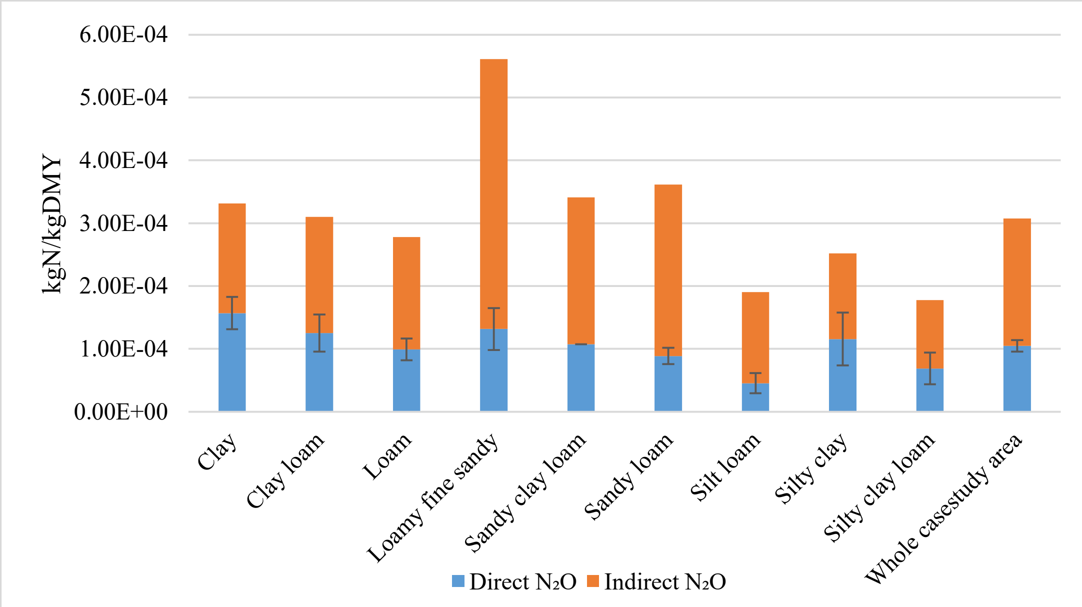

Figure 5-10 Direct and indirect N_2O emissions for per kg DMY grain produced (kgN/kg grain) for each soil types and across whole case study area; Error bars are for Standard Deviations of direct N_2O emission.

Both direct and indirect N_2O emissions for per kg grain production are graphed in Figure 5-10. For direct N_2O emissions, Clay soils have the highest NO_2/wheat grain ratio production (1.57×10^{-4} kgN/kgDMY, SD= 2.57×10^{-5} kgN/kgDMY), slightly(18%) higher than those on loamy fine sandy soils (1.32×10^{-4} kgN/kgDMY, SD= 3.34×10^{-5} kgN/kgDMY). When indirect N_2O emissions from NO_3^- leaching are accounted together, loamy find sandy soil still turns into the biggest N_2O efflux soil type, accounting for 15.02% of total N_2O flux in whole case study area.

5.2.3. NO_3^- and N_2O dynamics of MP scenario

In MP scenario, *Miscanthus* was assumed to be planted on all those soils with loamy fine sand texture. For those soils, simulated winter wheat yields are much lower than on the other soils while the nitrogen losses through leaching and N_2O emission are substantially higher than finer textured soils as indicated in Figure 5-6 and Figure 5-9.

Similar to winter wheat cultivation, daily N_2O and NO_3^- efflux were influenced by the timing of nitrogen fertiliser application and daily precipitation amounts. Using year

1989 and soil Crannymoor as an example (Figure 5-11), peaks of N_2O and NO_3^- efflux always occurs soon after nitrogen fertiliser application and heavy precipitation events.

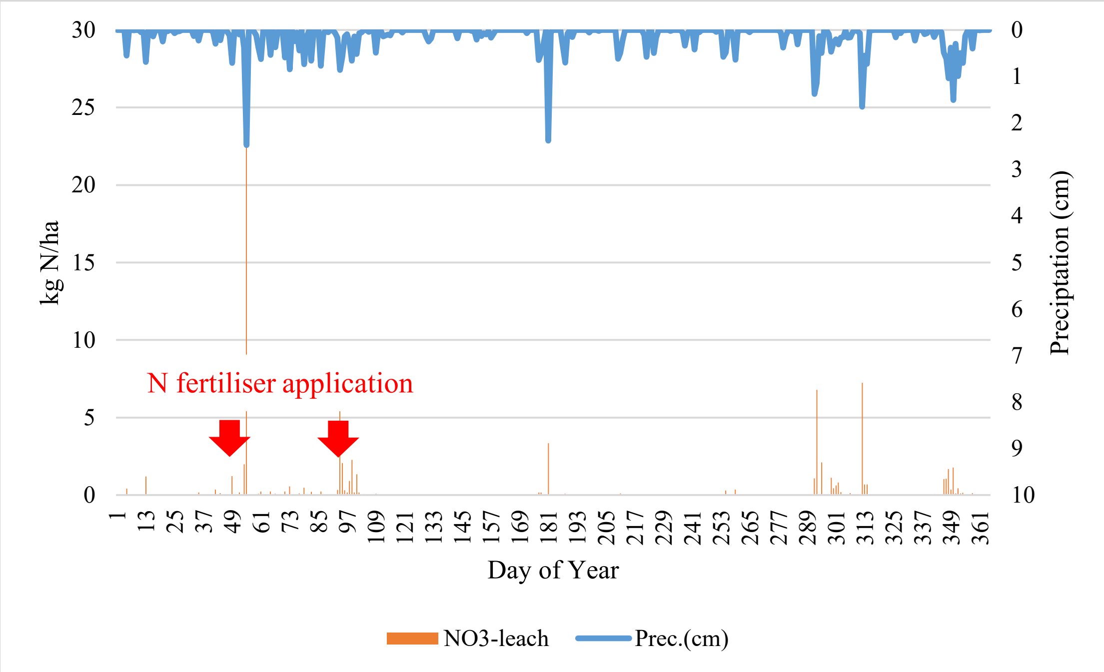

Figure 5-11Daily NO_3^- leaching from Miscanthus cultivation on soil Crannymoor and daily precipitation of year 1989; red arrow represents the date of N fertiliser application

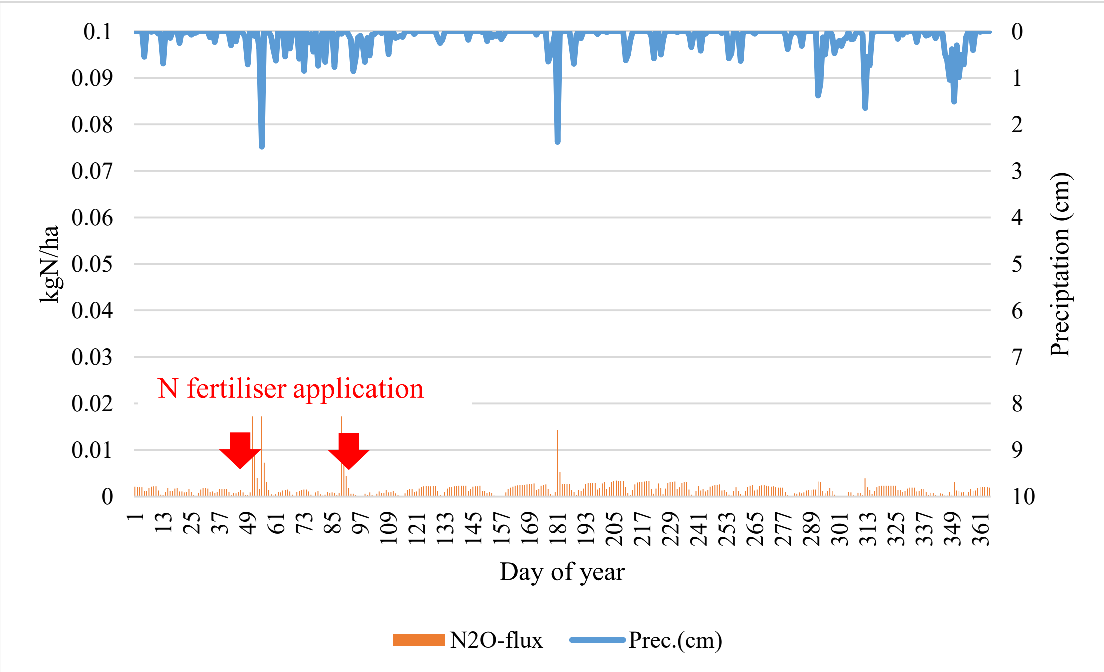

Figure 5-12 Daily N_2O emission from Miscanthus cultivation on soil Crannymoor and daily precipitation of year 1989; red arrow represents the date of N fertiliser application

On these four soils, *Miscanthus* produces about 12-13t/ha based on STAMINA model outputs, compared to only 1.5 to 2.0 t/ha of winter wheat straw were available on the same area. 8-year average NO_3^- leaching and N_2O emission are shown on Table 5-2. Comparison between *Miscanthus* and winter wheat growth were graphed in Figure 5-13 to Figure 5-15.

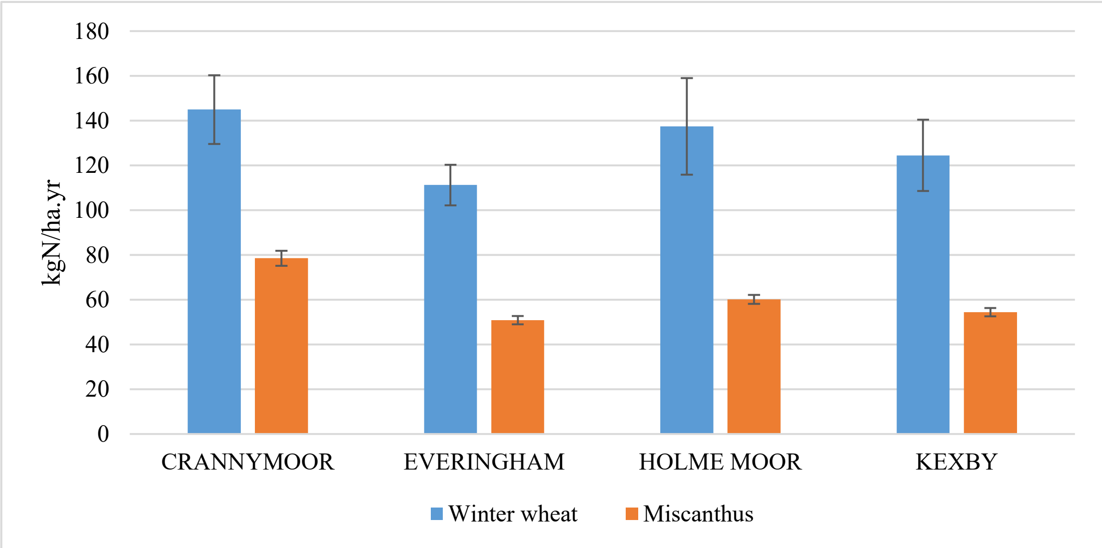

Figure 5-13 Comparison of NO_3^- leahcing from Miscanthus and Winter wheat cultivation on four loamy fine sand soils

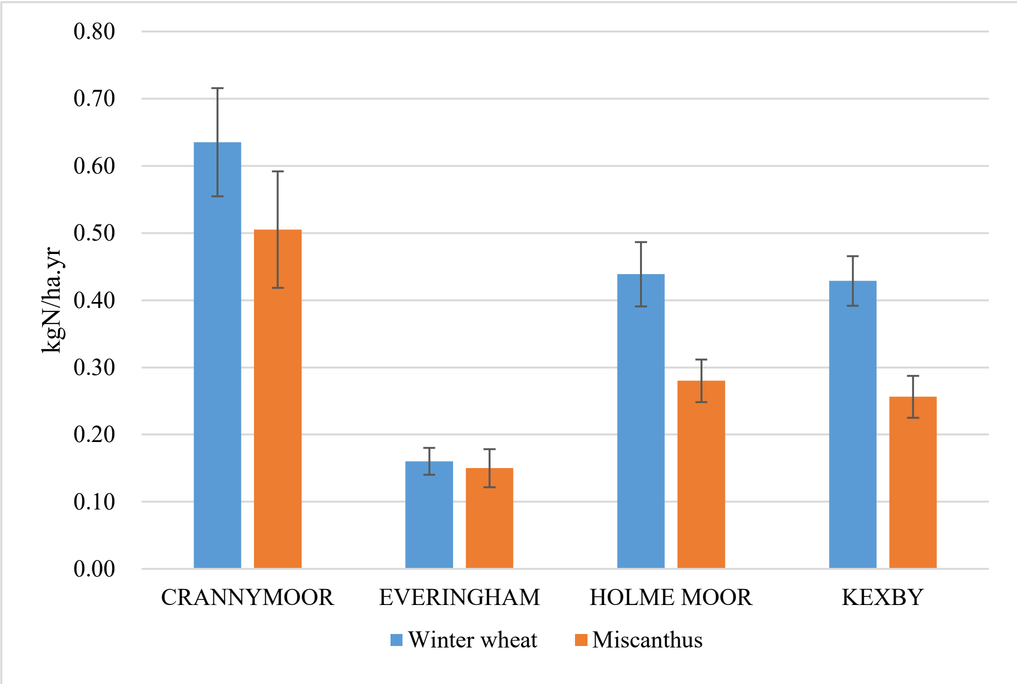

Figure 5-14 Comparison of direct N_2O emission from Miscanthus and Winter wheat cultivation on four loamy fine sand soils

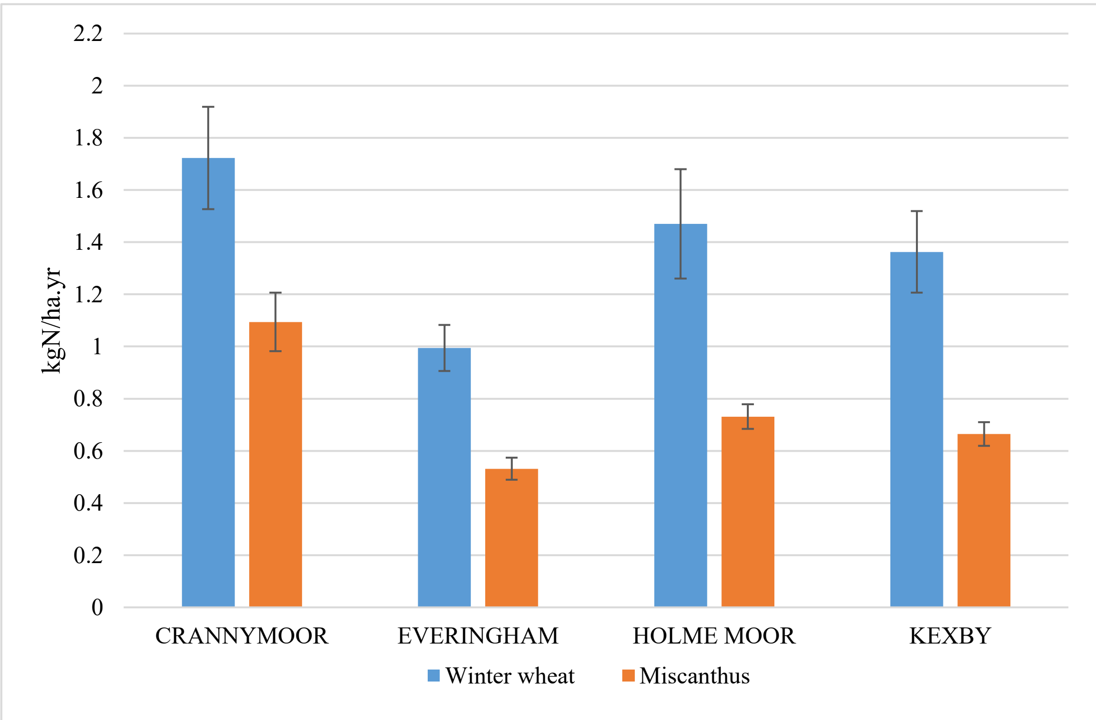

Figure 5-15 Comparison of total N_2O emission from Miscanthus and Winter wheat cultivation on four loamy fine sand soils

Table 5-2 8 years average value (and SD) of NO_3^- leaching, direct N_2O and indirect N_2O emissions of Miscanthus and winter wheat cultivation on four loamy fine sand soils.

			Leaching NO_3^-		Direct N_2O flux		Indirect N_2O	
			kgN/ha.yr	kgN/ kgDMY	kgN/ha.yr	kgN/ kgDMY	kgN/ha.yr	kgN/ kgDMY
CRANNYMOOR	*Miscanthus*	Mean	78.54	7.26E-03	0.51	4.65E-05	0.59	5.45E-05
		SD	3.36	1.73E-03	0.09	1.30E-05	0.03	1.30E-05
	Wheat grain	Mean	144.98	4.25E-02	0.64	1.83E-04	1.09	3.19E-04
		SD	15.41	8.42E-03	0.08	1.64E-05	0.12	6.31E-05
EVERINGHAM	*Miscanthus*	Mean	50.87	4.62E-03	0.15	1.36E-05	0.38	3.46E-05
		SD	1.91	1.02E-03	0.03	4.00E-06	0.01	7.62E-06
	Wheat grain	Mean	111.27	3.47E-02	0.16	4.90E-05	0.83	2.60E-04
		SD	9.07	6.76E-03	0.02	3.71E-06	0.07	5.07E-05
HOLME MOOR	*Miscanthus*	Mean	60.16	5.72E-03	0.28	2.69E-05	0.45	4.29E-05
		SD	2.04	1.27E-03	0.03	7.88E-06	0.02	9.54E-06
	Wheat grain	Mean	137.46	4.33E-02	0.44	1.37E-04	1.03	3.25E-04
		SD	21.57	9.49E-03	0.05	1.82E-05	0.16	7.12E-05
KEXBY	*Miscanthus*	Mean	54.40	5.04E-03	0.26	2.40E-05	0.41	3.78E-05
		SD	1.89	1.10E-03	0.03	6.93E-06	0.01	8.28E-06
	Wheat grain	Mean	124.52	3.94E-02	0.43	1.35E-04	0.93	2.95E-04
		SD	15.95	7.93E-03	0.04	1.75E-05	0.12	5.95E-05
Loamy find sand soil	*Miscanthus*	Mean	58.24	5.39E-03	0.25	2.35E-05	0.44	4.04E-05
		SD	5.54	5.39E-04	0.07	6.65E-06	0.04	4.04E-06
	Wheat grain	Mean	125.37	3.89E-02	0.34	1.02E-04	0.94	0.00E+00
		SD	8.14	2.33E-03	0.10	3.05E-05	0.06	1.69E-04

For per hectare land, NO_3^- leaching amount from *Miscanthus* cultivation ranges from 50.87 to 78.54 kgN/ha.yr, approximately half of the amounts that leached from winter wheat cultivation on the same soil series (Figure 5-13). Similar to winter wheat cultivation, the NO_3^- leaching rates of *Miscanthus* cultivation on loamy fine sandy soils were also high. Especially in the first year, the NO_3^- leaching amounts were even higher than the nitrogen inputs level. This is probably due to the low biomass productivity level of *Miscanthus* during the first year. Weighted average value for whole loamy fine sand soil category calculated to be 58.24 kgN/ha.yr for *Miscanthus* and 125.37 kgN/ha.yr for winter wheat. Direct N_2O fluxes of *Miscanthus* are also lower compared with winter wheat cultivation (Figure 5-13), 0.25 kgN/ha.yr for *Miscanthus* and 0.34 kgN/ha.yr for winter wheat.

When the figures were converted to kgN for per kg DMY production, the difference between *Miscanthus* and wheat yields become much bigger. For per kg *Miscanthus* DMY produced on loamy fine sand soils, 5.39 x 10^{-3}kgN will be lost through NO_3^- and 2.35 x 10^{-5}kg N emitted as direct N_2O, comparing to 3.89 x 10^{-2} kgN and 1.02 x 10^{-4} kgN for wheat grain respectively. Total direct and indirect N_2O emissions for per kg DMY *Miscanthus* is 6.39 x 10^{-5} kgN/kgDMY, less than ten times of the figure for wheat grain (1.02 x 10^{-4} kgN/kgDMY).

Across whole case-study area, when loamy fine sand soils are planted with *Miscanthus*, annual NO_3^- leaching dropped by 8.8% from 66.03 to 60.71kgN/ha.yr; annual total N_2O emissions dropped by 1.04% from 1.20 to 1.15 kgN/ha.yr. Thus, for the whole case study region with total area size of 396,400 ha, annual NO_3- leaching will be reduced by 2.11 kt N, annual N_2O emission reduced by 19.82 tN (2953 tCO_2eq).

5.3. Summary and discussion

5.3.1. Estimation of indirect N_2O emission based on IPCC 2006-AFOLU emission factors

Due to that DNDC only covers the estimation of NO_3^- leaching/run-off and direct N_2O emission of crops cultivation, EF5 in 2006-AFOLU was adopted to estimate indirect N_2O emission. Indirect N_2O emission accounts for one third of the total global agricultural N_2O source and leaching related N_2O accounts for more than 75% of total indirect N_2O emissions. As stated in IPCC Good Practice Guidance and Uncertainty Management in National Greenhouse Gas Inventories Indirect N_2O (Intergovernmental Panel on Climate Change 1998), indirect N_2O emissions account for 'inappropriate share of uncertainty' among all the N_2O sources.

According to IPCC (2006b), uncertainties of estimating leaching related N_2O emission come from three major areas. Firstly, the entire amount of fertiliser and manure, is subject to a default leaching fraction of 0.3. Secondly, under current practices, this default leaching fraction is commonly used by all countries, despite large variations within individual watersheds and agricultural systems. Finally, the N_2O emission factor assigned to leached nitrogen is estimated from a 3-step derivation which tracks the leached fraction through groundwater, rivers and estuaries, and broadly assumes some microbial N_2O production at each step on the basis of limited information. By using our DNDC model, using site specific climate and soil information, detailed field management practices, uncertainties come from the first and second areas have been significantly reduced.

EF5 of 0.0075 is used in this study in consistency with 2006-AFOLU guideline report, where reduced EF5 from 0.025 in its 1998 version to 0.0075. However, some studies suggested that the IPCC 2006-AFOLU underestimated riverine N_2O by up to threefold. (Turner et al. 2015)

Formation of N_2O in the atmosphere from NH_3 emissions originating from anthropogenic activities is also a source for indirect N_2O emission. (Intergovernmental Panel on Climate Change 1998) DNDC estimated positive results for NH_3 emissions for both winter wheat and *Miscanthus* cultivation, which may also lead to indirect N_2O emissions. However it is not possible to convert NH_3 emissions to N_2O emission, due to the lack of information and it was not considered in the IPCC guidelines. (Intergovernmental Panel on Climate Change 1998; Intergovernmental Panel on Climate Change 2006b)

5.3.2. Summary

In this work both NO_3^- and N_2O emissions were simulated with DNDC model for *Miscanthus* and winter wheat. Results from winter wheat simulation presented a large variance among the NO_3^- loss and N_2O emissions during all the simulated years. Among all the soil types, loamy fine sandy soils represented the highest N losses through both NO_3^- and N_2O. The NO_3^- leaching rates of winter wheat cultivated on these soils were up to 81%. By replacing winter wheat with *Miscanthus* on the four loamy fine sandy soils, the NO_3^- leaching rates were not reduced, while the across the whole area the total leaching amounts and N_2O emissions (direct and indirect) decreased by 2.11 kt N/yr and 19.82 tN/yr (2953 t CO_2eq/yr) respectively. This is due to the lower nitrogen fertiliser inputs level for *Miscanthus* cultivation compared with winter wheat cultivation.

Chapter 6. **Emissions from carbon stock changes of SPBC and MPBC scenario**

6.1. Introduction

In this chapter, the carbon emissions from terrestrial carbon stock changes were estimated using 2006-AFOLU Tier 2 and Tier 3 approaches for SPBC and MPBC scenarios. In both approaches, five carbon pools (AGB, BGB, SOC, dead wood and litter) were considered, while the carbon stock changes in deadwood and litter were assumed to be zero in this study, due to the relatively small carbon stocks in cropland. (Yin et al. 2004) According to 2006-AFOLU, both winter wheat and *Miscanthus* lands fall in to the cropland category. The objective of this chapter is to quantify the site specific potential carbon stock changes arising from replacing cereal crop winter wheat with perennial crop *Miscanthus* on selected low-quality soils.

6.2. Carbon stock change in AGB pool

6.2.1. 2006-AFOLU Tier 2 approach

As stated in Section 3.5.2.1, no carbon stock change in AGB is accounted for in either the SPBC or MPBC scenarios.

6.2.2. STAMINA based Tier 3 approach

As explained in Section 3.5.2.2, SPBC scenario does not induce any land use change. While for MPBC scenario, due to the yield difference between cultivated crops, carbon stock was expected to change in AGB pool.

Calculated based on STAMINA generated winter wheat and *Miscanthus* yields with Equation 5 (in Section 3.5.2), total AGB carbon stocks increase under the MPBC scenario by 3.22 ktC (shown on Table 6-1). For land under winter wheat cultivation, the biomass is harvested every year, so there is no further accumulation of ABG carbon stock beyond a one-year time frame. *Miscanthus* yields generally reach a peak after 3 to 5-year cultivation and no harvest applications are applied before the third year. In this study, it is assumed that the AGB carbon stock in *Miscanthus* land increases until the crop reaches its peak yield and the AGB carbon stock plateaus at this point and remains stable till the end of its lifecycle. As detailed in Section 3.3.2, a 30-year period consists of two *Miscanthus* cultivation cycles.

Table 6-1 Carbon stock changes in AGB pool estimated with Tier 2 and Tier 3 approaches

	Tier level	C stock changes in AGB		Averaged annual C stock changes in AGB				Cultivation area
				30 years	50 years	100 years	150 years	
		kt C	kgC/ha	kgC/ha.yr	kgC/ha.yr	kgC/ha.yr	kgC/ha.yr	ha
SPBC	Tier 2	0	0	0	0	0	0	396400
MPBC	Tier 2	0	0	0	0	0	0	396400
SPBC	Tier 3	0	0	0	0	0	0	396400
MPBC	Tier 3	3.22	8.11	0.27	0.16	0.08	0.05	396400
Winter wheat in MPBC	Tier 3	29.54	80.66	2.69	1.61	0.81	0.54	366200
***Miscanthus* in MPBC**	Tier 3	-26.32[1]	-871.58	-29.05	-17.43	-8.72	-5.81	30200

1. Negative figures indicate carbon stock decreases, in other words, carbon emissions.

The calculated 30-year average annual carbon accumulation rate for MPBC is 0.27 kgC/ha.yr. Averaged annual carbon stock change decreases when longer simulation timeframe was applied. It is worth mentioning that in MPBC scenario, for the soils under cultivation of *Miscanthus*, although *Miscanthus* yields are simulated to be higher than wheat grain, carbon stocks in AGB actually decrease comparing with previous winter wheat cultivation. The reason for this is AGB carbon stock in wheat cropping system involves not only grain, but also other AGB organs such as stems and leaves. When model simulated wheat grain yields/HI was higher than *Miscanthus* yields, carbon could be lost from AGB pool on those soils.

Table 6-2 Carbon stock change in BGB estimated with Tier 2 and Tier 3 approaches

		Cumulative C stock changes in BGB		Averaged annual C stock change in BGB				Cultivation area
				30 years	50 years	100 years	150 years	
		kt C	kgC/ha	kgC/ha.yr	kgC/ha.yr	kgC/ha.yr	kgC/ha.yr	ha
SPBC	Tier 2	0	0	0	0	0	0	396400
MPBC	Tier 2	0	0	0	0	0	0	396400
SPBC	Tier 3	0	0	0	0	0	0	396400
MPBC	Tier 3	421.85	1064.19	35.47	21.28	10.64	7.09	396400
Winter wheat in MPBC	Tier 3	6.82	18.63	0.62	0.37	0.19	0.12	366200
***Miscanthus* in MPBC**	Tier 3	415.02	13742.54	458.08	274.85	137.43	91.62	30200

6.3 Carbon stock change in BGB pool

6.3.1. 2006-AFOLU Tier 2 approach

As stated in Section 3.5.3.1, carbon stock changes in BGB pool were also considered as zero for both SPBC and SPMC scenarios when a Tier 2 approach was applied. This was due to both wheat and *Miscanthus* lands falling under the 'cropland' land use category and Tier 2 approach considered carbon stock changes in BGB pool for 'cropland remaining cropland' as negligible. (Intergovernmental Panel on Climate Change 2006a)

6.3.2. Literature and STAMINA based Tier 3 approach

Carbon stock changes in BGB pool were estimated based on literature data and STAMINA model outputs under Tier 3. In SPBC, carbon stock changes in BGB pool were assumed to be zero. For MPBC, total cumulative carbon stock changes in BGB was 421.85 ktC for the whole case study area (as presented in Table 6-2) and 98.4% of the sequestrated carbon is attributed to *Miscanthus* plantation. This further proves the strong BGB carbon sequestration ability of *Miscanthus*, as suggested by their studies. (Clifton-brown et al. 2007; McCalmont et al. 2015; Zatta et al. 2014)

Table 6-3Carbon stock changes in SOC estimated using a Tier 2 methodology

	Soil Classification	**Crop**	**Area**	**Starting level**	**End level**	**Cumulative carbon stock changes**		**Annual average change**			
								30 years	50 years	100 years	150 years
			ha	tC/ha	tC/ha	tC/ha	kt C	kgC/ha.yr	kgC/ha.yr	kgC/ha.yr	kgC/ha.yr
SPBC	whole area	ww[1]	396400	63.88	63.88	0.00	0.00	0.00	0.00	0.00	0.00
	Sandy soil	ww	30200	48.68	48.68	0.00	0.00	0.00	0.00	0.00	0.00
	HAC soil	ww	366200	65.13	65.13	0.00	0.00	0.00	0.00	0.00	0.00
MPBC	whole area	ww + Mis[2]	396400	63.88	67.07	3.20	1267.04	106.55	63.93	31.96	21.31
	Sandy soil	Mis	30200	48.68	90.63	41.96	1267.04	1398.50	839.10	419.55	279.70
	HAC soil	ww	366200	65.13	65.13	0.00	0.00	0.00	0.00	0.00	0.00

1. Winter wheat; 2. *Miscanthus*

6.4 Soil organic carbon

6.4.1 2006-AFOLU Tier 2 approach

Estimates of SOC stock changes under Tier 2 approach were calculated with Equation 7. Default SOC reference values were derived from 2006-AFOLU, based on climate conditions and soil classification (data shown on Table 3-6). Factors defined by the 2006-AFOLU Tier 2 guidance regarding land use, land management and carbon input levels are also shown in Table 3-7. In SPBC scenario, the cumulative SOC stock change is zero for all the soils. This is due to that, assuming previous land is crop land for winter wheat cultivation and the starting SOC level is already in equilibrium status, continuing the same land use with the same management and inputs conditions will not result in any further disturbance to SOC stocks. For MPBC scenario, the SOC contents of HAC soils also remain unchanged for the same reason as the SPBC scenario. The only SOC stock change happens on the selected loamy fine sandy soils, where the land management and biomass carbon inputs changed as a result of the introduction of *Miscanthus* on the loamy fine sand soils, replacing previous winter wheat cultivation.

6.4.2 RothC model as Tier 3 approach

6.4.2.1 SOC dynamic for winter wheat cultivation

In Tier 3 approach, SOC stocks were estimated using the RothC model. It was necessary to run the model to reproduce the same soil C content as originally presented in the soil (as the carbon stock levels of each soil series in the NATMAP 2014 database) for each individual soil series. In this preliminary run, annual plant inputs needed to reach the specific soil C contents prior to the start of the simulation are generated by the model (Appendix F). These preliminary run outputs were used in both SPBC and MPBC scenarios.

Table 6-4 presents the total SOC contents in the top 30 cm soil layers recorded at each time point for SPBC scenario. Total SOC at the starting point of the simulation (year 2021) was 38.31Mt C and gradually decreased to 37.49 Mt C over 150 years. When longer simulation periods were applied, the average annual SOC changes decreased. For the whole case study area, averaged annual SOC changes for 30-year, 50-year, 100-year and 150-year simulation periods were calculated to be -9.08 tC/yr, -7.82 tC/yr, -6.38 tC/yr and -5.59 tC/yr respectively. Averaged annual SOC change rates for each soil series ranged from -0.51% to 0.56% over the first 30 years of simulation; from -0.41% to 0.42% over 50 years; from -0.30% to 0.30% over 100 years and -0.24% to 0.25% over 150 years.

As graphed in Figure 6-1, under continues winter wheat cultivation, BLACKWOOD, BLACKTOFT, DENCHWORTH and WIGTON MOOR soils have the smallest SOC changes, from -0.45tC/ha to 0.62tC/ha during the total 150-year simulation period. CRANNYMOOR, DOWNHOLLAND, FLADBURY and ISLEHAM four soils suggested the largest SOC increases, from 16.20 tC/ha to 19.24 tC/ha. BURLINGHAM, CURDRIDGE, NEWPORT and TATHWELL four soils are those with the largest SOC losses, from 21.89 tC/ha to 104.25 tC/ha.

Although the total soil carbon content in whole case study area decreases for continuous winter wheat cultivation, it is notable that in some series, SOC contents accumulate for the whole or parts of the simulation period. In the first 30 years, 27 (out of total 47) soil series show increases in SOC contents. Among the 27 soil series, AGNEY, BLACKWOOD and BRICKFIELD start to decline after the 38th year, 24th year and 22nd year respectively.

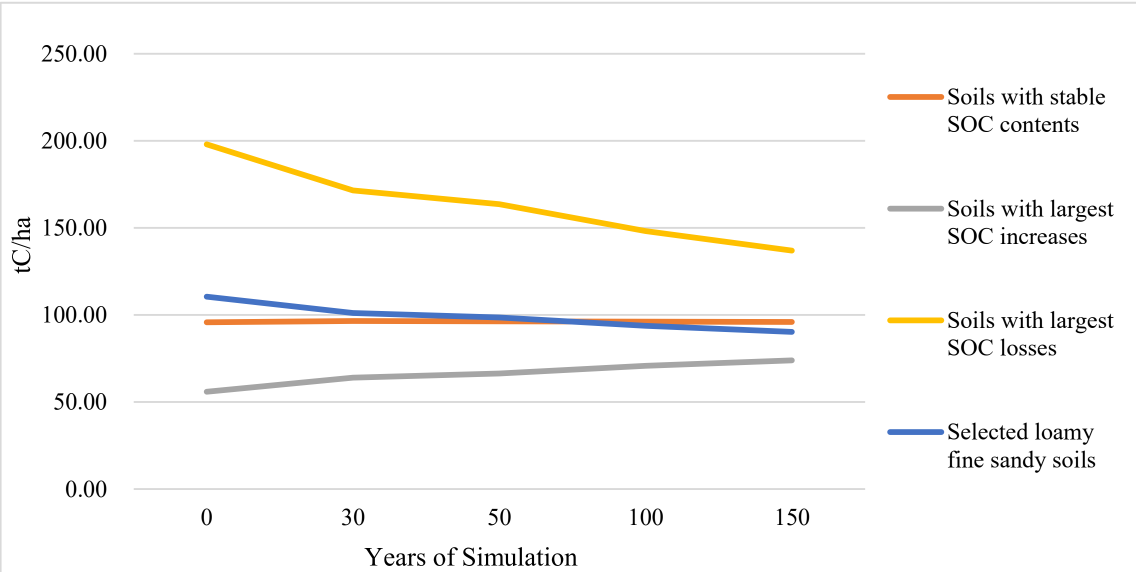

Figure 6-1 Graphed trends of averaged SOC contents of four soils with stable SOC contents (BLACKWOOD, BLACKTOFT, DENCHWORTH, WIGTON MOOR)(for which have the smallest SOC content changes); four soils with largest SOC increases(CRANNYMOOR, DOWNHOLLAND, FLADBURY, ISLEHAM); four soils with largest SOC losses (BURLINGHAM, CURDRIDGE, NEWPORT, TATHWELL) and the selected for loamy fine sandy soils(CRANNYMOOR, EVERNGHAM, HOLME MOOR and KEXBY)

Table 6-4 SOC level (top 30cm soil layers) at stating point (year 2021), 30th, 50th, 100th and 150th year simulation points for each soil series (continuous Winter Wheat cultivation)

		starting point	30th year	50th year	100th year	150th year
ABERFORD	t C/ha	98.82	98.20	98.00	97.63	97.35
AGNEY	t C/ha	106.02	109.50	109.41	108.91	108.51
BLACKWOOD	t C/ha	91.77	93.94	93.47	92.24	91.34
BRICKFIELD	t C/ha	102.48	104.42	103.88	102.52	101.50
BROCKHURST	t C/ha	86.94	88.80	89.36	90.42	91.19
BURLINGHAM	t C/ha	58.8	67.16	69.80	74.58	78.04
BLACKTOFT	t C/ha	95.58	95.78	95.85	95.97	96.06
BISHAMPTON	t C/ha	81.9	84.41	85.21	86.66	87.70
CONWAY	t C/ha	105.3	102.97	102.30	100.91	99.94
COOMBE	t C/ha	133.56	123.99	121.05	115.42	111.27
CRANNYMOOR	t C/ha	176.58	149.46	142.01	128.05	117.78
CURDRIDGE	t C/ha	52.56	61.37	63.73	68.53	71.92
CARSTENS	t C/ha	76.8	81.19	82.58	85.13	86.97
CANNAMORE	t C/ha	96.72	95.89	95.64	95.16	94.80
DENCHWORTH	t C/ha	100.05	100.32	100.40	100.56	100.67
DOWNHOLLAND	t C/ha	284.31	240.50	226.62	199.84	180.06
DUNKESWICK	t C/ha	105.27	102.69	101.86	100.28	99.11
ELLERBECK	t C/ha	85.8	86.89	87.21	87.81	88.26
ENBORNE	t C/ha	107.1	104.11	103.19	102.78	100.10
EVERINGHAM	t C/ha	76.14	76.91	77.12	77.53	77.83
EVESHAM	t C/ha	106.02	104.81	104.43	103.69	103.15
FLADBURY	t C/ha	139.38	130.20	127.28	121.65	117.49
FOGGATHORPE	t C/ha	96.39	97.36	97.67	98.26	98.70
FLINT	t C/ha	86.94	88.69	89.19	90.20	90.94
FROME	t C/ha	75	80.87	82.69	86.21	88.81
HOLME MOOR	t C/ha	102.96	94.38	92.13	87.97	84.91
HOLDERNESS	t C/ha	85.14	87.07	87.66	88.78	89.61
HUNSTANTON	t C/ha	78.09	80.70	81.47	82.93	84.00
ISLEHAM	t C/ha	191.58	165.75	158.03	143.32	132.50
KEXBY	t C/ha	86.31	83.56	82.82	81.41	80.42
METHWOLD	t C/ha	76.68	80.74	81.98	84.36	86.11
MILTON	t C/ha	88.32	89.61	90.00	90.75	91.30
NEWCHURCH	t C/ha	127.26	120.94	118.93	115.04	112.18
NEWPORT	t C/ha	49.83	57.83	60.01	64.07	67.07
RAGDALE	t C/ha	95.16	95.98	96.24	96.73	97.10
RIVINGTON	t C/ha	76.95	79.39	80.11	81.46	82.45
ROMNEY	t C/ha	85.56	86.09	86.24	86.52	86.74
RUSKINGTON	t C/ha	72.42	75.14	75.87	77.24	78.25
SALOP	t C/ha	99.63	97.83	97.29	96.25	95.49
SESSAY	t C/ha	127.65	118.36	115.57	110.24	106.33

		starting point	30th year	50th year	100th year	150th year
TATHWELL	t C/ha	62.55	69.66	71.77	75.79	78.75
WHIMPLE	t C/ha	92.25	93.14	93.42	93.95	94.34
WICK	t C/ha	70.89	74.68	75.77	77.84	79.36
WICKHAM	t C/ha	99.96	99.17	98.93	98.46	98.11
WIGTON MOOR	t C/ha	95.94	95.75	95.69	95.56	95.49
WORCESTER	t C/ha	78.75	83.94	85.56	88.70	91.03
WALLASEA	t C/ha	124.8	119.17	117.39	113.94	111.40
Whole case study area	t C/ha	38.31	38.04	37.92	37.67	37.49

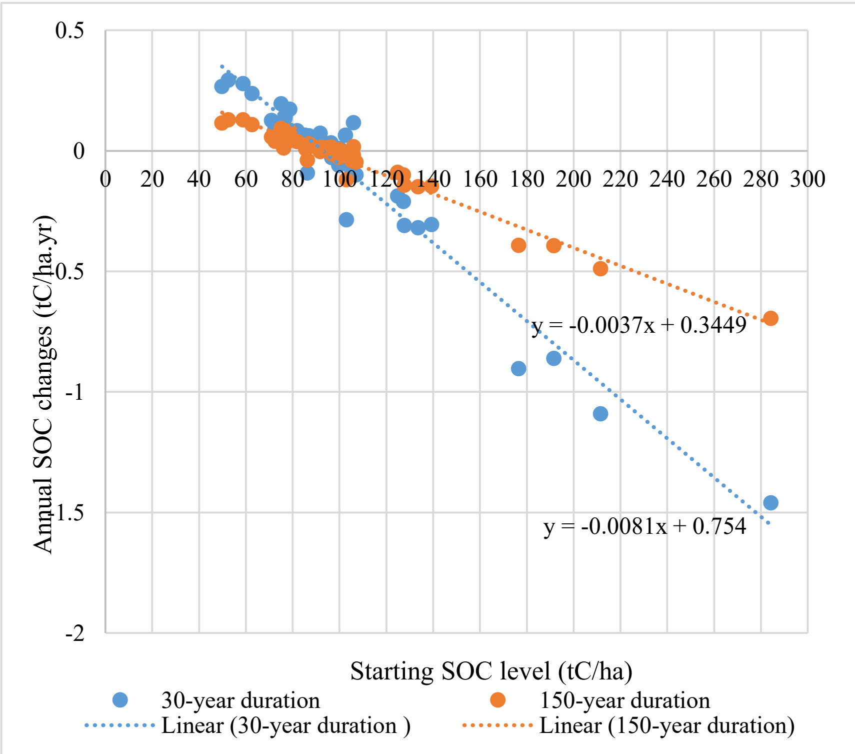

Figure 6-2 Annual SOC changes (top 30cm) (tC/ha.yr) vs starting SOC levels (tC/ ha) for each soil series for 30-year and 150-year continuous winter wheat simulation periods; each dot represents a soil series; negative values indicate carbon stock decreases (carbon emissions) in SOC pool; positive values indicate soil carbon sequestration

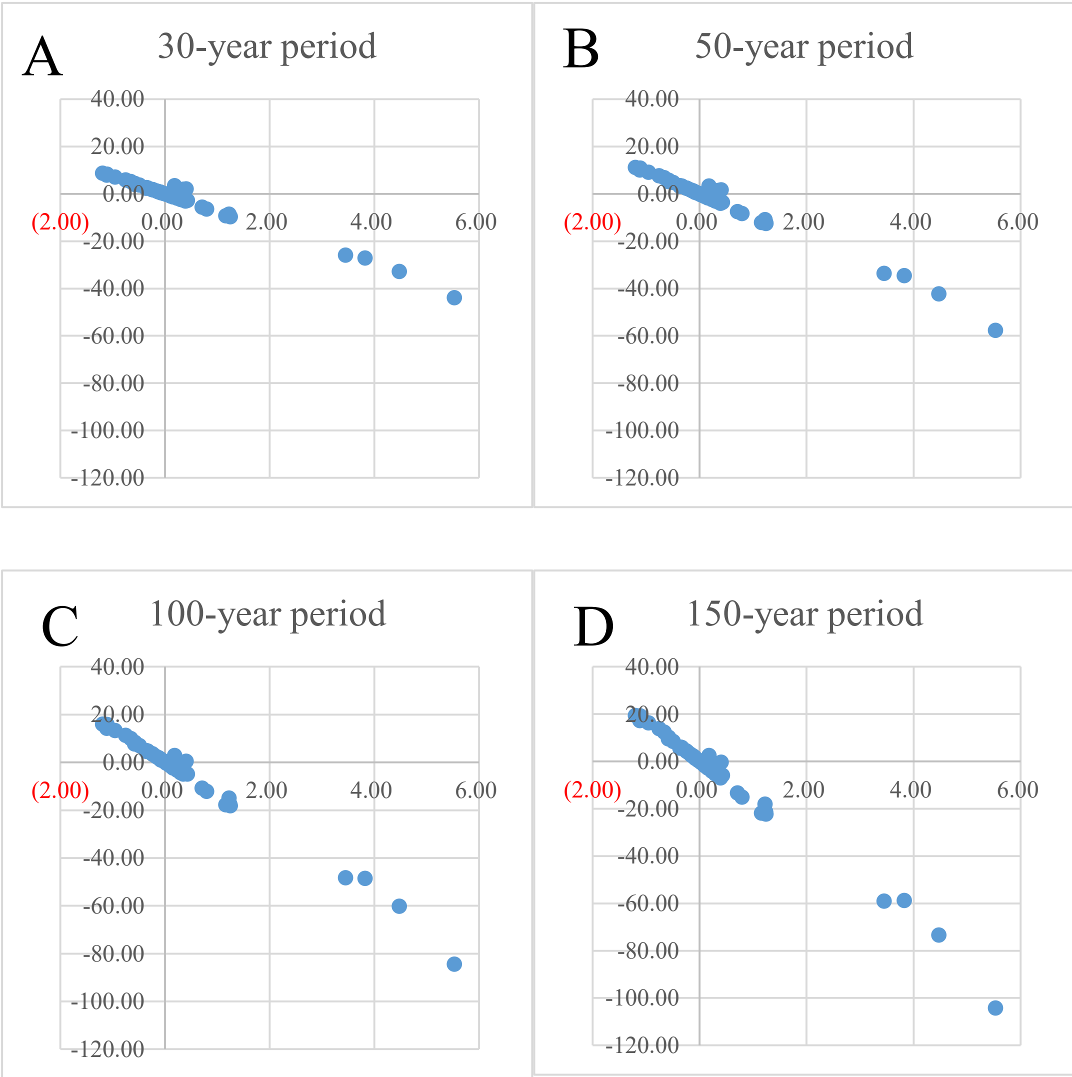

Figure 6-3 . Total SOC changes (top 30cm soil layers) (tC/ha) (y-axis) vs changes of annual biomass carbon inputs to soil (tC/ha) (x-axis) for each soil series for (A) 30-year, (B) 50-year, (C) 100-year and (D) 150-year simulation periods; each dot represents a soil series; negative values in y-axis indicate carbon stock decrease (carbon emissions).

Averaged annual SOC changes over the 30- and 150-year periods vs initial SOC content for each soil series were graphed in Figure 6-2. The strong correlations between averaged annual SOC changes and initial SOC levels suggested that initial SOC level is a crucial factor determining whether SOC would increase or decrease after land use change. This has been reflected in a number of assessments. (Peltre et al. 2016; Hillier et al. 2009) Peltre et al. suggested that when wheat was grown continuously, the losses of soil carbon were strongly determined by the initial soil carbon content, which reflects the management and land-use history of the soil. (Peltre et al. 2016) Hillier et al. (2009)

assessed the soil carbon change of potential expansion of perennial energy crops onto arable, grassland and forest land in the whole UK land cover. A similar correlation between initial soil carbon content and the carbon stock change was suggested in Hillier et al.'s work, while an extreme land use scenario adopted in that study, were an extreme case, where assumed that the whole UK area would be converted to energy crop cultivation. Calculated from the two equations displayed by the trend lines on Figure 6-2, breakeven values for SOC sequestration for 150-year duration was 93.22 tC/ha and for 30-year duration was 93.09 tC/ha. Similarly, breakeven values for 50 years duration and 100 years duration was calculated to be 93.23 tC/ha and 91.91 tC/ha respectively.

Secondly, another strong correlation has also been seen between changes of the annual biomass carbon inputs to soil and total SOC changes over all the four simulation periods (Figure 6-3). Regardless of the initial SOC level, the more significant the annual biomass carbon inputs changes with land use change, the faster the SOC accumulates (or decreases).

6.4.2.2 SOC stock changes for MPBC

SOC changes from Miscanthus cultivation on selected soils

Miscanthus was assumed to be planted in four soil series in MPBC scenario, namely; EVERINGHAM, HOME MOOR, CRANNYMOOR and KEXBY. Similar to the simulation applied to winter wheat, annual biomass carbon inputs from *Miscanthus* to soil were generated based on STAMINA simulated *Miscanthus* DMYs using Hillier's approach (Hillier et al. 2009) with Equation 10 (Appendix G).

As illustrated in Figure 6-4, for the EVENINGHAM, HOLME MOOR and KEXBY soil series, SOC contents increased with *Miscanthus* cultivation through the whole simulation period. However for CRANNYMOOR soil, SOC content first accumulated before it started to decrease gradually at an average rate of 0.0165 tC/ha.yr for 115 years after the 55th year of simulation. Despite this decrease during the later part of simulation, its SOC content at the end of the simulation (182.28 tC/ha) was still higher than the starting status (176.58 tC/ha).

Similar to winter wheat cultivation, SOC changes under *Miscanthus* were significantly influenced by both initial SOC contents (as shown in Figure 6-5) and the changes of carbon inputs from biomass after land use change (as shown in Figure 6-6). SOC accumulated faster on those soils with lower initial SOC contents and received more carbon from biomass after land was converted to *Miscanthus* cultivation. It indicates the possibility that for soils with high initial SOC contents, SOC changes after *Miscanthus* plantation would be difficult to detect. This helps explain the work conducted by Robertson et al.(2017), in which no SOC enrichment was detected under a 4-years *Miscanthus* land.

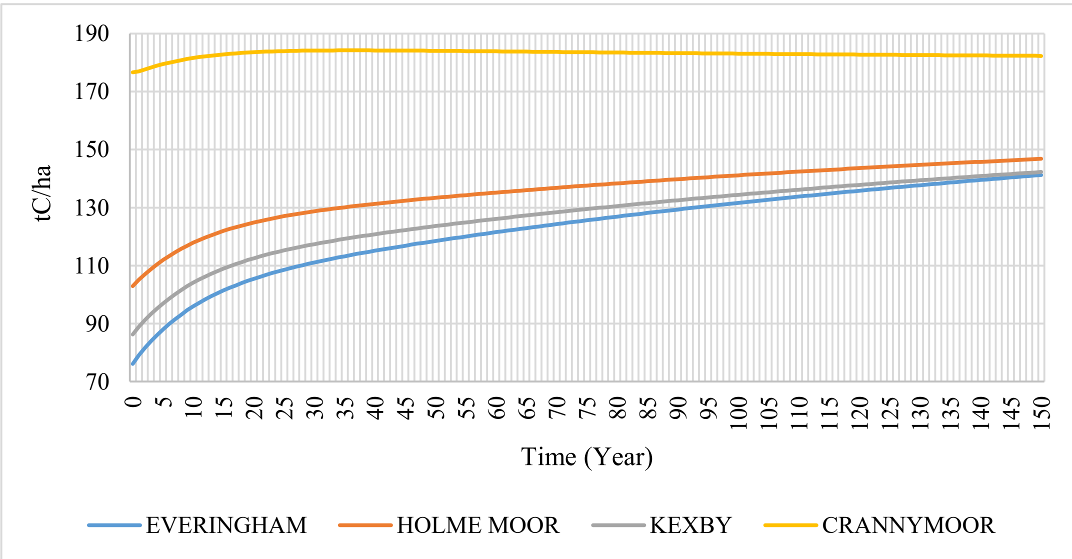

Figure 6-4 RothC model simulated SOC content trends under Miscanthus cultivation for EVENINGHAM, HOLME MOOR, KEXBY and CRANNYMOOR soil series over 150-year simulation period

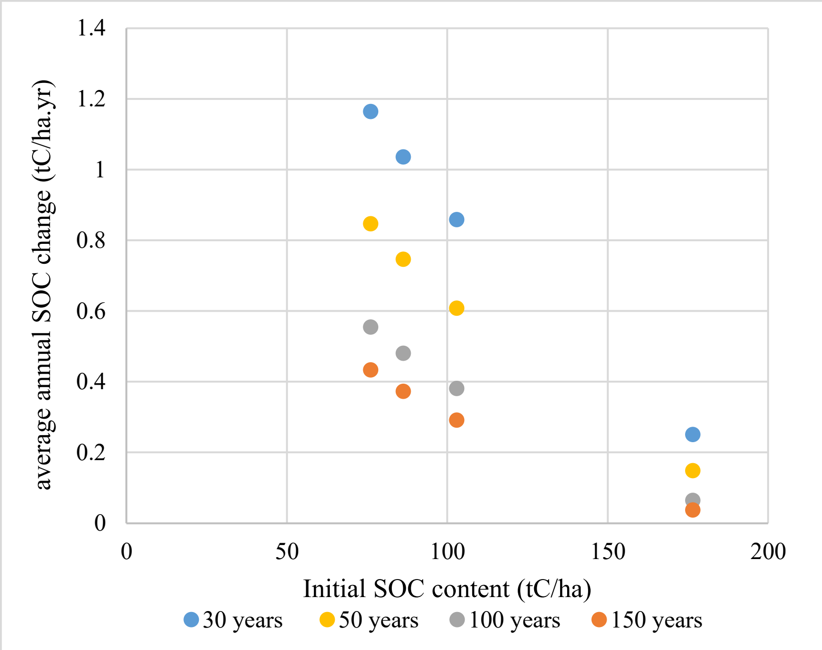

Figure 6-5 Average annual SOC content changes of Miscanthus cultivation for 30-year, 50-year, 100-year and 150-year periods vs initial SOC contents (top 30cm soil layers) on CRANNYMOOR, EVERNGHAM, HOLME MOOR and KEXBY soil series.

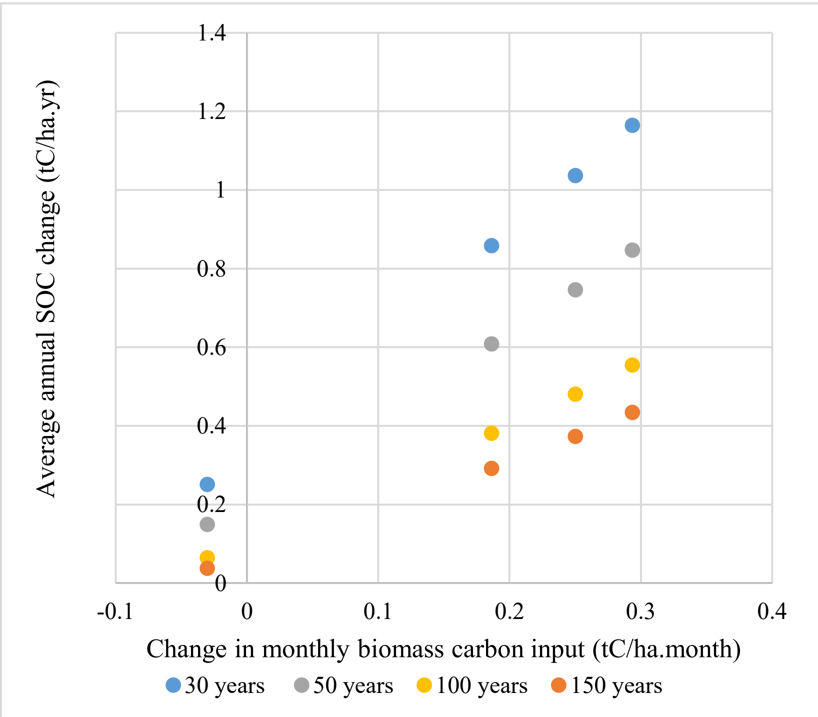

Figure 6-6 Average annual SOC content changes of Miscanthus cultivation over 30-year, 50- year, 100-year and 150-year periods vs monthly biomass carbon input changes on CRANNYMOOR, EVERNGHAM, HOLME MOOR and KEXBY soil series.

Graphing SOC content trend of *Miscanthus* and winter wheat cultivation on the same soil series (Figure 6-7) indicates the strong ability of *Miscanthus* sequestering carbon back to soil, even on soils with higher initial SOC content above 170 tC/ha. Over the 30-year simulation period, the average SOC content increase of *Miscanthus* compared with winter wheat cultivated on the same soil series is 24.84 tC/ha (SD= 12.13 tC/ha). For 50 years, 100 years and 150 years periods, the values are 29.39 tC/ha (SD=15.42tC/ha), 37.05 tC/ha (SD=21.58 tC/ha) and 42.64 tC/ha (SD= 26.12 tC/ha) respectively. The considerable variation among different soil series is mainly caused by the wide range of the initial SOC contents (MEAN=110.50 tC/ha, SD=45.42 tC/ha).

SOC changes from MPBC scenario

Total SOC content at top 30cm layer of whole case study area under MPBC scenario and SPBC scenario were illustrated in Figure 6-8 and Table 6-6. Comparing with SP, SOC content of MP could increase by 2.72% after 30 years; 3.30% after 50 years; 4.32% after 100 years and 5.08% after 150 years. As the SOC accumulation of MPBC is attributed to the *Miscanthus* cultivated on four selected sandy soils, it shares the same trends with SOC changes under *Miscanthus* cultivation. SOC contents accumulate rapidly in the first 30-year period and the increase rates decrease gradually when the simulation time gets longer.

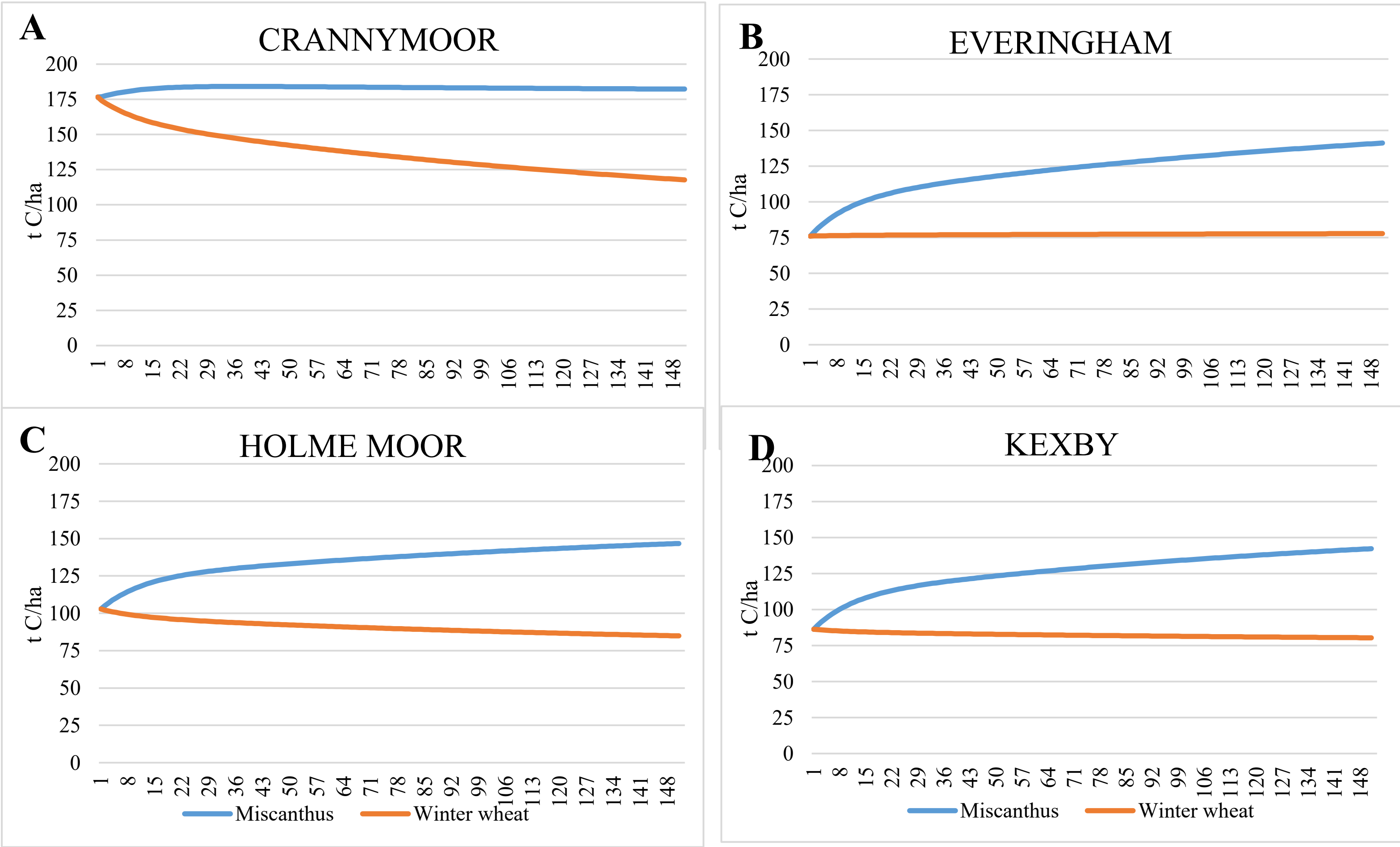

Figure 6-7 Trends in SOC contents from Miscanthus and winter wheat cultivation on (A) CRANNYMOOR (B) EVERINGHAM (C) HOLME MOOR and (D) KEXBY soil series

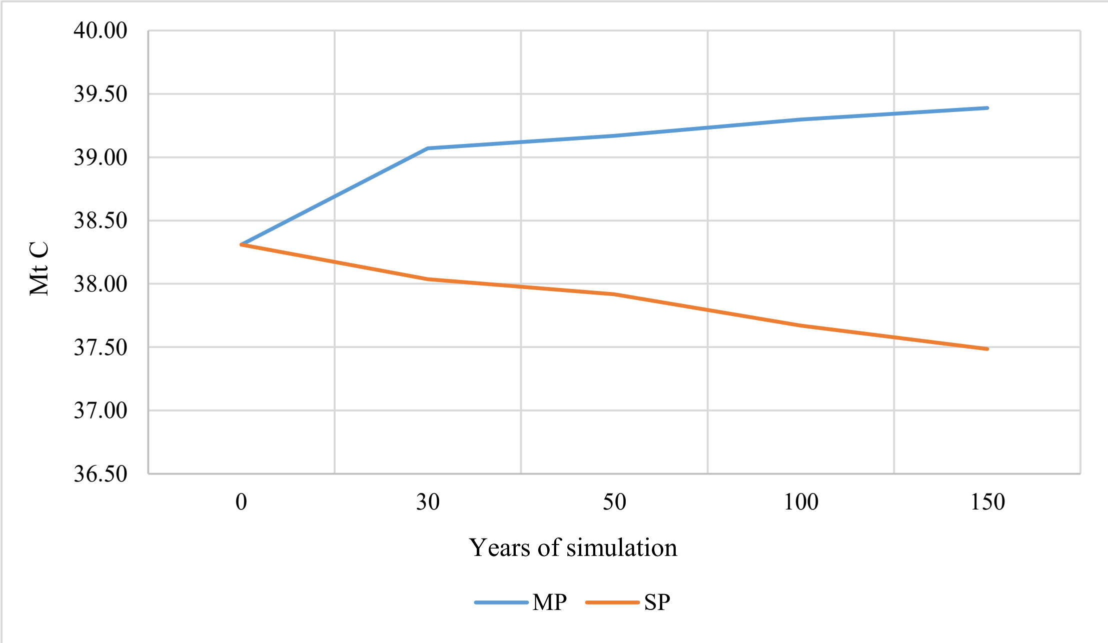

Figure 6-8 Trends of SOC stock change for SPBC and MPBC scenarios based on RothC model outputs.

Table 6-5 Carbon stock change in SOC estimated using a Tier 3 approach based on RothC model outputs.

Timeframe			**Area**	**Starting level (2021)**	**End level (2170)**	**Cumulative carbon stock change**		**Annual average**
years			ha	tC/ha	tC/ha	tC/ha	kt C	kg C/ha.yr
30	SPBC	whole area	396400	96.64	95.96	-0.69	-272.53	-22.92
	MPBC	whole area	396400	96.64	98.57	1.92	762.47	64.12
		Mis[1]	30200	100.62	128.23	27.62	834.07	920.60
		ww[2]	366200	96.32	96.12	-0.20	-71.60	-6.52
50	SPBC	whole area	396400	96.64	95.66	-0.99	-391.02	-13.75
	MPBC	whole area	396400	96.64	98.81	2.17	859.24	38.47
		Mis	30200	100.62	133.57	32.96	995.25	552.36
		ww	366200	96.32	95.94	-0.37	-136.01	-7.43
100	SPBC	whole area	396400	96.64	95.03	-1.61	-638.41	-6.88
	MPBC	whole area	396400	96.64	99.14	2.49	988.67	19.23
		Mis	30200	100.62	142.71	42.09	1271.12	276.18
		ww	366200	96.32	95.54	-0.77	-282.46	-7.71
150	SPBC	whole area	396400	96.64	94.56	-2.08	-823.83	-4.58
	MPBC	whole area	396400	96.64	99.36	2.72	1078.65	12.82
		Mis	30200	100.62	149.37	48.75	1472.36	184.12
		ww	366200	96.32	95.24	-1.08	-393.70	-7.17

1. *Miscanthus* 2. Winter wheat

6.5 Summary and discussion

6.5.1 Carbon stock changes results from introducing *Miscanthus* into winter wheat production system

Total carbon stock changes calculated by Tier 2 and Tier 3 approaches for SPBC and MPBC scenarios are presented in Table 6-6. The results are used to evaluate the question 'what are the carbon stock changes that result from introducing *Miscanthus* into a winter wheat production system?' The total carbon stock increases when moving from the reference SPBC to the MPBC scenarios. Results from both of the two tiered approaches suggested a carbon stock credit when *Miscanthus* was introduced to the wheat production system. Especially over the first 30-year time-frame, the results from Tier 2 and Tier 3 are similar; Tier 2 predicted that 1,267 kt C will be stored if *Miscanthus* is cultivated on selected soils; Tier 3 predicted 1,460 kt C. However, the value gap between Tier 2 and Tier 3 gets bigger when adopting a longer timeframe. Tier 2 generally assumes that soil carbon stocks reach the equilibrium status and remain stable after a 20-year period, while in this work Tier 3 predicted continuous carbon stock sequestration benefits from *Miscanthus* cultivation, although the annual rate of increase decreases when longer simulation periods are applied.

Table 6-6 Total carbon stock change predicted with Tier 2 and Tier 3 approaches

Approach	**Scenario**	**Total carbon stock change (kt C)**			
		30 years	50 years	100 years	150 years
Tier2	SPBC	0	0	0	0
	MPBC	1267.04	1267.04	1267.04	1267.04
	MPBC-SPBC	1267.04	1267.04	1267.04	1267.04
Tier3	SPBC	-272.53	-391.02	-638.41	-823.83
	MPBC	1187.53	1284.30	1413.73	1503.71
	MPBC-SPBC	1460.06	1675.32	2052.14	2327.54

6.5.2 Comparing Tier 2 and Tier 3 approaches

The basic structure provided by IPCC 2006-AFOLU is considered capable for predicting the carbon stock changes for the specific land use and management activities applied in this study. The fundamental difference between the two Tiers is in the methods they use to estimate the carbon stocks for each carbon pool at each simulation point. Tier 3 requires using process-based models to simulate the carbon stock change continuously across the whole simulation period. Tier 2 approach calculates the carbon stock levels according to the functions, default values and climate-, management-related factors, which are generally provided by the IPCC guidelines.

When using a Tier 2 approach, carbon stock changes estimated for SPBC scenario are zero across all the three considered carbon pools. For AGB and BGB, Tier 2 considers only the carbon stock in perennial wood crops. For SOC, as the land is assumed under the same use and management, thus the SOC at both the beginning and the end of each timeframe are all at the equilibrium status, so the stock change in SOC can be considered as zero as well. For MPBC scenario, ABG and BGB carbon stock changes are estimated as zero for the same reason as for SPBC. The only carbon stock change that happens is in the SOC under *Miscanthus* cultivation. However, there is no cumulative SOC beyond 20 years as 2006-AFOLU considers that SOC will reach equilibrium status after the first 20 years of cultivation.

While Tier 3 estimates that carbon stock continues decreasing even in 100th to 150th year in SPBC. All the decrease is attributed to SOC changes from continuous winter wheat cultivation. This is quite different from the Tier 2 approach, which assumes SOC reach equilibrium when the land remains under the same management regime for 20 years. RothC results clearly indicate that both the trends and spends of SOC change are both strongly influenced by its starting value, for soil with higher initial SOC level, the assumption of 20 years appears too ambitious for SOC to reach a new stable equilibrium.

6.5.3 Three accounted carbon pools

As both land for *Miscanthus* and winter wheat cultivation fall into ‘crop land category’ as defined in 2006-AFOLU and are non-wood crops, carbon stock changes in the BGB and AGB biomass are negligible when using the Tier 2 approach. However, under the Tier 3 approach conducted in this work, the outcomes clearly indicate that the carbon stock differences in AGB and BGB between *Miscanthus* and winter wheat can be significant and should not be neglected when *Miscanthus* is cultivated in predominantly arable cropped land. Regarding the AGB pool, replacing winter wheat with *Miscanthus* does not always result in a carbon stock credit, as carbon is stored in both grain and non-grain AGB parts. Regarding BGB pool, although literature data is used for BGB accounting, *Miscanthus* allocates significant amounts of carbon in below-ground pools e.g. rhizomes and roots, as confirmed by previous published works. (Hansen et al. 2004; Zatta et al. 2014; Richteret al. 2015)

The 30 years simulation of RothC model (Tier 3) suggests that planting *Miscanthus* on the selected sandy soils could increase SOC sequestration at an annual rate of 920.60 kgC/ha.yr. This is similar to the result from previous field experiments established by Poeplau and Don. (2014), which measured a mean rate of SOC increase of 0.78 ± 0.19 tC/ha.yr over a 10 year cultivation period. Confidence can also be gained from a review of work conducted by Don et al.(2012), which summarized the average SOC increase from ‘cropland converted to *Miscanthus*’ as 0.66 tC/ha.yr. Tier 2 predicted a slightly larger annual SOC increase rate of 1,398.50 kgC/ha.yr for cereal land converted to *Miscanthus* land. As stated above, this is probably due to the Tier 2 assumption that SOC reaches its equilibrium status in the 20th year, which could be too soon for soils with low or high initial SOC contents, compared with RothC results.

Although the Tier 2 approach estimates the carbon stock change for continuous winter wheat cultivation is negligible, RothC predicted an average rate of decrease of 22.92 kgC/ha.yr across the whole study area for continuous winter wheat cultivation. This rate is a little lower than Tier 2, and the results reported by other similar research provide a range from 200 to 550 kgC/ha.yr (Malça & Freire 2009; Anthoni et al. 2004). This is probably due to the reported figure 22.92 kgC/ha.yr in this study is a weighted average value for the whole case study region which covers a wide range of soil series. Some soils in the case study area might have been under cereal production for a long period and equilibrium has been established already, thus the SOC changes can be minor. Indeed, for some specific soil series, consistency can be found between this study and previous publications. Anthoni et al. reported SOC stock decreased at an average rate of 166 kgC/ha.yr (5000 kgC/ha for 30 years) for a site with initial SOC content of 103.3 tC/ha (Anthoni et al. 2004), which is close to the HOLME MORE soil series (as shown in Table 6-4) in this study and its 30-year average SOC decrease rate is 286 kgC/ha.yr under winter wheat cultivation.

6.5.4 SOC equilibrium under long time *Miscanthus* cultivation

Although the SOC enrichment potential of cereal land converted to *Miscanthus* land has been suggested by both previous publications (Poeplau & Don 2014; Richter, Agostini, Redmile-Gordon, White & Keith W.T. Goulding 2015; Zatta et al. 2014) and also the results predicted by RothC results in this work. There have been conversations regarding the SOC equilibrium under *Miscanthus* cultivation. (Agostini et al. 2015; Poeplau & Don 2014; Stockmann et al. 2013) Although such effects have not been observed in in-situ measurements for *Miscanthus* cultivation (Don et al., 2012), the possibilities have been suggested by several model based research applications. (Pepper et al. 2005; Andress 2002)

The RothC predicted SOC trends of *Miscanthus* cultivated on selected sandy soils also indicted the potential SOC equilibrium under *Miscanthu*s cultivation for soil with high initial SOC content, this is probably due to the increased annual biomass carbon inputs to soil when wheat land converted to *Miscanthus* land. According to Figure 6-7, simulated trends for SOC contents in EVERINGHAM, HOLME MOOR and KEXBY soils showed continuous increase of SOC till the 150th year. While for soil CRANNYMOOR, not only its SOC increase rate is much smaller than other three soils even at the beginning of land conversion, but also its SOC content reached a maximum threshold at the 55th year. As the carbon inputs level among the four soils are close, the different SOC trends are most likely due to their different initial SOC contents. The simulated results for CRANNYMOOR even showed slight decreases after reaching its peak value (Figure 6-7), for which the underlying mechanism needs further investigation. Based on a modelling work conducted accessing SOC contents of Switchgrass on the US national-level, Andress (2002) suggested that most of the accessed soils reached SOC equilibrium status after 125 years cultivation and it was also affected by local climate conditions such as temperature. This also contributes to the argument in Section 6.4.2 that, it is a bit too simplified for the IPCC Tier 2 approach to assume after 20 years, new SOC equilibrium would be reached after land use change.

Chapter 7. **LCA of LCB feedstocks and associated Bio-SA life cycle**

7.1 Introduction

As one of the most widely applied approaches used to estimate global warming impacts and the GHG balances associated with Bio-based products, a 'field to upstream factory gate' LCA of delivered LCB feedstocks was conducted to assess the GHG emissions resulting from the SPBC and MPBC production scenarios. The system boundaries and analysis framework were shown in Figure 3-1. The LCA integrates nitrogen emissions from fertiliser applications and CO_2 emissions arising from carbon stock changes due to land use change. Additionally, the GHG balance associated with LCB feedstocks supply was further integrated into a 'cradle to end-of-life' LCA of a lignocellulosic succinic acid life cycle to evaluate the impacts of the agricultural production stage and the activities within this stage, especially N_2O emissions from fertiliser application and terrestrial carbon stock changes on whole lignocellulosic succinic acid life cycle.

The LCAs conducted were an attributional LCA which aimed to quantify the site and management specific GHG balances associated with an LCB feedstock supply for a Lignocellulosic succinic acid life cycle, whilst investigating the further GHG reduction potential from integrating *Miscanthus* into an existing winter wheat system. Regarding carbon stock change, Tier 3 level data generated by RothC with 30-year timeframe were used in this study, while Tier 2 level data was included in the sensitivity analysis work. The consequential effects, such as the reduction of grain production and the emissions might be arising from producing it outside the case study area were not considered in this chapter, while will be addressed in Section 8.1.

There are four phases in an LCA study, Goal and Scope Definition, LCI, LCIA and Interpretation. For LCA of LCB feedstocks, the 'Goal and Scope Definition' phase has been described in Section 3.4, results for LCI, LCIA and Interpretation phrases are presented in this section. For LCA of bio-based plastic end products, only the LCIA results are present in this chapter. As most of the LCI data from upstream factory gate to end-of-life treatments were provided by project partners, the data and sources are included in Appendix D and Appendix E. Assumptions and descriptions regarding some key processes in LCI development were provided in Section 3.6. Interpretations for both studies are reflected in Discussion section.

7.2 Cradle to upstream factory gate LCA of LCB feedstocks

7.2.1 LCI analysis

The LCI contains all inputs, outputs and flows relevant to the product system and impacts to be assessed. (Table7-1) Background data used for LCI development are listed in Appendix C. All the inputs and activities were converted to the functional unit per kg LCB.

In MPBC scenarios, per unit delivered LCB feedstock is assumed as mixed of wheat straw and *Miscanthus*, thus the inventory data for MPBC were calculated based on the inputs required for producing unit wheat straw and *Miscanthus* and their mass ratios among the total delivered LCB feedstock. The mass ratios were based on the results presented in Chapter 4. In MPBC scenario, annual supply capacity of potential LCB feedstock for lignocellulosic succinic acid production across whole case study area is 363.37 t/ha (14.5% moisture content), consisting of 18.11 t wheat straw and 345.26 t *Miscanthus*.

Table 7-1 LCI for delivered LCB feedstock

			SPBC			MPBC		
allocation			Economic	Energy	RED	Economic	Energy	RED
Functional unit: 1 kg lignocellulosic feedstock delivered								
Seed application/ Rhizomes	Wheat seeds	kg	7.84E-03	1.84E-02	0.00	3.86E-04	9.05E-04	0.00
	Miscanthus rhizomes	p	0.00	0.00	0.00	0.44	0.44	0.44
Nitrogen fertiliser	Ammonium nitrate	kg N	9.19E-03	2.15E-02	0.00	4.93E-03	5.55E-03	4.47E-03
	Ammonium sulphate	kg N	0.00	0.00	0.00	0.00	0.00	0.00
	Calcium ammonium nitrate	kg N	0.00	0.00	0.00	0.00	0.00	0.00
	Urea	kg N	0.00	0.00	0.00	0.00	0.00	0.00
Phosphate fertiliser	Monoammonium phosphate	kg P_2O_5	0.00	0.00	0.00	0.00	0.00	0.00
	Diammonium phosphate	kg P_2O_5	0.00	0.00	0.00	0.00	0.00	0.00
	Single superphosphate	kg P_2O_5	0.00	0.00	0.00	0.00	0.00	0.00
	Triple superphosphate	kg P_2O_5	1.75E-03	4.09E-03	0.00	6.11E-04	7.27E-04	5.25E-04
Potassium fertiliser	Potassium chloride	kg K_2O	2.15E-03	5.04E-03	0.00	1.06E-04	2.48E-04	0.00
	Potassium sulphate	kg K2O	0	0	0.00	7.82E-03	7.82E-03	7.82E-03
Calcium oxide		kg CaO	0	0	0.00	1.30E-02	1.30E-02	1.30E-02
Pesticides		kg	4.63E-05	1.08E-04	0.00	8.80E-05	9.10E-05	8.57E-05
Manganese sulphate		kg	0	0	0.00	4.17E-04	4.17E-04	4.17E-04
Diesel consumption at farm		kg	1.03E-02	2.41E-02	0.00	5.63E-04	1.24E-03	5.55E-05
Direct and Indirect Emissions	Direct N_2O emissions	kg N_2O	5.00E-05	1.17E-04	0.00	3.18E-05	3.52E-05	2.93E-05
	NO_3^- leaching	kg N	2.96E-03	6.93E-03	0.00	4.47E-03	4.65E-03	4.34E-03
	Indirect N_2O	kg N_2O	3.49E-05	8.17E-05	0.00	5.27E-05	5.48E-05	5.12E-05
Emissions from land use change	AGB	kg C	0.00	0.00	0.00	2.16E-03	2.15E-03	2.17E-03
	BGB		0.00	0.00	0.00	-3.41E-02	-3.41E-02	-3.41E-02
	SOC		1.03E-03	2.41E-03	0.00E+00	-6.86E-02	-6.86E-02	-6.86E-02
	Deadwood		0.00	0.00	0.00	0.00	0.00	0.00
	Litter		0.00	0.00	0.00	0.00	0.00	0.00
Transport	Road transport to storage (roundtrip)	t.km	0.05	0.05	0.05	0.05	0.05	0.05

	Road transport to plant (roundtrip)	t.km	0.05	0.05	0.05	0.05	0.05	0.05
Loading & Offloading	Diesel consumption at farm	kg	7.68E-04	7.68E-04	7.68E-04	7.68E-04	7.68E-04	7.68E-04
	Diesel consumption at storage	kg	1.54E-03	1.54E-03	1.54E-03	1.54E-03	1.54E-03	1.54E-03
	Diesel consumption at plant	kg	7.68E-04	7.68E-04	7.68E-04	7.68E-04	7.68E-04	7.68E-04

As described in Section 3.6.1.2, three allocation methods were used in this work, Economic allocation following PAS2050, energy allocation and RED allocation. The latter two differ from each other in that, RED considers that no GHG emissions shall be attributed to wheat straw up to the collection stage (RED, 2009), whilst in energy allocation, GHG emissions were attributed to straw and grain according to their energy contents (calorific values).

7.2.2 Results of LCIA

7.2.2.1 Characterization factors

In the LCIA phase, the results from previous LCI were interpreted to calculate their potential impact on climate change. The LCIA was conducted using the characterization factors derived from the ReCiPe Midpoint (H) LCA impact assessment methodology. (Table 7-2)

Table 7-2 Characterization factors for Climate change impact category derived from ReCiPe Midpoint (H) model in Simapro 8

Activities/Emissions	unit	kg CO_2 eq	Activities/Emissions	unit	kg CO_2 eq
Wheat seeds	1 kg	0.58581	Triple superphosphate	1 kg P_2O_5	1.712646
Maize seeds	1 kg	2.144087	Potassium chloride	1 kg K_2O	0.456069
***Miscanthus* rhizomes**	1p	0.005691	**Potassium sulphate**	1 kg K_2O	1.446689
Willow cuttings	1p	0.018075	**Calcium oxide**	1 kg CaO	0.008619
Ammonium nitrate	1 kg N	9.36565	**Pesticides**	1 kg	10.24819

Ammonium sulphate	1 kg N	2.433147	**Magnesium sulphate**	1 kg	0.675913
Calcium ammonium nitrate	1 kg N	9.451795	**Diesel consumption**	1 kg	3.735445
Urea	1 kg N	4.452966	**N_2O emissions**	1 kg N_2O	298
Monoammonium phosphate	1 kg P_2O_5	1.665657	**Indirect N_2O**	1 kg N_2O	298
Diammonium phosphate	1 kg P_2O_5	1.720134	**C stock change**	1kg C	44
Single superphosphate	1 kg P_2O_5	1.826698	**Road transportation**	tkm	0.084728

7.2.2.2 Characterization

LCIA outputs are presented in Table 7-3 and Figure 7-1 for both the SPBC and MPBC scenarios. The overall field to upstream factory gate climate change impacts for SPBC scenario ranges from 0.02 to 0.50 CO_2eq/kg LCB delivered, depending on difference allocation choices. For MPBC scenario, the overall climate change impact ranges from -4.42 to -4.30 CO_2eq/kg LCB delivered depending on the allocation choice applied to wheat straw. Compared with SPBC scenario, the variation of the overall GHG emissions of MPBC appears smaller and less dependent on the allocation choice. This is due to the small proportion of wheat straw among total delivered mixed LCB feedstocks, as indicted in previous LCI development.

For SPBC scenario, when RED allocation was applied to winter wheat, the total climate change impact is significantly smaller than the results generated with economic allocation and energy allocation, as RED considers zero emissions should be allocated to straw before its collection from fields. When economic and energy allocation were used, nitrogen fertiliser production was the biggest contributor amongst all the considered resource inputs and emission outputs, representing 38.4% to 40.5% of the total climate change impact. On-farm diesel consumption resulted in 17.2% and 18.1% of the total impacts for economic and energy allocation respectively. Combined N_2O emissions (direct and indirect) caused by nitrogen fertiliser application accounts for 11.3% of the total impact under economic allocation and 11.9% under energy allocation. Emissions from SOC stock change caused 20.2% and 21.3% of the total impacts for economic and energy allocation respectively. These four components added up to 87.1% of the total pre-delivered impacts under economic allocation, increasing to 91.7% when energy allocation was applied. Regarding pre-harvest emissions, the contribution ratio of each component was the same for economic and energy allocation, with the absolute values in energy allocation approximately 2.3 times of those calculated based on economic allocation.

Regarding MPBC scenario, the overall GWP figures were similar for the three allocation choices for wheat straw. Under economic allocation, SOC stock change from 'wheat land converted to *Miscanthus* land' represented the most significant components among all the sources and was also the largest carbon sink, accounting for approximately 66.8% of total carbon stock. BGB carbon stock change from 'wheat land converted to *Miscanthus* land' constituted another important carbon sink, accounting for the rest 33.2% of total carbon stock. Nevertheless, AGB carbon stock change appeared to be the largest carbon emission source, rather than a carbon sink in this case, accounting for 46.4% of total GHG emissions (see Section 6.2 for more detail). Nitrogen fertiliser production (excluding N_2O emissions from its applications) resulted in 22. 6% of total emissions, ranking as the second GHG emissions source. Similar to SPBC, combined direct and indirect N_2O emissions together contributed to 12.29% of total emitted GHGs. A considerable reduction was seen for on-farm diesel consumption emissions, which only accounting for 0.1% to 2.2% of the total emissions, depending on the allocation approach applied. This is due to the significant decrease in annual average machinery use for the perennial crop *Miscanthus* when compared to the cereal crop.

Table 7-3 Characterised LCIA profiles of SPBC and MPBC scenarios

			SPBC			MPBC		
Allocation			Economic	Energy_ non RED	RED	Economic	Energy_ non RED	RED
Net emissions		CO_2 eq/ kg delivered LCB	0.22	0.50	0.02	-4.32	-4.30	-4.32
Seed application/ Rhizomes	Wheat seeds		4.59E-03	1.08E-02	0	2.26E-04	5.30E-04	0
	Miscanthus rhizomes		0	0	0	2.51E-03	2.51E-03	2.51E-03
Nitrogen fertiliser	Ammonium nitrate		8.60E-02	2.02E-01	0	4.62E-02	5.20E-02	4.19E-02
	Ammonium sulphate		0	0	0	0	0	0
	Calcium ammonium nitrate		0	0	0	0	0	0
	Urea		0	0	0	0	0	0
Phosphate fertiliser	Monoammonium phosphate		0	0	0	0	0	0
	Diammonium phosphate		0	0	0	0	0	0
	Single superphosphate		0	0	0	0	0	0
	Triple superphosphate		2.99E-03	7.01E-03	0	1.05E-03	1.25E-03	9.00E-04
Potassium fertiliser	Potassium chloride		9.81E-04	2.30E-03	0	4.83E-05	1.13E-04	0
	Potassium sulphate		0	0	0	1.13E-02	1.13E-02	1.13E-02
Calcium oxide			0	0	0	1.12E-04	1.12E-04	1.12E-04
Pesticides			4.74E-04	1.11E-03	0	9.02E-04	9.33E-04	8.78E-04
Manganese sulphate			0	0	0	2.82E-04	2.82E-04	2.82E-04
Diesel consumption on-farm			3.85E-02	9.02E-02	0	2.10E-03	4.65E-03	2.07E-04
Direct and Indirect Emission	Direct N_2O emissions		1.49E-02	3.49E-02	0	9.48E-03	1.05E-02	8.72E-03
	Indirect N_2O		1.04E-02	2.43E-02	0	1.57E-02	1.63E-02	1.52E-02
Emission from land use change	AGB		0	0	0	9.50E-02	9.47E-02	9.53E-02
	BGB		0	0	0	-1.50E+00	-1.50E+00	-1.50E+00
	SOC		4.52E-02	1.06E-01	0	-3.02	-3.02	-3.02
	Deadwood		0	0	0	0	0	0
	Litter		0	0	0	0	0	0
Transport	Road transport to storage (roundtrip)		4.24E-03	4.24E-03	4.24E-03	4.24E-03	4.24E-03	4.24E-03
	Road transport to plant (roundtrip)		4.24E-03	4.24E-03	4.24E-03	4.24E-03	4.24E-03	4.24E-03
Loading & Offloading	Diesel consumption at farm		2.87E-03	2.87E-03	2.87E-03	2.87E-03	2.87E-03	2.87E-03
	Diesel consumption at storage		5.74E-03	5.74E-03	5.74E-03	5.74E-03	5.74E-03	5.74E-03
	Diesel consumption at plant		2.87E-03	2.87E-03	2.87E-03	2.87E-03	2.87E-03	2.87E-03

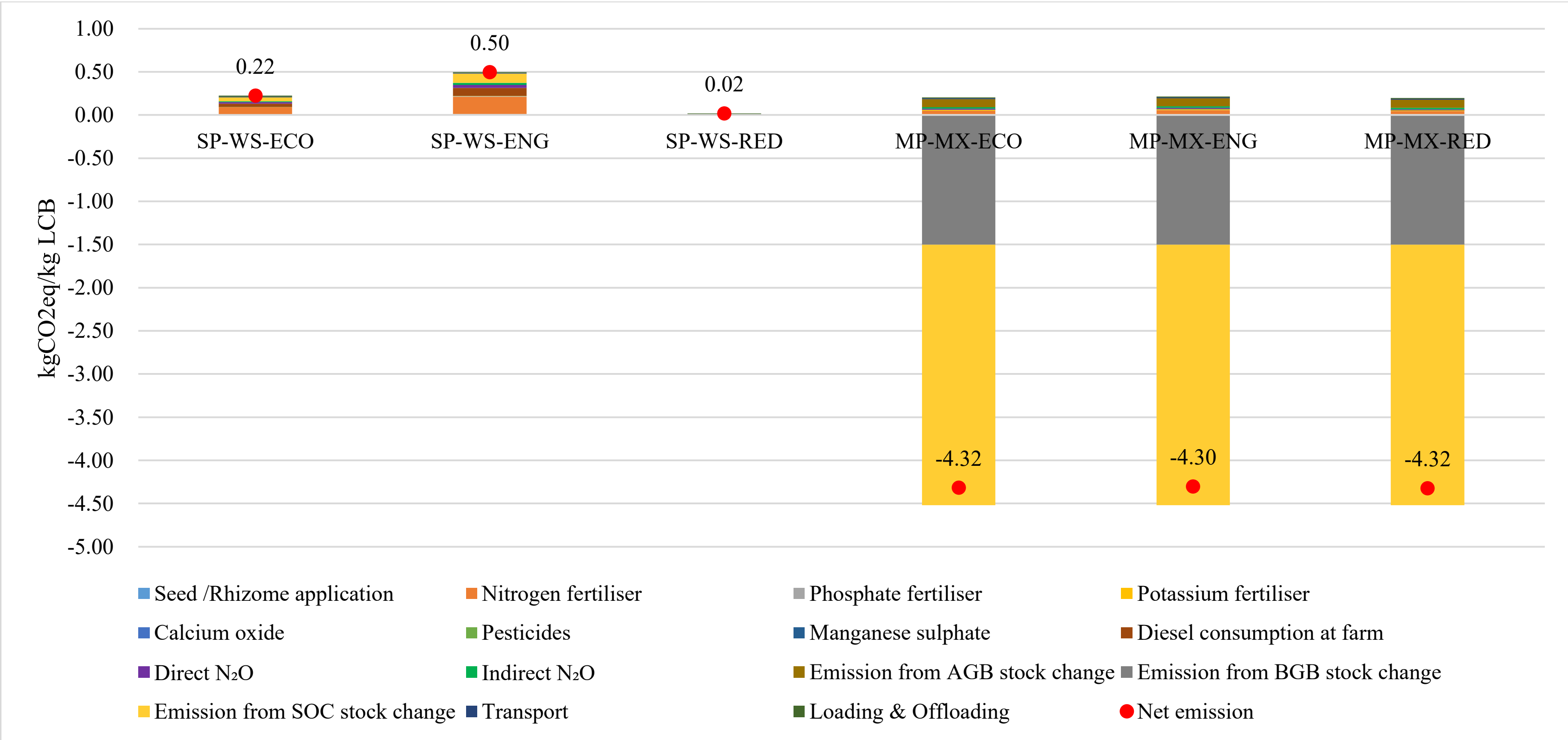

Figure 7-1 Characterised LCIA profiles of delivered LCB feedstock for difference production scenarios and allocation methods. SP-WS-ECO: SPBC production scenario producing only wheat straw feedstock using Economic allocation; SP-WS-ENG: SPBC production scenario producing only wheat straw feedstock using energy allocation(based on calorific values); SP-WS-RED: SPBC production scenario producing only wheat straw feedstock using RED allocation; MP-MX-ECO: MPBC production scenario producing mixed feedstock and using Economic allocation for wheat straw; MP-MX-ENG: MPBC production scenario producing mixed feedstock and using energy allocation for wheat straw; MP-MX-RED: MPBC production scenario producing mixed feedstock and using RED allocation for wheat straw.

7.2.3 Discussion

7.2.3.1 Allocation approach in RED

Figure 7-1 shows considerable disparities among the climate change impacts generated when comparing economic, energy and RED allocation approaches, especially when RED allocation was selected. The allocation methodology used in the RED is a simplified approach, aiming at encouraging the utilization of agricultural residues for bioenergy production, instead of reflecting the actual GHG emissions of straw production. The analysis in this thesis and the improved understanding of the potential impacts of integrated land management can then be used to inform the policy makers on how to improve current or future policy in programmes aimed at stimulating the bioeconomy. (European Commission 2018)

Additionally, if *Miscanthus* is grown on fields that are currently primarily tasked with wheat production then the biomass produced should not be categorized as a 'waste' or 'residue' and in fact, if wheat straw is harvested and baled for markets then nor should it. This means that the LCA boundary used for accounting for any form of lignocellulosic biomass provision whether food, biomaterials and/or bioenergy, should begin with field prep, prior to planting and not at the field gate.

The outcomes of this study indicate that the current allocation methodology in RED is too simple to reliably reflect the real GHG dynamics, especially when comparison with perennial crops is made. Further modification on the RED allocation is suggested.

7.2.3.2 Sensitivity analysis

Aiming to explore the variations of the climate change impacts associated with LCB provision under SP and MP scenarios, sensitivity analyses were conducted on:

- longer timescales extended to 50-year,100-year and 150 year periods
- exclusion of N_2O emissions and emissions from terrestrial carbon stock changes
- scenarios of different grain and straw prices

7.2.3.3 Influence of longer timescales on estimated climate change impacts of LCB provision

As indicated in Chapter 6, the choice of the analytical time horizon resulted in significantly different outcomes with regard to the annual average carbon stock changes calculated and which might also influence the overall climate change impacts associated with feedstock supply. Apart from the 30-year timescale applied in the LCA, longer timescales of 50 years, 100 years and 150 years were considered in the sensitivity analyses presented below.

Shown in Figure 7-2, as expected, SPBC scenario with RED allocation was the only case where GWP figures did not change with extended timescales. For other cases, when timescales longer than 30 years were applied, the yearly averaged GWPs increased, albeit in terms of a reduced carbon sink potential of MPBC scenario. The rates of change decreased with time.

Figure 7-3 presents to what degree the GHG emissions during LCB supply stage will be influenced by extended timescales, compared to 30-year timescale. Generally, MPBC scenario appeared to be more sensitive to applied timescales, compared with SPBC scenario. Applying a longer timescale beyond 30 years and till 150 years would reduce the climate change mitigation potential by 27.0% to 54.3%, depending on allocation method and timescale applied for MPBC cases. For SPBC, the reduction of estimated GHG emissions caused by extended timescales ranged from 0.0% to 17.0% depending on allocation approach and timescale applied.

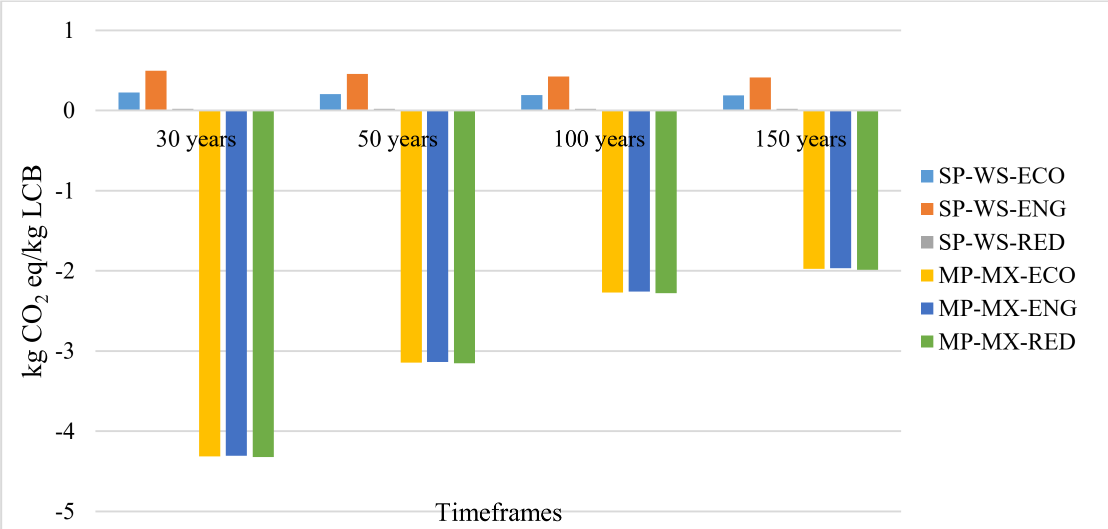

Figure 7-2 Sensitivity analysis on different timescales applied in LCA; specifications of the legends can be found in Figure 7-1.

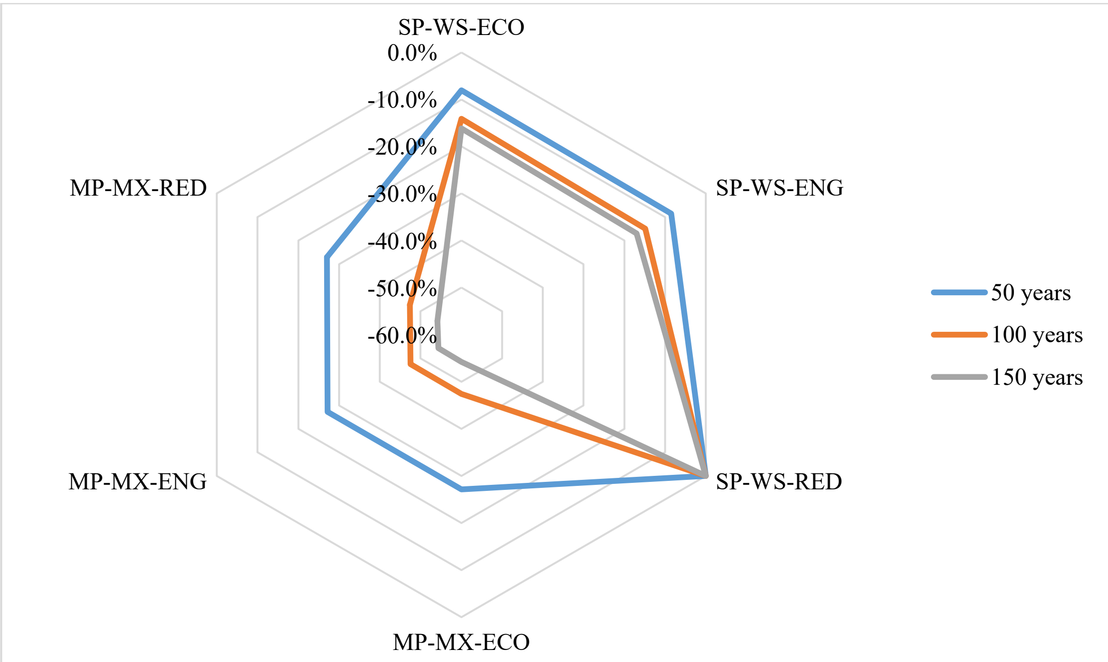

Figure 7-3 Influences of longer timescales (50, 100 and 150 years) on GHG emissions associated with LCB provisions compared with 30-year timescale; specifications of the legends can be found in Figure 7-1. Negative percentages indicate the reduction percentages of simulated sequestrations of MP scenario and GHGs emissions of SP scenario.

7.2.3.4 Influence of terrestrial carbon stock changes and N_2O emissions on estimated climate change impacts of LCB provision

As recognized by Don et al.(2012) and Pawelzik et al. (2013), whether carbon stock changes in feedstock cultivation stage were accounted was a critical aspect in provides robust outcomes from the LCAs of biomaterials, especially for those using perennial crops as feedstocks. Additionally, Guo et al. (2012) stated that the N_2O emissions were another significant component in calculating the GWP of wheat production. This section aims to investigate the impacts of including/excluding biogenic carbon stock changes and N_2O emissions during the feedstock cultivation stage on the overall GWPs associated with LCB provision for the bioeconomy.

The GWPs calculated with different accounting cases are shown in Figure 7-4 and the extents to which they influenced the GWPs compared with the 'Include carbon stock changes and N_2O accounting' case are graphed in Figure 7-5. Similar to the previous section, the GWPs from the SPBC production scenario under RED allocation remained independent from the N_2O emissions and carbon stock accounting. Figure 7-5 confirms that accounting for carbon stock changes is crucial in evaluating the GWPs of perennial LCB feedstocks. If carbon stock changes are excluded, the cultivation stage of *Miscanthus* appears as a carbon source rather than a sink.

Additionally, when the RED allocation approach was applied to wheat straw, failure to consider carbon stock change would lead to a wrong conclusion that the GHG emission factors associated with LCB feedstock could increase when *Miscanthus* was introduced into the conventional wheat production system. When either economic or energy content-based allocation was conducted, regardless of whether biogenic carbon stock changes were accounted for or not, introducing *Miscanthus* into a wheat production system would reduce the GHG emissions of the LCB feedstock production and supply stages.

Figure 7-5 demonstrates the influence on the overall climate change impacts if terrestrial carbon stock changes were excluded from the accounting framework for the MPBC scenario. The carbon sequestration potential under the MPBC scenario would be underestimated by 102.4% to 102.8% depending on allocation approach applied to wheat straw, whilst the influence of N_2O emissions on the overall GHG emissions performance appeared less significant for MPBC scenario. Excluding the accounting for N_2O emissions would overestimate the mitigation potential of MPBC by 0.55% to 0.62% all depending on allocation approach used for straw.

Compared with MPBC, SPBC scenario was more sensitive to the inclusion of N_2O emissions. Excluding N_2O emissions would underestimate GHG emissions by 11.3% for SPBC with economic allocation and 11.9% with energy content allocation. Excluding emissions from changes in carbon stocks would underestimate GHG emissions by 20.2% for SPBC with economic allocation and 21.3% with energy content allocation.

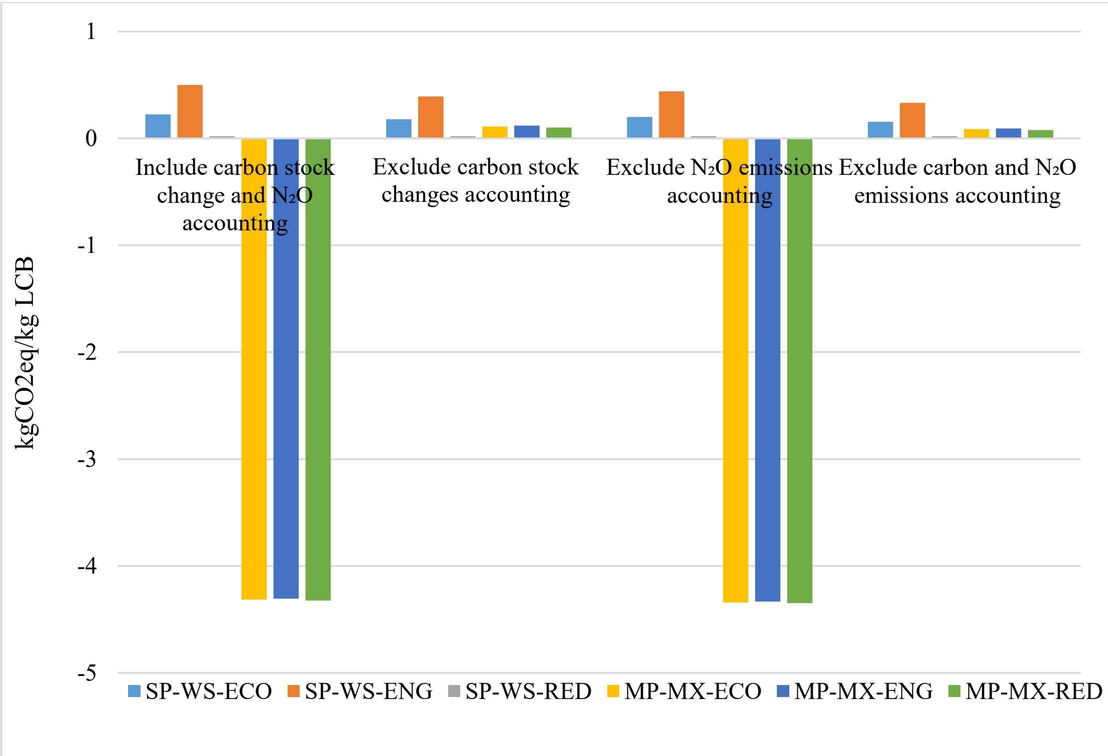

Figure 7-4 Including/excluding biogenic carbon stock changes and N_2O emissions during feedstock cultivation stage on the overall GHG emissions associated with LCB provisions; specifications of the legends can be found in Figure 7-1.

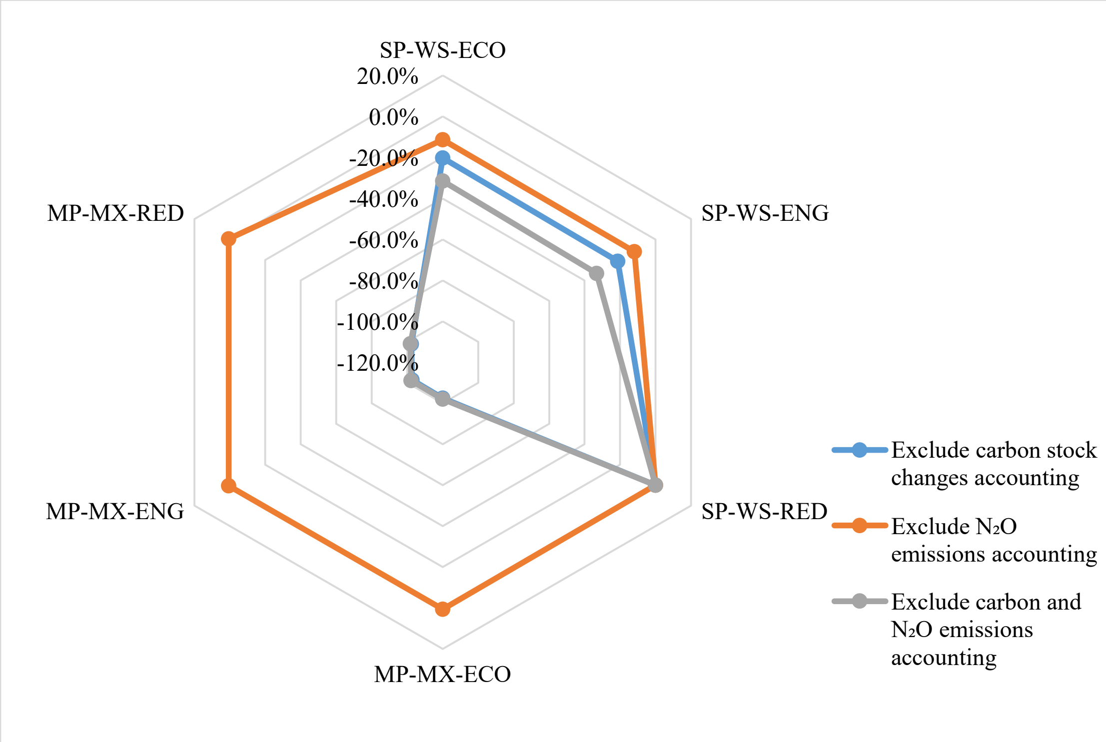

Figure 7-5 Influence of excluding terrestrial carbon stock changes and N_2O emissions on GHG emissions performance associated with LCB provisions, compared with 'Include carbon stock changes and N_2O counting' scenario; specifications of the legends can be found in Figure 7-1. Negative percentage figures indicate the levels of underestimation of GHG sequestration for MP scenario and GHG emissions of SP scenario.

7.2.3.5 Straw and grain prices

Straw price is a key factor influencing the sustainability performance of lignocellulosic biomaterial production systems from social, economic and environmental aspects. Lignocellulosic bioethanol or biomaterial production plants would benefit financially from access to straw at lower prices as production costs are reduced. (Littlewood et al. 2013) However, a 'higher' straw price which is attractive to farmers would be needed to secure the conversion plant's feedstock supply, as feedstock availability has been identified as one of the uncertainties regarding the development of lignocellulosic bioenergy and biomaterial systems. (Carriquiry et al. 2011; Spatari et al. 2005) Moreover, as a basis of economic allocation, straw prices also influence the reported GWP associated with LCB supply when an LCA is conducted.

Straw prices are highly volatile (Appendix B). They can triple during a year of poor supply. (Whittaker et al. 2011) It is also predicted that straw price may increase when Lignocellulosic succinic acid plants are established. (Kaufman et al. 2010) This section investigates the impacts of different levels of grain and straw prices on the LCA results by perturbing the economic allocation. Four price scenarios were established based on the three-year historical highest/lowest wheat grain and straw prices from June 2015 to June 2018 (Appendix B)[12]. Those four price scenarios were High Grain Low Straw (HGLS), High Grain High Straw (HGHS), Low Grain High Straw (LGHS) and Low Grain Low Straw (LGLS).

Table 7-4 Wheat straw and grain prices for different price scenarios; three-year average values were used to decide the economic allocation factor in the LCA.

Price scenarios	Straw price (£/t)	Grain Price(£/t)
LSHG	31	159
HSHG	91	159
LSLG	31	100
HSLG	91	100
Three-year average	49	127

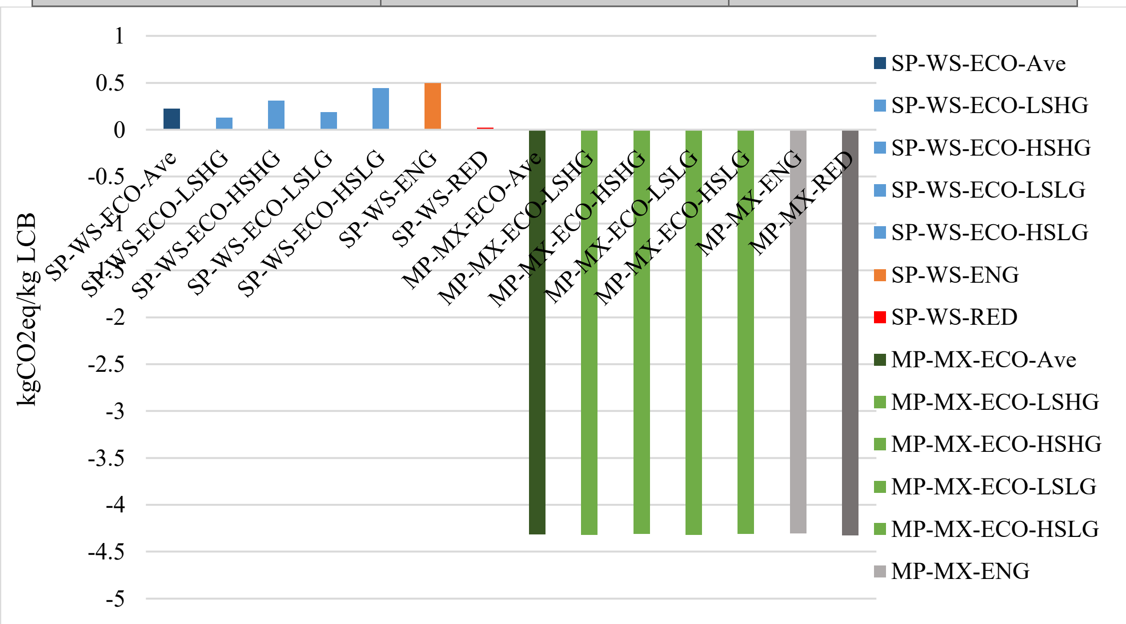

Figure 7-6 Climate change impacts associated with LCB supply under different wheat grain and straw price scenarios; Ave, LSHG, HSHG, LSLG and HSLG refer to different price levels for wheat grain and straw used in economic allocations with the details given in Table 7-4; specifications of the other legends can be found in Figure 7-1.

[12] Online data sources from AHDB database, information available at: https://dairy.ahdb.org.uk/market-information/farm-expenses, accessed on 21 Nov 2018.

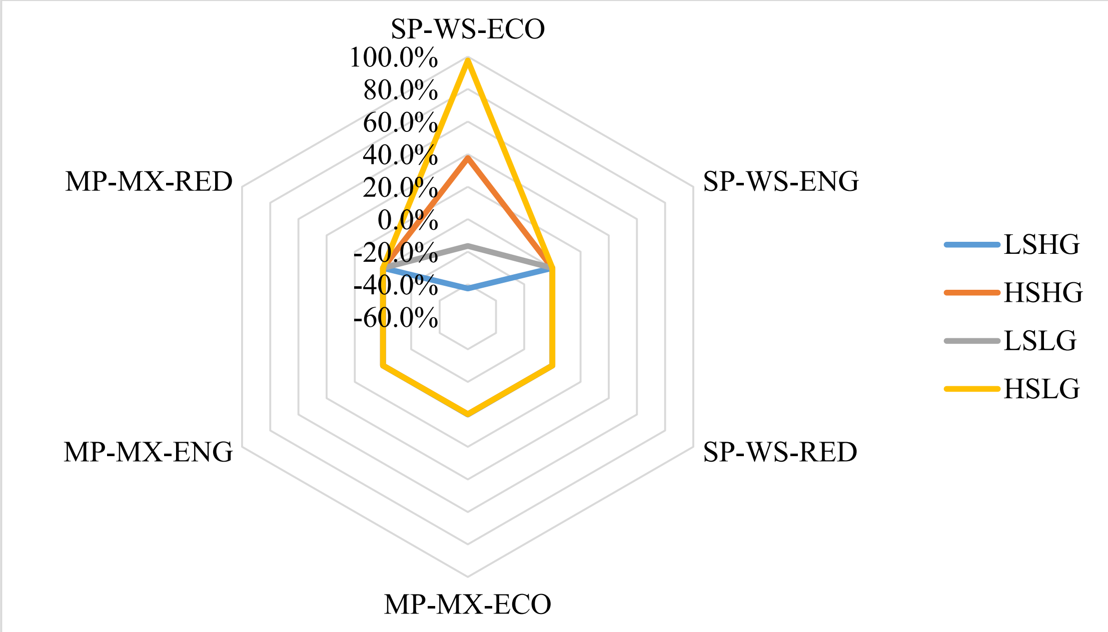

Figure 7-7 Influences of different wheat grain and straw prices levels on GHG emissions associated with LCB supply; compared with the price level (three-year averaged prices) used in this study; positive figures indicate the increase level of estimated GHGs emitting effects for SP scenario; negative figures indicate the decrease of estimated GHG sequestrations of MP scenario and GHGs emitting effects of SP scenario.

Generally, when economic allocation was applied, reported GHG emissions associated with LCB provision tended to increase under high straw prices and/or low grain price scenario, and tended to decrease when straw prices decline or grain price increase. As the larger price of straw/price of grain is, the larger proportion of emitted GHGs would be attributed to the production of straw.

In this work, the influences of different straw and grain prices on MPBC production scenario were limited due to the limited proportion of straw in total LCB supply.as shown in Figure 7-7, for MPBC, the carbon sequestration potential would be reduced by 0.2% in the HSLG price scenario and increase by 0.1% in the LSHG scenario.

For SPBC provision scenario, the changes of straw or grain prices would have considerable influences on the LCA generated figures for climate change impacts (Figure 7-7). Under the HSLG price scenario, the GHG emissions associated with LCB provision would increase by 97.6% and under LSHG scenario, the reported emissions would decrease by 42.6%.

7.3 Cradle to end-of-life LCA of bio-plastic end-products

7.3.1 LCIA Characterization results

As described in Section 3.6.2, cradle to end-of-life climate change impacts of plastic tray and mulch film production were presented (Table 7-5) and graphed for SE (Figure 7-8) and OS (figure 7-9) pretreatment options. LCB-based succinic acid were assumed be produced in an integrated site (integration of pretreatment and SA production)

7.3.1.1 Maize grain-based plastic products and petrochemical products

Climate change impacts of maize grain-based plastic products ranges from 4.11 to 6.72 kg CO_2 eq/kg product, depending on product type (partly-bio ‘pb’ or fully-bio ‘fb’, tray or film) and end-of-life treatment options. For maize grain-based fb PBS tray, if incineration was chosen as the end-of-life treatment, the climate change impact was 14.3% lower than one of its petro-based alternative PET trays, while 1.7% higher than PP trays. Composting as another end-of-life treatment for fb PBS tray would increase the GHG emissions by 9.8% compared with incineration. Similarly, the climate change impact of maize grain-based fb PBS film was 16.9% lower than PE film. However, all maize grain-based pb PBS products were higher than the current incumbent petro-based products in terms of GHG emissions.

7.3.1.2 Climate change impacts of LCB-based plastic end products

As illustrated in Figure 7-8 and Figure 7-9, there are significant variations among GHG emissions of different LCB-based PBS production scenarios. The lowest GHG emissions (-25.10 kg CO_2eq/kg product) occurred at MP-FB-Tray-Inc case (Table 7-5), when fb PBS trays were produced from mixed feedstocks, with SE pretreatment and incineration as end-of-life treatment. The highest GHG emissions (6.71 kg CO_2 eq/kg product) was a consequence of SP-PB-Tray-Com case, when pb PBS trays were produced from single feedstock (wheat straw) with OS pretreatment and composting as the end-of-life treatment.

The impacts of different end-of-life options on the overall climate change impacts of LCB-based plastics were relatively small. Generally, regardless of other production choices (feedstock composition, provision scenario, fully or partly biobased and pretreatment options), incineration could result in a reduction of 0.5 kg CO_2eq per kg product compared with composting.

GHG emissions were lower for fb cases than pb cases. This was caused by no fossil fuel-based BDO requirement during fb polymer production, extra energy credits from bio-DBO production, no fossil-based CO_2 emissions during end-of-life treatment. Although during the end-of-life stage, biogenic carbon emissions appeared to be higher in fb products compared with pb products, these biogenic emissions were offset by the biogenic carbon embedded in the products. In the MP scenarios where *Miscanthus* was used as feedstock in addition to wheat straw, extra carbon credits were also achieved as a result of increased terrestrial carbon storage.

Compared with OS pretreatment option, GHG emissions of products produced through SE method were around 1.05 to 2.3 kg CO_2 eq per kg fb products and 0.44 to 0.99 kg CO_2 eq per kg pb products.

For LCB-based plastics produced from MPBC feedstock provision scenario, GHG emissions ranged from -23.62 to -25.10kg CO_2eq/kg product for fp products and ranged from -5.98 to -6.54 kg CO_2eq/kg product for pb products. In all the cases when feedstock was sourced from the MPBC scenario, carbon sequestration could be achieved even for pb products.

Table 7-5 Production cases and associated total climate change impacts (kg CO_2eq/kg product) of considered LCB-based, maize grain-based and petrochemical products.

Case		Feedstock(s)	Pretreatment[5]	Product type		End-of-life	Total impact
LCB-based	SP[1]-FB[2]-Tray-Inc[3]	ws[4]	SE	FB	Tray	Incineration	2.49
	SP-FB-Tray-Com	ws	SE	FB	Tray	Composting	2.91
	MP-FB-Tray-Inc	Mis+ws	SE	FB	Tray	Incineration	-25.10
	MP-FB-Tray-Com	Mis+ws	SE	FB	Tray	Composting	-24.68
	SP-FB-Tray-Inc	ws	OS	FB	Tray	Incineration	4.79
	SP-FB-Tray-Com	ws	OS	FB	Tray	Composting	5.21
	MP-FB-Tray-Inc	Mis+ws	OS	FB	Tray	Incineration	-24.08
	MP-FB-Tray-Com	Mis+ws	OS	FB	Tray	Composting	-23.66
	SP-PB-Tray-Inc	ws	SE	PB	Tray	Incineration	5.30
	SP-PB-Tray-Com	ws	SE	PB	Tray	Composting	5.72
	MP-PB-Tray-Inc	Mis+ws	SE	PB	Tray	Incineration	-6.54
	MP-PB-Tray-Com	Mis+ws	SE	PB	Tray	Composting	-6.12
	SP-PB-Tray-Inc	ws	OS	PB	Tray	Incineration	6.29
	SP-PB-Tray-Com	ws	OS	PB	Tray	Composting	6.71
	MP-PB-Tray-Inc	Mis+ws	OS	PB	Tray	Incineration	-6.11
	MP-PB-Tray-Com	Mis+ws	OS	PB	Tray	Composting	-5.69
	SP-FB-Film-BDG	ws	SE	FB	Film	Biodegradation	2.38
	MP-FB-Film-BDG	Mis+ws	SE	FB	Film	Biodegradation	-24.92
	SP-FB-Film-BDG	ws	OS	FB	Film	Biodegradation	4.65
	MP-FB-Film-BDG	Mis+ws	OS	FB	Film	Biodegradation	-23.90
	SP-PB-Film-BDG	ws	SE	PB	Film	Biodegradation	5.12
	MP-PB-Film-BDG	Mis+ws	SE	PB	Film	Biodegradation	-6.43
	SP-PB-Film-BDG	ws	OS	PB	Film	Biodegradation	6.09

	MP-PB-Film-BDG	Mis+ws	OS	PB	Film	Biodegradation	-6.00
Starch-based	MG-FB-Tray-Inc	Maize grain	NA	FB	Tray	Incineration	4.29
	MG-FB-Tray-Com	Maize grain	NA	FB	Tray	Composting	4.71
	MG-PB-Tray-Inc	Maize grain	NA	PB	Tray	Incineration	6.72
	MG-PB-Tray-Com	Maize grain	NA	PB	Tray	Composting	7.14
	MG-FB-Film-BDG	Maize grain	NA	FB	Film	Biodegradation	4.11
	MG-PB-Film-BDG	Maize grain	NA	PB	Film	Biodegradation	6.51
Petro-based	PP-Tray-Inc	PP	NA	NA	Tray	Incineration	4.22
	PET-Tray-Inc	PET	NA	NA	Tray	Incineration	5.01
	PE-Film-Inc	PE	NA	NA	Film	Incineration	4.95

1. *SP =SPBC; MP =MPBC; MG =maize grain;*
2. *FB =fully bio-based; PB=partly bio-based;*
3. *Inc =Incineration; Com =Composting; BDG =bio-degradation on field;*
4. *NA = not applicable.*
5. *Pretreatment options: ‘SE’ = steam explosion. ‘OS’ = organic solvent*

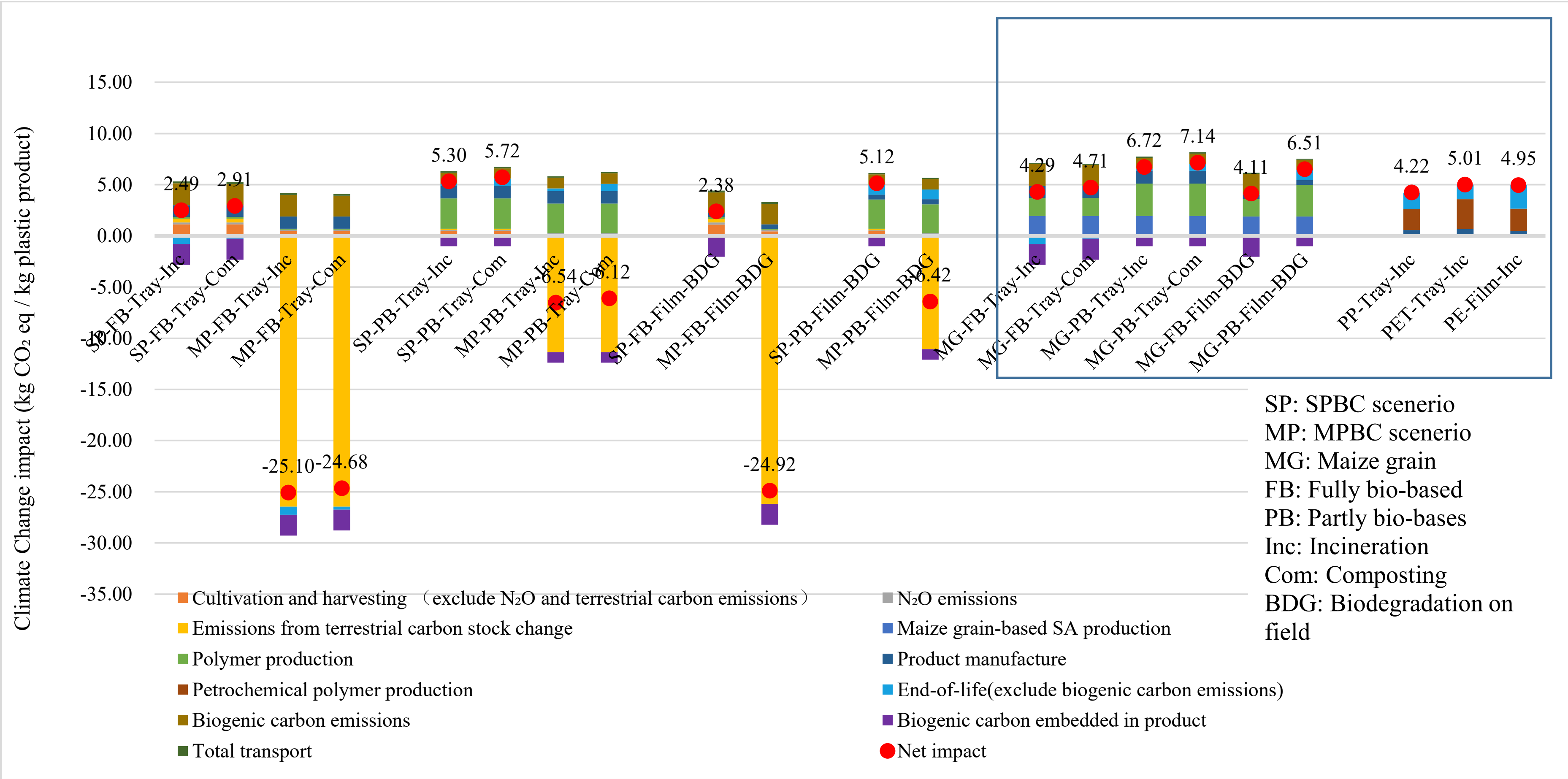

Figure 7-8 Characterised LCIA profiles: cradle to end-of-life climate change impacts for plastic trays and mulch films made from LCB (through SE pretreatment in an integrated site) and maize grain based PBS, for both fully bio-based (fb) and partly bio-based (pb), as well as petrochemical (PP,PET and PE) products. Reference products (maize grain based and petrochemical products) are grouped on the right side.

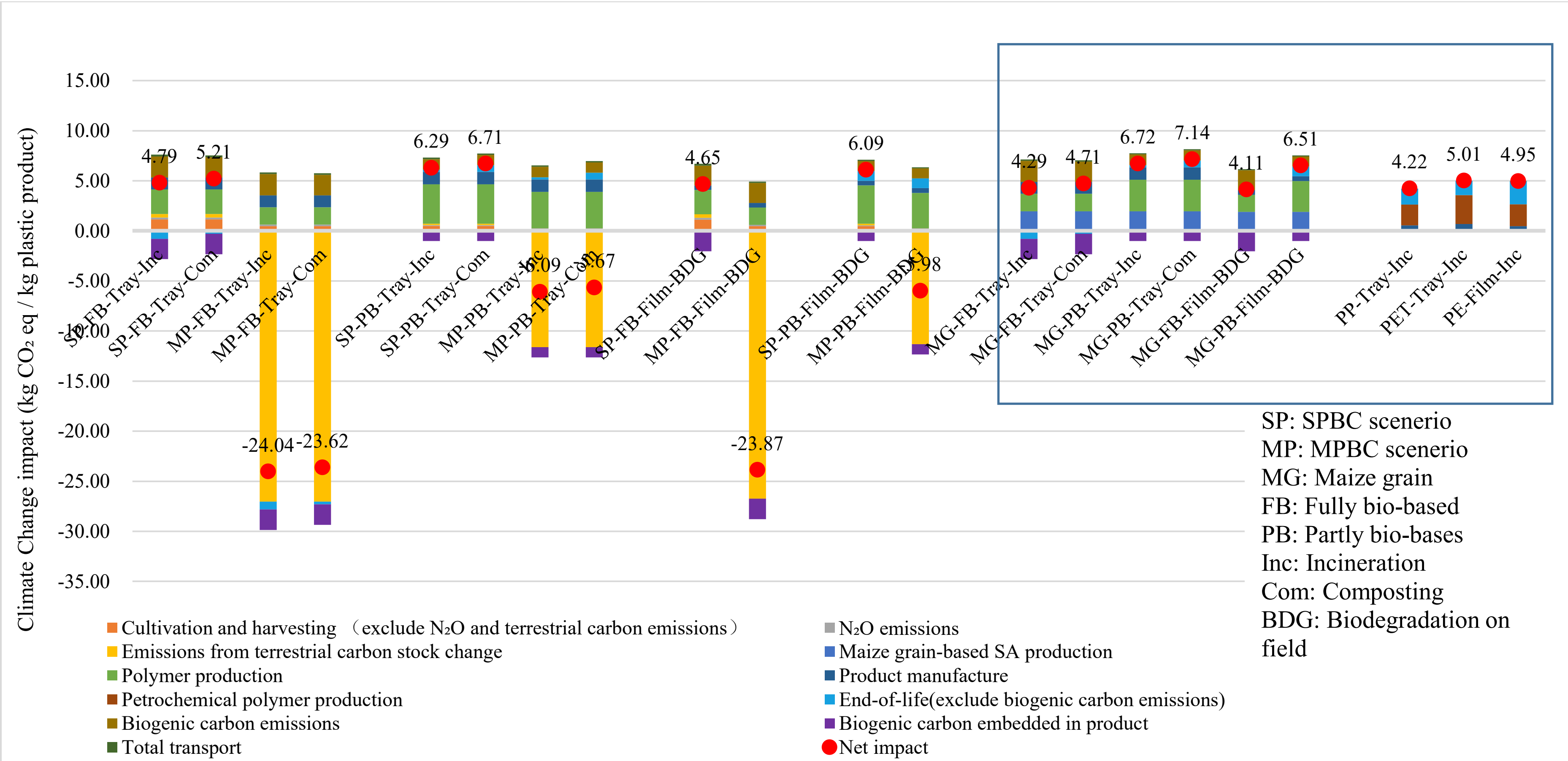

Figure 7-9 Characterised LCIA profiles: cradle to end-of-life climate change impacts for plastic trays and mulch films made from LCB (through OS pretreatment in an integrated site) and maize grain based PBS for both fully bio-based (fb) and partly bio-based (pb), as well as petrochemical (PP,PET and PE) products. Reference products (maize grain based and petrochemical products) are grouped on the right side.

For LCB-based plastics produced from SPBC feedstock provision scenario, GHG emissions ranged from 2.38 to 5.21 kg CO_2 eq/kg product for fb products and ranged from 4.65 to 6.71 kg CO_2 eq/kg product for pb products. Compared with maize grain-based fb tray, SP-LCB-based fb tray could reduce GHG emissions by around 40% when produced through SE pretreatment. Similarly, SP-LCB-based fb film produced through SE could reduce GHG emissions by 42% compared with the grain-based product. When produced through OS pretreatment, SP-LCB-based fb products could result in GHG emissions reduction by 11% to 13%, compared with grain-based alternatives with the same end-of-life treatment options. While compared with maize grain-based pb tray and film, SP-LCB-based pb products were able to achieve GHG emissions reduction by approximately 20% under SE pretreatment and by 6% under OS pretreatment.

7.3.1.3 Climate change impacts in bio-polymer production through SE and OS pretreatment options

Apart from the different GHG emissions performance associated with feedstock cultivation, another major difference between LCB-based SA production and starch-based SA production is that pretreatment process required for LCB feedstock to increase rate of the enzyme accessibility and improve digestibility of cellulose. (Alvira et al. 2010) SE and OS, two pretreatment options were considered in this project, and the impacts of these two methods were mainly on the polymer production stage (Figure 7-8, Figure 7-9 and Table 7-6). While the difference of C6 monomers yields between the two options were minor. For wheat straw, C6 yields produced through OS was 324kg/t biomass and through SE was 326 kg/t biomass. (Patel et al. 2018) Similarly, for *Miscanthus*, C6 yields through OS was 418 kg/t biomass and through SE was 427 kg/t biomass.(Patel et al. 2018) The table below presented the climate change impacts of polymer production stage for SE and OS pre-treated LCB-based products, as well as maize grain-based products.

For LCB-based fb cases, SE option could reduce GHG emissions in polymer production stage by 2.26 to 2.28 $kgCO_2eq$ for per kg SP-based product compared with OS option.

This figure for MP-based product was 1.64 to 1.65 $kgCO_2eq/kg$ product. For LCB-based pb cases, the GHG emission reductions of SE compared with OS were around 0.69 to 0.98 $kgCO_2eq/kg$ product, depending on product type (tray or film) and difference feedstock provision scenario. For grain-based products, emissions during polymer production stage were around 1.70 to 3.15$kgCO_2eq/kg$ product depending on different production scenario.

Table 7-6 Climate change impacts ($kgCO_2eq/kg$ product) of polymer production stages for LCB-based products with different pretreatment options (SE and OS) and maize-grain based productions (with no pretreatment required).

Cases		Polymer production through SE pretreatment	Polymer production through OS pretreatment	Difference (SE-OS)	Polymer production with no pretreatment
LCB-based	SP-FB-Tray-Inc	0.16	2.44	-2.28	
	SP-FB-Tray-Com	0.16	2.44	-2.28	
	MP-FB-Tray-Inc	0.09	1.74	-1.65	
	MP-FB-Tray-Com	0.09	1.74	-1.65	
	SP-FB-Film-BDG	0.15	2.41	-2.26	
	MP-FB-Film-BDG	0.08	1.72	-1.64	
	SP-PB-Tray-Inc	2.94	3.92	-0.98	
	SP-PB-Tray-Com	2.94	3.92	-0.98	
	MP-PB-Tray-Inc	2.91	3.62	-0.71	
	MP-PB-Tray-Com	2.91	3.62	-0.71	
	SP-PB-Film-BDG	2.87	3.82	-0.96	
	MP-PB-Film-BDG	2.84	3.53	-0.69	
Maize grain-based	MG-FB-Tray-Inc				1.75
	MG-FB-Tray-Com				1.75
	MG-FB-Film				1.70
	MG-PB-Tray-Inc				3.15
	MG-PB-Tray-Com				3.15
	MG-PB-Film-BDG				3.08

It is noticeable that when the SE pretreatment method was applied, the total GHG emissions in polymer production appeared to be much smaller than all the other bio-based cases. Even when compared with grain based-cases, where pretreatment processes were not required, polymer production emissions were 1.55 to 1.66

$kgCO_2eq$/kg product lower in fb-SE cases and 0.21 to 0.25 $kgCO_2eq$/kg product lower in pb-SE cases. This is due to the energy credits gained from biogas produced in both pretreatment and fermentation processes. Compared with pb, additional energy savings in fb were also achieved through bio-DBO production.

7.3.2 Contribution analysis

The contributions of each stage and component to the overall climate change impact of each considered plastic production case were reflected in Figure 7-8 and Figure 7-9, with detailed percentages presented in Table 7-7.

As illustrated in Figure 7-8 and 7-9, for the cases with carbon sequestrations (shown as negative climate change impacts factors in Table 7-7), terrestrial carbon sequestration during feedstock cultivation provided the dominating contribution, accounting for 90% to 93% (Table 7-7) of total carbon sequestration. For LCB-based cases with positive GHG emissions figures, emissions from agricultural production (including cultivation, harvesting, N_2O emissions and terrestrial carbon emissions) accounted for 10% to 37% of the life cycle GHG emissions.

As reference cases, fewer production scenarios were established for maize-grain based products, thus smaller variance was observed for the contribution of each stage and component compared with LCB-based cases. Emissions associated with feedstock (wheat grain) production accounted for 24% to 31% of the life GHG emissions. Another major contribution was from the polymer production stage, which accounted for 27% to 41% of the total GHG emissions. This is higher than some of the LCB-based cases, due to the lack of energy credits from pretreatment and/or bio-BDO production. Detailed explanation was given in 7.2.1.3.

Table 7-7 Contributions (in %) of each stage and component to the overall climate change impact (kg CO_2eq/kg product) of considered plastic production case. (Specifications of cases were included in Table 7-5; In terms of total climate change impacts, GHG emissions are presented in black and GHG sequestration (negative figures) are highlighted in red; For contributions of each component, figures coloured in black are the contributing proportions to emissions, while figures in red are the proportions to sequestrations)

Case		Total climate change impact	Cultivation and harvesting (exclude N_2O and terrestrial C emissions)	N_2O emissions	Emissions from terrestrial C stock change	Maize grain-based SA production	Polymer production	Product manufacture	Petrochemical polymer production	End-of-life (exclude biogenic carbon emissions)	Biogenic C emissions	Biogenic C embedded in product	Transportation
LCB - (SE pre-treated) product	SP-FB-Tray-Inc	2.49	21.1%	3.7%	6.6%		3.0%	22.3%		27.8%	39.9%	72.2%	3.4%
	SP-FB-Tray-Com	2.91	21.5%	3.7%	6.7%		3.0%	22.7%		12.2%	39.0%	87.8%	3.4%
	MP-FB-Tray-Inc	-25.10	10.9%	3.6%	90.3%		2.1%	28.3%		2.7%	50.7%	7.0%	4.4%
	MP-FB-Tray-Com	-24.68	11.1%	3.7%	91.9%		2.2%	28.9%		1.0%	49.7%	7.1%	4.5%
	SP-PB-Tray-Inc	5.30	7.6%	1.3%	2.4%		46.5%	19.6%		3.6%	16.8%	100.0%	2.2%
	SP-PB-Tray-Com	5.72	7.2%	1.2%	2.2%		43.6%	18.4%		10.2%	15.1%	100.0%	2.1%
	MP-PB-Tray-Inc	-6.54	3.4%	1.1%	91.7%		51.6%	21.2%		3.9%	18.2%	8.3%	2.5%
	MP-PB-Tray-Com	-6.12	3.1%	1.0%	91.7%		48.0%	19.8%		11.0%	16.3%	8.3%	2.3%
	SP-FB-Film-BDG	2.38	25.1%	4.4%	7.8%		3.4%	10.3%		0.0%	45.0%	100.0%	4.0%
	MP-FB-Film-BDG	-24.92	13.6%	4.5%	92.8%		2.5%	13.7%		0.0%	60.2%	7.2%	5.5%
	SP-PB-Film-BDG	5.12	7.7%	1.3%	2.4%		46.6%	7.8%		15.8%	16.2%	100.0%	2.2%
	MP-PB-Film-BDG	-6.42	3.4%	1.1%	91.6%		50.0%	8.4%		17.1%	17.5%	8.4%	2.5%
LCB - (OS pre-treated) product	SP-FB-Tray-Inc	4.79	14.9%	2.6%	4.6%		32.1%	15.6%		27.8%	27.9%	72.2%	2.4%
	SP-FB-Tray-Com	5.21	15.0%	2.6%	4.7%		32.4%	15.8%		12.2%	27.1%	87.8%	2.4%
	MP-FB-Tray-Inc	-24.04	8.0%	2.6%	90.5%		29.9%	20.4%		2.6%	36.5%	6.8%	2.6%
	MP-FB-Tray-Com	-23.62	8.1%	2.7%	92.1%		30.4%	20.7%		1.0%	35.6%	7.0%	2.6%

	SP-PB-Tray-Inc	6.29	6.7%	1.2%	2.1%		53.6%	16.9%		3.1%	14.5%	100.0%	1.9%
	SP-PB-Tray-Com	6.71	6.3%	1.1%	2.0%		50.7%	16.0%		8.9%	13.2%	100.0%	1.8%
	MP-PB-Tray-Inc	-6.09	3.1%	1.0%	91.9%		57.1%	18.9%		3.5%	16.3%	8.1%	1.9%
	MP-PB-Tray-Com	-5.67	2.9%	0.9%	91.9%		53.6%	17.8%		9.9%	14.7%	8.1%	1.8%
	SP-FB-Film-BDG	4.65	16.8%	2.9%	5.2%		36.0%	6.8%		0.0%	29.7%	100.0%	2.6%
	MP-FB-Film-BDG	-23.87	9.4%	3.1%	92.9%		34.9%	9.2%		0.0%	40.4%	7.1%	3.0%
	SP-PB-Film-BDG	6.09	6.7%	1.2%	2.1%		53.8%	6.7%		13.7%	14.0%	100.0%	1.9%
	MP-PB-Film-BDG	-5.98	3.1%	1.0%	91.7%		55.5%	7.5%		15.3%	15.6%	8.3%	2.0%
Maize grain-based product	**MG-FB-Tray-Inc**	4.29				27.4%	24.5%	16.7%		27.8%	29.8%	72.2%	1.6%
	MG-FB-Tray-Com	4.71				27.7%	24.8%	16.9%		12.2%	29.0%	87.8%	1.6%
	MG-PB-Tray-Inc	6.72				25.2%	40.8%	16.0%		2.9%	13.7%	100.0%	1.5%
	MG-PB-Tray-Com	7.14				23.9%	38.7%	15.2%		8.4%	12.5%	100.0%	1.4%
	MG-FB-Film-BDG	4.11				30.9%	27.6%	7.4%		0.0%	32.3%	100.0%	1.8%
	MG-PB-Film-BDG	6.51				25.2%	40.9%	6.3%		12.9%	13.2%	100.0%	1.5%
Petrochemical product	**PP-Tray-Inc**	4.22						13.3%	48.6%	38.1%			
	PET-Tray-Inc	5.01						13.7%	57.7%	28.5%			
	PE-Film-Inc	4.95						9.7%	44.0%	46.1%			0.2%

During the life cycle of petrochemical tray products, polymer production from petroleum occupied the largest proportion (approximately 50% to 60%) of total climate change impacts. It was then followed by end-of-life treatments, which accounted for 29% to 38% of total emissions as a result of petro-based CO_2 emitted to air. In contrast, emissions from end-of-life treatment represented as the biggest component of PE-film life cycle, due to an extra baling process was needed to collect films (having been used as plastic mulches) from field. Moreover, extra transport was caused for films being transported from farms to incineration plants.

7.3.3 Discussion

7.3.3.1 Accounting for biogenic carbon stock in bio-based plastic end-products

In this study biogenic carbon embedded in bio-based end products were accounted for in both LCB-based and maize grain-based life cycles. Due to a lack of specific guidance provided by ISO (ISO 2006) standards on considering embedded biogenic carbon as carbon-neutral or as a carbon store for bio-based material life cycles, there have been ongoing debates and inconsistency in different approaches in dealing with this issue. (Pawelzik et al. 2013)

Although even considered as temporary/transient carbon storage, it has proved to be necessary to account for the embedded biogenic carbon in this study. If biogenic embedded carbon was not accounted for in the bio-products, then in the end-of-life treatments the biogenic carbon emission should also be considered as neutral and excluded from inventory development. This would result in the same estimated climate change impact figures when products were actually treated with different end-of-life management options. As shown in table 7-5, there was approximated 5% difference in biogenic CO_2 emissions between the incineration and compositing options.

7.3.3.2 Sensitivity analysis

Sensitivity analyses were conducted on four areas, including using of Tier 2 approaches estimated terrestrial carbon stock change figures (Figure 7-10); exclusion of N_2O and terrestrial carbon emissions in accounting framework (Figure 7-11); extended timeframes of 50-year, 100-year and 150-year periods (Figure 7-12); and four assumed price levels of wheat grain and straw (Figure 7-13).

The influences from applying Tier 3 or Tier 2 estimated values within 30-year timeframe and for the overall climate change impacts were relatively limited (Figure-10). This suggested the capability of IPCC 2006-AFOLU default Tier 2 approaches in estimating carbon stock changes for the purpose under 'crop-land remaining cropland' management regime, within 30-year timeframe.

As indicated in Figure 7-12, when extended timeframes were applied, the carbon sequestration effects associated with mixed production strategy become less significant compared with 30-years' timeframe. For SP-based case, the application of different timeframes shows limited impacts on the LCA outputs. However for MP cases, the choice of different timeframes generated significantly different outcomes with regard to potential climate mitigation potential. For MP-fb cases, the biggest decline in carbon sequestration effect happens during the 30^{th} to 50^{th} year, from around 25kgCO_2eq/kg product to 9 kgCO_2eq/kg product, while the difference between 50-year, 100-year and 150-year timeframes were only 1-2 kgCO_2eq/kg product. For MP-pb cases, applications of 50-year and longer timeframes have offset the original carbon sink effects appeared in the 30-year simulations, and turned the MP-pb-PBS products into a carbon pool with the emission factors of 0.06-1.7 kgCO_2eq/kg product.

Excluding N_2O and terrestrial carbon stock changes imposed significant limitations on the overall climate change impacts of LCB-based feedstocks. Based on the sensitivity analysis conducted in 7.1.3.2, the alteration on MP-based cases was largely attributed to the carbon sequestration during *Miscanthus* cultivation. While for SP-based cases, this alteration was mainly caused by N_2O emissions.

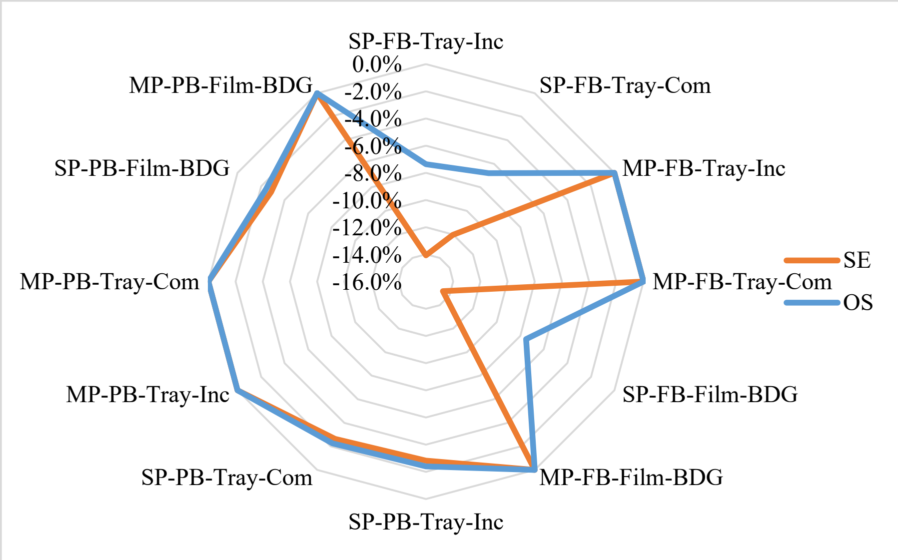

Figure 7-10 Sensitivity analysis results: replacing Tier 3 estimated terrestrial carbon stock changes with Tier 2 estimated values (for 30-year timeframe) compared with Tier 3-based results; negative percentages indicate the level of reduction for GHG sequestrations of MP-based cases and GHG emissions of SP-based cases compared with Tier 3-based results

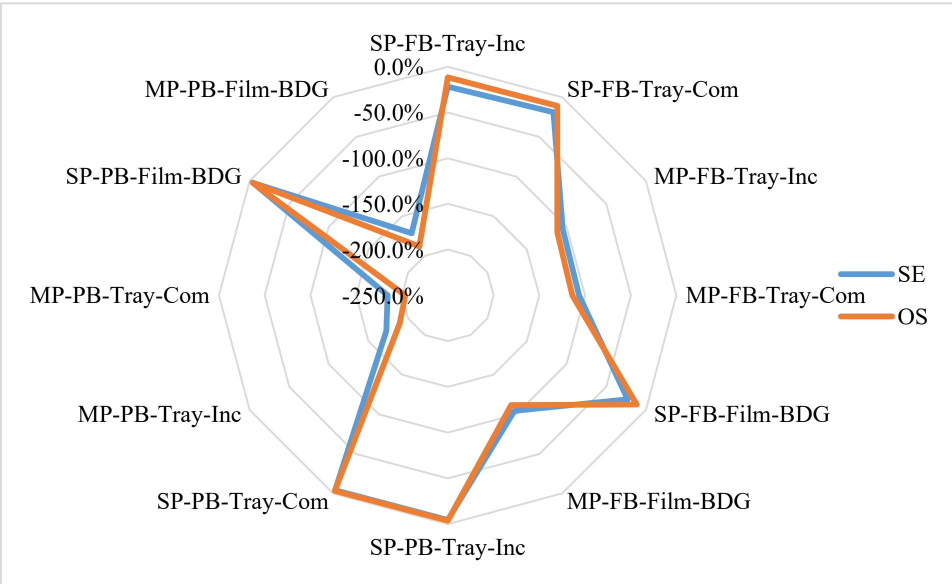

Figure 7-11 Sensitivity analysis results: excluding N_2O emissions accounting and terrestrial carbon stock changes, compared with 'both accounted figures'; negative percentages indicate the level of reduction for estimated GHG sequestrations of MP-based cases and GHG emissions of SP-based cases; negative percentages lower than -100% indicate that in this specific case, excluding N_2O and terrestrial carbon stock changes has turned the GHGs sequestrating effects into GHGs emitting effects for all MP-based cases.

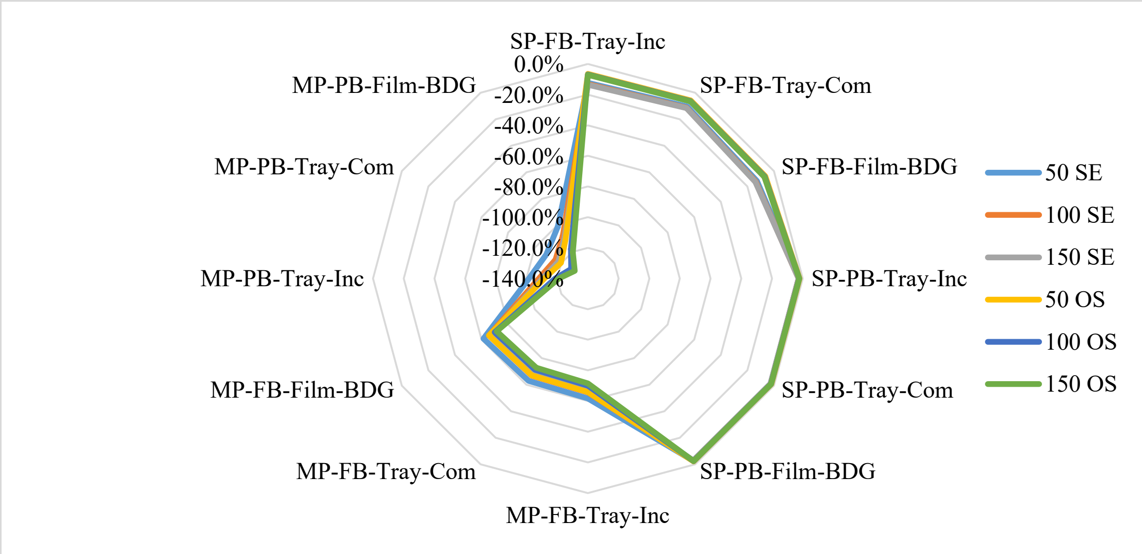

Figure 7-12 Sensitivity analysis results: influences of extended timeframes applied in LCA of LCB; negative percentages indicate the level of reduction for estimated GHG sequestrations of MP-based cases and GHG emissions of SP-based cases, compared with 30-year timeframe used in this study; negative percentages lower than -100% indicate that in this specific case, the extended timeframe has turned the GHGs sequestrating effects into GHGs emitting effects for some of the cases.

Table 7-8 Sensitivity analysis results: Climate change impacts (kgCO$_2$eq/kg product) of PBS products from difference production scenarios, under 30-, 50-, 100- and 150-year simulation timeframes.

Timeframe	**30-year**	**50-year**	**100-year**	**150-year**	**30-year**	**50-year**	**100-year**	**150-year**
	SE pre-treatment				OS pre-treatment			
SP-FB-Tray-Inc	2.49	2.18	2.16	2.15	4.79	4.48	4.45	4.45
SP-FB-Tray-Com	2.91	2.60	2.58	2.57	5.21	4.90	4.88	4.87
MP-FB-Tray-Inc	-25.10	-9.61	-8.61	-8.28	-24.04	-8.21	-7.20	-6.86
MP-FB-Tray-Com	-24.68	-9.18	-8.19	-7.86	-23.62	-7.79	-6.78	-6.44
SP-PB-Tray-Inc	5.30	5.17	5.16	5.15	6.29	6.15	6.14	6.14
SP-PB-Tray-Com	5.72	5.59	5.58	5.58	6.71	6.57	6.56	6.56
MP-PB-Tray-Inc	-6.54	0.11	0.53	0.68	-6.09	0.70	1.14	1.28
MP-PB-Tray-Com	-6.12	0.53	0.96	1.10	-5.67	1.12	1.56	1.70
SP-FB-Film-BDG	2.38	2.07	2.05	2.05	4.65	4.35	4.33	4.32
MP-FB-Film-BDG	-24.92	-9.59	-8.60	-8.28	-23.87	-8.21	-7.20	-6.87
SP-PB-Film-BDG	5.12	5.00	4.99	4.98	6.09	5.96	5.95	5.95
MP-PB-Film-BDG	-6.42	0.06	0.48	0.62	-5.98	0.65	1.07	1.21

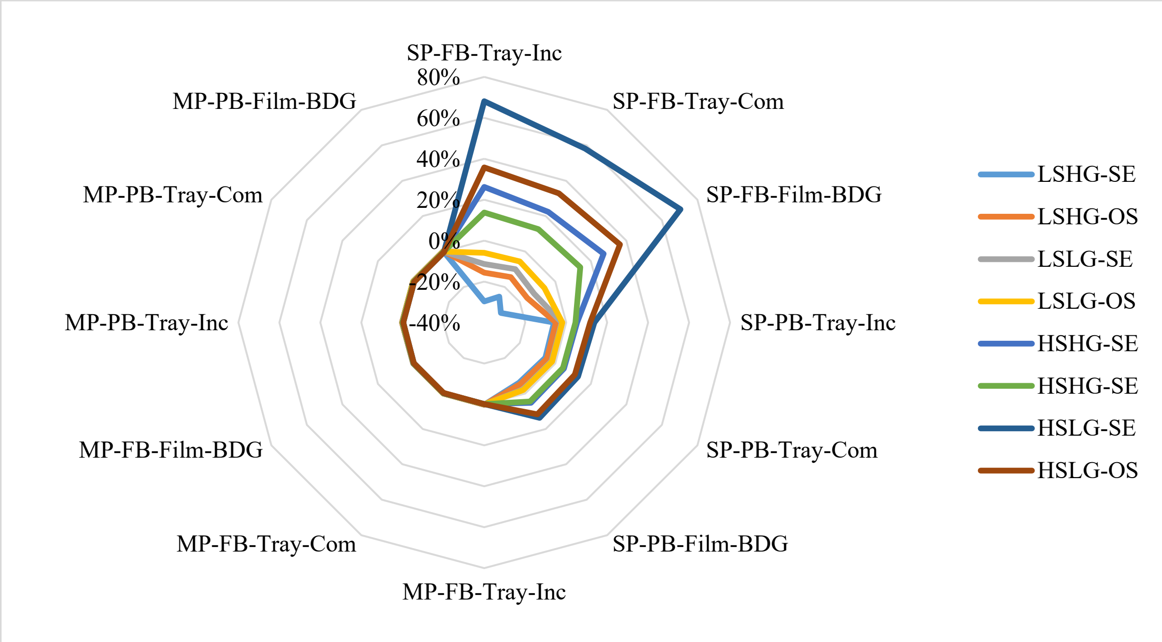

Figure 7-13 Sensitivity analysis results: influence of applying different levels of grain and straw prices on LCA of LCB; negative percentages indicate the level of reduction for estimated GHG sequestration of MP-based cases and GHG emissions of SP-based cases, compared with 3-year average values used in this study, positive figures indicate the level of increase of sequestrating or emitting effects.

7.4 Summary

This chapter included two LCAs. The cradle to up-stream-factory gate LCA for LCB feedstocks aimed at estimating and comparing the climate change impacts associated with SPBC and MPBC provision scenarios and identifying key components in terms of climate change mitigation potential within the LCB provision stage.

Cradle to end-of-life LCA for plastic end product was conducted through integrating the case- and site- specific climate change impacts figures from previous chapters with climate change impacts of polymer production, product manufacture and end-of-life treatment data provided by project partners. (Patel et al. 2018)

The climate change mitigation potential of proposed MP scenario compared with SP scenario was reflected in both LCAs. Comparing with SP, LCB produced through MP scenario would achieve a GHG reduction of 2.0 to 2.5kg CO_2eq for per kg delivered LCB feedstock, 2.14kgCO_2eq/kg LCB, 2.35kg CO_2eq/kg LCB and 1.97kgCO_2/kg LCB for Economic, energy and RED allocations respectively. Nitrogen fertiliser production and consequent N_2O emissions represented the dominant GHG emission sources in the winter wheat (straw) provision system.

For most of the cases, climate change impacts of the feedstock provision stage represented the major contributor to the overall performance of bio-based plastic's life cycle. The proposed MP strategy would not only achieve significant reductions of climate change impacts, it even offset all the GHGs emitted from other processes and stages, indicating that this mixed cropping-PBS production system holds out the tantalising potential of being considered as a 'negative emissions technology' Sensitivity analysis suggested that accounting for terrestrial carbon stock changes is critical when LCA is conducted for *Miscanthus* -based biomaterials. Similar conclusions have been drawn from LCAs for *Miscanthus* based bioenergy production that terrestrial carbon stock change appeared to be the most important component for *Miscanthus*' GHGs sequestration potential. (Shemfe et al. 2016)

Chapter 8. **Discussion and conclusions**

8.1 Summary and integration of results

In this work, a mixed (winter wheat and *Miscanthus*) production strategy (MP) was proposed to provide lignocellulosic biomass feedstocks for the production of bio-plastics. By modelling the replacement of winter wheat with *Miscanthus* on the low-quality sandy soils in an area predominantly growing winter wheat, the research aimed to investigate the climate change impacts of providing sufficient feedstock for a lignocellulosic biomass (LCB)-based PBS plastics plant within a defined biomass resourcing area. The research outcomes were generated and hypothesis was tested using a spatially explicit case-study-based approach developed using two process-based crop models STAMINA and DNDC, coupled to a Life Cycle Assessment (LCA). The counterfactual adopted was the continued use of existing winter wheat Single crop Production strategy (SP) without supplementary *Miscanthus* production in the case study area.

Based on the biomass availability (Chapter 4), and under the assumption that the current markets for wheat straw continue to be supplied, only about 18kt of wheat straw could be considered as available for bio-succinic acid production without increasing market competition for straw. With a feedstock requirement for a commercial scale production plant of 350kt straw per year (CIMV 2015, private communication), the establishment of the hypothetical SA production plant accessing LCB feedstocks exclusively from within the case study catchment, will generate significant competition for straw.

If the wheat production and land management were to continue unchanged as SP with winter wheat straw being the only LCB source, two regimes were predicted in the context of the potential bio-economy development. An SPBC1 (SPBC = Single crop Production strategy under Baseline Climate condition） scenario which assumes that no LCB-plastic trays are produced from succinic acid (SA), then 60.72 kt plastic products would be produced from conventional polyethylene terephthalate (PET) polymers

(Table 8-1), requiring 61.33 kt PET polymer granules (Patel et al, 2018). The SPBC2 scenario assumes the establishment of the hypothetical SA plant with 363 kt of locally sourced wheat straw being the sole feedstock option. As competition for straw would result, a simplified assumption was made that straw deficits were compensated by wheat cultivated elsewhere but with the same emission level as this study. Other possible changes such as improved resource use efficiency or alternative feedstocks for other straw uses were not considered.

Table 8-1 Overview of MPBC and SPBC production outputs, GHG emissions and potential indirect impacts (resources and GHG emissions); fb tray produced through SE pretreatment was assumed; economic allocation applied on wheat straw and grain.

	Products (kt/yr)		**Indirect impacts (kt/yr)**		
	Grain DM	fb plastic tray	Grain losses	straw deficit	PET polymer consumption
SPBC 1	1746	0	0	-18[1]	61.33[2]
SPBC 2	1746	46.90[3]	0	345[4]	13.96[5]
MPBC	1631	60.72[6]	115	0	0
	Emission factors (t CO_2eq /t)		**Emission factors (t CO_2eq /t)**		
	Grain DM	GHG savings by fb trays	Grain DM	Straw	
SPBC 1	1.99	0	-	-	
SPBC 2	1.99	-2.52[7]	-	0.22[10]	
MPBC	1.61	-30.10[8]	1.61[9]		
	Emissions (kt CO_2eq/yr)		**Indirect emissions may be caused (kt CO_2eq/yr)**		
	Emission from Grain production	GHG savings by bio-plastics	From grain losses	From straw deficits	PET polymer consumption
SPBC 1	3487.06	0	0	-3.96	Accounted[11]
SPBC 2	3487.06	-118.19	0	75.90	Accounted
MPBC	2625.23	-1827.67	185.15	0	Accounted
	Total emissions (kt CO_2eq/yr)		**Total indirect emissions (kt CO_2eq/yr)**		**Total emissions including indirect impacts (kt CO_2eq/yr)**
SPBC 1	3487.1		-3.96		3483.1
SPBC 2	3368.9		75.90		3444.8
MPBC	797.6		185.15		982.72

1. Negative figure indicates that in SPBC1, there would be 18 kt straw surplus when no SA production;
2. calculated based on the amount of plastic tray products that could be replaced by MPBC-fb scenario, and assuming a resource efficiency of 0.99 based on Patel et al. (2018);

3. calculated based on the assumption that in SPBC2, a total 363 kt straw (LCB provision capacity of MPBC) would be used to produce SA; production rates of LCB feedstocks to PBS was based on Patel et al. (2018);
4. in SPBC2, due to the commercial scale SA plant utilised total 363 kt straw and this would cause 345 kt straw deficits for current straw uses;
5. in SPBC2, due to the lower conversion rate of straw compared to *Miscanthus*, 363kt of straw LCB only produce 46.9 kt fb PBS trays, so another 13.96 kt PET would be consumed to produced plastic trays to match MPBC scenario;
6. in MPBC scenario, a total 363 kt LCB were available to produce 60.72 kt fb trays based on production rate in Patel et al. (2018);
7. difference of climate change impacts between 'SP-FB-Tray-Inc' an 'PET-Tray-Inc' cases, produced in Chapter 7;
8. difference of climate change impacts between 'MP-FB-Tray-Inc' an 'PET-Tray-Inc' cases, produced in Chapter 7;
9. if the wheat grain production lost in MPBC was produced elsewhere outside the case study area, it is assumed the emission factor of grain production being the same with this study; all figures coloured in dark blue were based on assumptions regarding indirect impacts, in which there is a high level of uncertainty;
10. due to the straw deficits for other uses in SPBC2, simplified assumption was made that extra straw needed to be produced outside the case study area but with the same emission level; similar to No.9 a high level of uncertainty remains;
11. Emissions from PET trays have been already accounted in 'GHG savings by bio-plastics'.

In MPBC (Mixed winter wheat and *Miscanthus* production under Baseline Climate condition) scenario, 8% of the wheat land (30,200 ha from a total 396,400 ha) was assumed to be replaced by *Miscanthus* cultivation, resulting in a 6% reduction in grain production (115 kt/year). It is possible that the grain yield would increase under enhanced CO_2 fertilization, wetter and warmer climate conditions in the context of climate change, as indicated by the results presented in Chapter 4 and other research. (Röder et al. 2014; de Souza et al. 2013) Additionally, improved plant breeding and other agronomy techniques, together with tactical and strategic farm management practices could achieve a smaller 'yield gap' (the difference between the yield that is theoretically possible in a field and that, which is achieved in practice) without additional resource inputs and energy consumption.(Anderson et al. 2016) Nevertheless, a simplified and conservative assumption was made in dealing with the indirect climate change impacts of grain reduction, assuming reduced grain in MPBC would be produced elsewhere and with the same emissions level as the wheat production in the case study area.

The annual wheat grain and polybutylene succinate (PBS)-products production outputs and associated GHG emissions are presented in Table 8-1. Data for fb-trays produced using steam explosion (SE) pretreatment and incineration as the end-of-life stage were assumed. The influences of the different pretreatment and end-of-life treatment options are discussed in Chapter 7.

If emissions from indirect impacts are not considered, establishing a lignocellulosic biomass (LCB)- succinic acid (SA)-bioplastic production chain, under the assumptions in the SPBC2 scenario, GHG emissions would be reduced by 3.4% (118.19 kt CO_2eq/year). 46.90 kt bio-based trays would be produced per year and competition for straw with the current users would result. When emissions from indirect impacts are included, the annual GHG emissions in SPBC2 are only 1.1% (38.33 kt CO_2eq) lower than SPBC1.

The MPBC scenario resulted in a significant climate change mitigation potential compared to SPBC1 and SPBC2. By using the proposed mixed feedstock provision strategy, annual GHG emissions savings of 77% (2689.5 kt CO_2eq/year) are calculated. In addition, 60.72 kt polybutylene succinate (PBS) trays could be produced annually and correspondingly could save 61.33 kt of conventional polyethylene terephthalate (PET) polymer production per year. This would happen at a cost of the 6% (115 kt/year) reduction of wheat grain. When the emission from indirect impacts are included, GHG emission reduction of 72% result from the deployment of the MPBC scenario (2,500.4 kt CO_2eq/year) compared with SPBC1 scenario. In MPBC, GHG sequestration credits would also be obtained from the optimised emission factor for per unit of wheat grain produced. These credits resulted from the loamy fine sandy soils being excluded from wheat (straw) production, with reduced nitrogen leaching and associated emissions and increased soil organic matter and carbon stocks, emission factor of per kt grain produced could be reduced by 19% (from 1.99 to 1.61 kg CO_2eq/kg grain).

This work highlights the significance of integrating a perennial crop such as *Miscanthus* into a conventional winter wheat production system to not only facilitate but also optimise the climate change mitigation performance of a bioplastic (LCB-PBS) value chain. By comparing the GHG emissions of SPBC2 and MPBC, in both scenarios, a hypothetical lignocellulosic biomass-based bioplastics production system was established. However, without the targeted deployment of *Miscanthus* relatively minor GHG reduction benefits would result (3.4% compared with a no SA scenario and only 1.1% when emissions from indirect impacts were considered).

8.2 Main findings and contributions

8.2.1 Climate change mitigation potential of bio-based materials

This work tested and clearly challenged a hypothesis that bio-based materials are carbon neutral. Academia and industries have long been seeking options to replace petro-based plastics with bio-based alternatives to address concerns regarding climate change and plastics pollution, especially marine pollution. As petro-based single use plastic products were proposed to be completely banned by the European Commission in May 2018[13], production and supply of sustainable alternatives to petro-based plastics seems to be more urgent than ever to help a societal transition to a post-petroleum era.

Although research has been conducted and the climate change impacts of lignocellulosic biomass (LCB)-based bio-plastics reported, (Cok et al. 2014; Patel et al. 2018; Patel et al. 2006) this is the first work which integrates site-specific climate change impacts associated with lignocellulosic biomass (LCB) feedstocks supply in a

[13] 'New EU rules to reduce marine litter', information available at https://ec.europa.eu/commission/news/single-use-plastics-2018-may-28_en, accessed on 28 Nov 2018;

whole systems analysis framework, considering both, management-specific N_2O emissions and emissions from terrestrial carbon stock changes.

As indicated in Chapter 7, the Life cycle assessment (LCA) results shows a large variance in the climate change impacts among different LCB-based production cases, from -25.1 to 6.71 kg CO_2eq/kg bioplastic product. The impacts of grain-based plastics production remain relatively stable, around 4.11 to 7.14 kg CO_2eq/kg product. The results demonstrate the GHG reduction potential of LCB-based plastics products compared with grain- and petrol-based ones. However, in order to achieve the climate change mitigation potential of an LCB-based SA-plastics value chain, advanced land management is considered necessary during the feedstock provision stage. The proposed mixed production strategy in this study possesses considerable capacity in meeting this potential.

8.2.2 Bioeconomy, a threat to Sustainable Development Goal 15?

Bioeconomy, a threat to Sustainable Development Goal 15?

Whether bio-economy is a threat to Sustainable Development Goal 15 depends on how each individual case is implemented.

This work tested and challenged another perception that have emerged for the non-food bioeconomy, that increased non-food biomass demand would exacerbate competition for land and environmental impacts of crop production. Several works have predicted the potential competition for biomass and cropland for EU to meet the agreed 2030 GHGs reduction target through LCB feedstock. (Frank et al. 2016; Bianco Fonseca et al. 2010)

The visualized future evolution of lignocellulosic biomass (LCB)-based material production in addition to the current bioenergy commitment, has posed a challenging but critical question on the ability of the farming system to continue to provide land-based ecosystem services as well as improvements in the overall sustainability performance of agriculture. Competition for land resources and jeopardising the Sustainable Development Goal 15 (land-based resource restoration) have been considered the biggest potential threat associated with the bioeconomy strategy, however as suggested by O'Brien et al. (2017), the actual 'sustainability' performance of bioeconomy strategy depends on how it implemented. It is possible to achieve a range of sustainability benefits when each individual plan is carefully tested and implemented. 'Trade-offs' are unavoidable, however they should only be accepted when all other scenarios have been explored and deemed worse (Gibson, cited in Rack 2017).

The outputs of this thesis suggested various sustainability potential of the proposed 'integrated LCB cultivation-PBS production' strategy, with minimum and 'acceptable' trade-offs. Based on the results of Chapter 4, the assessment of straw availability indicated that the potential expansion of an LCB-based bioeconomy would cause intense competition amongst current straw users if the bio-plastics industry were to rely solely on agricultural residues. However, meeting the feedstock demands for commercial scale bio-SA production by integrating dedicated non-food crop production into existing farming systems (MP strategy) would avoid feedstock competition, with a range of other sustainability benefits, including the considerable system-level reduction achieved by MPBC scenario; the 24% reduction of the carbon footprints associated with wheat grain production (compared with SPBC 1 and MPBC), and avoiding 61.33kt year petro-based PET polymer production. The 'unavoidable' trade-off refers to the 6% decline in local grain production, although it is possibly manageable that the estimated grain loss could be at least partly compensated by the increasing atmospheric CO_2 concentration (direct fertilisation and increased temperature) and improved agronomy and breeding techniques. If the reduction could be compensated through the CO_2 fertilisation effects and techniques improvement, the mixed production strategy can be deemed as an effective approach to help the farms 'produce more from less', without any compromises to the SDG15, land restoration.

It also suggests EU's potential capability in meeting its bio-PBS feedstock requirement without extra land occupation either within or beyond its continental boundaries， avoiding further anfractuous ecological, social and economic issues might be brought with imported feedstocks. (Bruckner et al. 2018)

Land for 'food vs fuel vs material'?

It is still not possible to confidently answer the questions of 'land for food or fuel or material?' Such conclusion can only be drawn when system level sustainability assessments have been conducted and a full range of relevant indicators have been tested. In order to robustly address sustainability concerns, a much wider range of issues should be considered from social and economic perspectives. This also requires better understanding of the interrelation among different dimensions and indicators. (Rack 2017)

Even for the case study area used in this research, a conclusive outcome could not be provided regarding which would be the best land/biomass use strategy (or strategies) among the choices of 'land/biomass for food', 'land/biomass for energy' and/or 'land/biomass for bioplastics', in terms of carbon mitigation. As concluded by Fajardy and Mac Dowell (2017), determining the sustainability or otherwise of a given land-based bioenergy project as a candidate for climate change mitigation is therefore only possible on a case-to-case basis. Such conclusion can only be drawn when case- and site- specific LCA works have also been conducted for other land use options (land/biomass for food and land/biomass for energy) as well, considering the climate change impacts of bioenergy production systems were also highly variable (Shen et al. 2015), so was food production systems as reflected in the N_2O emission outputs presented in Chapter 5. Nevertheless it is worth mentioning that this work has developed a robust framework and underpinning evidence base to estimate the gains and losses of this proposed mixed feedstock supply and bio-PBS production scenario compared with reference systems (SPBC1 and 2) that reflect a more business-as-usual approach. The research framework established in this work could also facilitate further investigation of other land/biomass use and production scenarios, such as land/biomass used for bioenergy production. Then to better understand where this limited resource (land/biomass) can be prioritised for the best cases to maximize the climate change mitigation across bioeconomy.

8.2.3 Methodological contributions

Several methodologies from different estimation tiers were applied in this study. This section discusses the modifications and improvements that have been made in this thesis to serve the specific purposes of this work. Issues that have been highlighted during the research are also discussed with suggested solutions.

8.2.3.1 Estimation of straw availability

Many works have been conducted and published investigating the availability of wheat straw, while most of them were only based on recorded grain yields and use the Harvest Index (HI) to estimate straw production. (Donaldson et al. 2001; Nelson 2002) Neglecting the amounts already allocated to other uses of straw could cause overestimation of its potential availability. This overestimation might lead to a competition in the market and consequently increase the straw market price. Some estimations were based on farm survey results. (Glithero et al. 2013) This approach possibly underestimates the total straw production, due to the poor recording of farmers as the value of straw is generally low, and thus receives less attention by the farmers. (Glithero et al. 2013)

The improved estimation approach developed in this study used both, the field production and market demand components. Using process-based crop models generated wheat grain and straw yields thus providing site-specific estimates of wheat production potentials. Information regarding local straw incorporation rates and current active users in straw markets were obtained from literature, government surveys and reports.

8.2.3.2 Simulating nitrogen dynamics of *Miscanthus* growth with DNDC model

As one of the most widely used process-based agro-ecosystem models, DNDC has been used to provide site-specific data regarding N_2O and other emissions from agricultural systems, and integrated into downstream LCAs. (Goglio et al. 2018; Guo et al. 2012) While the uses of DNDC in simulating *Miscanthus* cultivation were still limited (Borzcka-Walker et al. 2010; Gopalakrishnan et al. 2012), due to there being no default parameters given in the model for a *Miscanthus* crop. This work firstly tested and validated the Miscnathus parameters under UK condition based on parameters published by Gopalakrishnan et al. (2012).

8.2.3.3 IPCC 2006-AFOLU Tier 2 approach in estimation emissions from terrestrial carbon stock change

Both Tier 2 and Tier 3 approaches were applied in estimating carbon emission from terrestrial carbon stock changes. The general 'five carbon pools' structure and 'Stock-Difference Method' provided by 2006-AFOLU (Agricultural, Forestry and Other Land Uses) (Intergovernmental Panel on Climate Change, 2006a) were applied in a comparative Tier 2 and Tier 3 evaluation framework. The fundamental difference between the two tiers lies in the specific methods used to estimate the carbon values at the first and last year of the defined timeframe for each carbon pools. Comparing the results generated by Tier 2 with Tier 3, confidence could be gained when estimating land-based carbon stock change within a 30-year simulation period. However some assumptions in Tier 2 appeared to be too simplistic to generate robust results. The main areas where confident outcomes or significant limitations were noted are summarised below, based on the results presented in Table 6-6. Detailed dissections were included in Section 6.4.2.

- The annual carbon emissions over a 30-year timeframe (2021 to 2050) estimated by the Tier 2 and Tier 3 were comparable. The annual emissions predicted by Tier 3 are 15% high than Tier 2. This indicted the level of confidence in using Tier 2 as a less time-consuming while well standardised and instructed approach in the short term (20- to 30-year) estimations.

- The 20 years period for land to reach new equilibrium after use change is too simplistic. Gaps between the results generated from the two approaches began to occur for longer timeframes beyond 30 years. This is mainly due to the Tier 2 assumption that SOC would reach equilibrium after 20 years for lands remaining in the same use. The RothC model used for the Tier 3 evaluations predicted continuous carbon stock changes independent from the timeframe but influenced by the initial soil carbon levels and annual biomass carbon inputs.

- It is also too simplified to consider both, lands for wheat and for *Miscanthus* as 'cropland' under the Tier 2 guidance. For SOC, it is possible to distinguish stock levels for land under wheat and *Miscanthus* cultivation. This is done by selecting the carbon stock change factors for different land managements in Equation 7 (Chapter 3). However, the difference for AGB and BGB pools, could not be distinguished between wheat and *Miscanthus* lands in Tier 2. This appeared to be acceptable for ABG pool as the ABG were close for the two crops. However, for BGB pool, the strong potential of *Miscanthus* in sequestering carbon in roots and rhizomes would be ignored with the Tier 2 approach.

8.2.3.4 Other methodological concerns

Other methodological concerns raised in this study include,

- In RED, the energy-based allocation approach suggested to attribute cultivation-related emissions between grain and agricultural residues needs to be modified. As discussed in Section 7.1.3.1, it would lead to an underestimation of emissions associated with straw production and fail to adequately reflect the real emissions.

- Biogenic carbon embedded in bio-based plastics products is suggested to be accounted for rather than being considered as carbon neutral. This would influence the approach in accounting biogenic carbon emissions during end-of-life stage for different treatment options.

8.2.4 Policy implications

8.2.4.1 Strategy of integrating *Miscanthus* into arable system

Increasing evidence has emerged demonstrating the climate change mitigation potential of *Miscanthus* through both field trials and modelling work. (Richteret al. 2015; Shemfe et al. 2016; Zatta et al. 2014; McCalmont et al. 2015; Dondini et al. 2017; Dondini et al. 2009) Important issues remain in developing the practical deployment strategies for introducing *Miscanthus* into the agricultural landscapes. As indicated by the outputs from this study (Chapter 6) and Goetz et al. (2015), the sequestration potential could be marginal for soils with high initial soil carbon content. Additionally, for soils which were productive for cereal production, the carbon sequestration credits from *Miscanthus* cultivation could be deducted when considering other ecosystem services such as food production provided by wheat cultivated on the same land.

The strategy proposed in this study i.e. replacing *Miscanthus* on the sandy soils currently used for wheat cultivation provided a promising approach for integrating *Miscanthus* into agricultural landscapes as a tool for achieving significant reductions in GHG emissions. At national level, limited information is available regarding the areas of land with sandy textures. Based on the UK Soil Observatory from Canfield University (Canfield University, 2017)[14] (Appendix I) and mapped 'estimation of sandy

[14] Digital map of 'UK Soil Observatory' is available on http://www.ukso.org/SoilsOfEngWales/englandAndWales.html, accessed in 28 Nov 2018;map is also attached in Appendix I;

soil location in England and Wales' (DEFRA, 2011)[15] (Appendix J), a conservative estimation can be made that there are about 3% of the total areas in England and Wales were covered with sandy soils, taking up to 4,534 km^2. Most of the sandy areas are located in the eastern parts of England, which are also the major arable areas in England according to CORINE land cover map (CORINE Land Cover 2012)[16] (Appendix K). As indicated in Section 8.1, in the MPBC scenario, the total 30200ha of sandy soils are able to achieve 2,689.5 kt CO_2eq GHG reduction per year without considering the indirect potential impacts, which is equivalent to 89.1t CO_2/ha. Based on the same GHG reduction rate, deployment of mixed production strategy at the national scale could achieve a climate mitigation potential of approximately 40.4 Mt CO_2eq/year, without considering the emission from indirect impacts. This 40 Mt CO_2eq/year GHG reduction potential was calculated based on a simple assumption that all the sandy soils were converted to *Miscanthus* cultivation from conventional arable land, with fully bio-based PET products being the end-products. To further contribute to the UK Committee on Climate Change proposed 'Net Zero' ambition by 2050[17], the UK National Farm Union (NFU)[18] has announced the target of achieving 'Net Zero farming' across England and Wales by 2040. According to the UK GHG Inventory, 1990 to 2017, (Brown et al. 2019) the national GHG emissions in 2017 was 464.5Mt CO_2eq/year, among which agricultural is responsible for 41.2Mt CO_2eq/year. The figures for the year 1990 was 798.2Mt CO_2eq/year in total and 49.2Mt for agricultural sector. Although UK has achieved a national GHG reduction by 42% since1990, the emissions from agricultural

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[15] 'Approximate Locations of Sandy Soils in England and Wales', link at: http://adlib.everysite.co.uk/adlib/defra/content.aspx?id=000HK277ZW.0A9O2YFJMYQFSG, accessed in 28 Nov 2018;map is also attached in Appendix J

[16] CORINE Land Cover, available at https://land.copernicus.eu/pan-european/corine-land-cover; accessed in 28 Nov 2018; map is also attached in Appendix K.

[17] 'UK becomes first major economy to pass net zero emissions law', available at https://www.gov.uk/government/news/uk-becomes-first-major-economy-to-pass-net-zero-emissions-law, accessed in 08 July 2019.

[18] 'NFU reiterates its net zero aims for agricultural', available at https://www.nfuonline.com/news/latest-news/nfu-reiterates-its-net-zero-aims-for-agriculture/; accessed in 10 July 2019.

production were only decreased by 16.3%. Considering the relatively lower reduction rate of agriculture resulted GHG emissions compared with the national average, the proposed 'integrated land use-PBS production' strategy present considerable potential and significant importance to help the farming sector achieve its 'Net Zero' plan.

Analysing from the consumption-side, the total consumption of packaging plastic in the UK was estimated to be around 3.2 Mt/yr (Davis & Song 2006), if petro-based plastics packaging material could be fully replaced by PBS-based alternatives produced from the mixed production strategy, the total GHG reduction potential is estimated to be 96.3 Mt CO_2eq/year for the UK plastic packaging market.

8.2.4.2 Integrated sustainability assessment tools required in policy making

Although this work suggests a significant climate change mitigation potential of MPBC scenario compared with SPBC scenarios, it is difficult to make a robust sustainability comparison, due to a lack of robust and agreed methodologies as reviewed in Section 2.5.1. From the current understanding, sustainability assessment should be conducted from the environmental, social and economic dimensions, although a much more granular Sustainable Development Goal-based approach has recently emerged.

It has been suggested that perennial crops outperform traditional cereal crops in other environmental metrics, such as biodiversity (Heaton et al. 2010), soil qualities (Heaton et al. 2010), material efficiency (Pinazo et al. 2015), energy efficiency (Pinazo et al. 2015), land use efficiency (Pinazo et al. 2015).

From economic sustainability perspective, theoretically planting perennial crops such as *Miscanthus* on low cereal-productivity land should reduce the farm's vulnerability compared with single output systems. Especially in the context of the recently proposed new UK Environmental Land Management scheme[19], according to which farmers will

[19] 'Environmental farming scheme given green light', information available at: https://www.gov.uk/government/news/environmental-farming-scheme-given-green-light, accessed in 28 Nov 2018.

receive subsidies according to the environmental performance of their farming systems, farms' incomes would be predicted to increase with significant carbon credits brought by the proposed mixed production strategy. On the other hand, uncertainties and inconsistencies remain regarding the production costs of LCB-based PBS or energy production systems compared with grain-based productions. Heaton et al. (2010) and Littlewood et al. (2013) concluded that economic concerns were the biggest barrier for the development of LCB-based energy or material productions. However, Pinazo et al. (2015) demonstrated a LCB-SA production case with lower costs compared with petrochemical-based.

Permanence issue associated with soil carbon sequestration is another sustainably concern from the economic perspective. (Hediger 2009) As indicated in Chapter 6 and Chapter 7, the climate change mitigation potential of the mixed production-lignocellulosic PBS plastics production scenarios is largely attributed to the terrestrial carbon storage under *Miscanthus* cultivation. Maintenance of the sequestrated carbon in the soil to avoid the threat of future carbon release when land use change happens is needed to be considered.

The potential increase of landscape complexity and change in farm production in the proposed perennial-arable production scenario would require farmers to move from arable specialisation to be more generalist producers, which requires more knowledge and complexity in farming and management practices. Research has suggested that if climate change will offer new opportunities of increasing incomes, either through expansion of cash crop cultivation or novel land-use options such as perennial dedicated biomass crops, these opportunities will always be welcome and seized. (Pröbstl-Haider et al. 2016)

From the social sustainability perspective, several works suggested poverty alleviation and job creation potentials from biomass-based energy or material production, especially in developing regions. (Heaton et al. 2010; Littlewood 2013) However, Diaz-Chavez indicted that the increased use of biomass for non-food production may raise conflicts, such as land competition along with synergies between socio-economic and environmental impacts. (Diaz-chavez 2014) Moreover, the underlying consequence of the 6% reduction in grain production predicated in this work is still uncertain.

Although trade-offs are unavoidable, they should only be accepted when all other scenarios have been explored and deemed worse.(Gibson, cited in Rack 2017) However, different scenarios can only be comparable when standardised and accepted sustainability assessment methodologies exist and are widely deployed. Such tools with robust methodologies, criteria, standards and certification schemes, should be developed to facilitate policy-making with minimized bias and uncertainties.

8.2.4.3 Improvements and modifications needed in carbon accounting methodologies

As indicated in Section 8.2.3, concerns have been raised that some of the current GHG emissions accounting methodologies appeared to be unfavourable to perennial crops such as *Miscanthus* in terms of reflecting their real GHG reduction potentials. These methods include the Tier 2 approach in 2006-AFOLU (see details in Section 8.2.3.3) and the allocation approach of agricultural residues in the RED guideline (see details in Section 7.2.3.1).

8.3 Limitations of this study and recommendations for further research

The limitations of this work and recommendations for further work fall into three categories: 1) data limitations; 2) limitations of the methodological approaches; and 3) limitations regarding the focus and scope of this PhD study. The research and analysis for this thesis focused on the climate change impacts of the cultivation and feedstock provision of lignocellulosic succinic acid derived bioplastics. Details within the pre-processing, processing, polymer production, products manufacture and end-of-life treatment stages, as these processes were mainly modelled and provide by BioSuccInnovate project partners, and any downstream life-cycle components were taken from project reports and internal working documents and data, much of which is available in Patel et al. (2018).

8.3.1 Data limitations and future work

8.3.1.1 Validation of DNDC model with measured nitrogen effluxes values

The process-based model DNDC, was used in study to simulated nitrogen dynamics during the cultivation of *Miscanthus* and winter wheat. For winter wheat, the model has been parametrized for England by the author using crop yield data recorded by Rothamsted Research. For *Miscanthus,* the parameters were obtained from (Gopalakrishnan et al. 2012), as this cultivar (*Miscanthus x giganteus*) and associated propagation and land management practices were adopted for the research in this thesis. For both crops, model performance has been evaluated against the locally measured yield data in England. No model validation was conducted on nitrogen dynamics due to the lack of site measurement of N_2O emissions and NO_3^- leaching. Although the simulated yields agreed well with the measured ones, and the simulated N_2O and NO_3^- losses were in accordance with other reported research for both winter wheat (Lassaletta et al. 2014) and *Miscanthus* (Behnke et al. 2012; Christian & Riche 1998), there were still uncertainties regarding the nitrogen fluxes simulated by DNDC model. The author could not assess if the simulated fluxes are likely to be representative of those from the specific environment and management conditions of the case study. Future field measurement of nitrogen effluxes should be established and used to validate the DNDC model performance. Especially for *Miscanthus*, as the application of DNDC to simulate its nitrogen dynamics were still limited. Only three works have been published so far on *Miscanthus* simulation with DNDC model, and they were only evaluated against field measured yields data. (Borzcka-Walker et al. 2010; Gopalakrishnan et al. 2012; Ni et al. 2019)

8.3.1.2 UKCP09 datasets and the updated version UKCP18

In the simulation of wheat and *Miscanthus* production under medium emission (ME) and high emission (HE) climate change scenarios, the climate data sets used were derived from the 2009 version of UKCP model, which was the latest version when this project started. The new version of UKCP (UKCP18) was released in November 2018[20]. It was recognized by the Met Office that the UPCP09 should still be capable for land-based research, but changes would be made regarding the winter precipitation patterns in the UKCP18 (Met Office 2016). It would be beneficial to retest the biomass production with the UKCP18 datasets to reduce the level of uncertainties, considering the UKCP18 is the reflection of the latest scientific understanding and modelling capability.

8.3.1.3 Better understanding of nitrogen fertiliser requirements during *Miscanthus* cultivation

A knowledge gap was identified regarding the appropriate nitrogen fertiliser application levels for *Miscanthus* cultivation. Although an application rate of 60-80kgN/ha.yr was suggested by RB209, it is considered as a 'preliminary guidance' and more field experimentation is required to understand the appropriate application levels under different conditions.

It was indicated by several individual case studies that generally the main response to nitrogen fertilisation was in young plants. (Monti et al. 2019) For *Miscanthus*, it has also been suggested that more nitrogen fertiliser was required for the growth of rhizomes in addition to the amount being removed in harvested biomass. (Agriculture and Horticulture Development Board 2017) However, other researches have reported that as the amount of nitrogen removed in the early stages of growth was smaller than

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[20] Information regarding the UKCP18 is available at http://ukclimateprojections.metoffice.gov.uk/

in subsequent years, it was unnecessary to increase the nitrogen inputs for rhizome development. (DEFRA 2010) Moreover, a significantly higher level of NO_3^- leaching during the first year was observed in some filed studies than the subsequent year with the same N-input level. (Christian & Riche 1998) This lower nitrogen intake level by young *Miscanthus* crop is also seen in the results of this research (Chapter 5), that surplus nitrogen application would lead to increased levels of N_2O emissions and NO_3^- leaching, especially during the first two years after *Miscanthus* establishment. A recent study conducted by Monti et al. (2019) reported that young *Miscanthus* showed negligible benefits from nitrogen fertiliser application during the first three years. (Monti et al., 2019) Consequently, a question has been raised whether a reduced, instead of increased, nitrogen fertiliser application level would be more appropriate for *Miscanthus* at its early growth stage.

8.3.2 Limitations regarding methodological approaches

8.3.2.1 Crop rotations during winter wheat cultivation

In the UK, winter wheat is generally cultivated in a three- or four-course wheat-dominated rotation with oilseed rape, barley or potato. (DEFRA 2010) In this study the effects of rotation on the crop production was only considered in calculating the annual provision capacity of grain and straw by Equation 2, assuming 2/3 of the total area were covered by winter wheat due to rotation. The effects of rotation on other aspects related to wheat production were not considered for several reasons as discussed below.

Firstly, rotation practice is a site- and farm- specific decision, which makes it difficult to develop a robust assumption that would adequately represent the whole case study area over the time periods considered in this research. There was also a lack of sufficiently detailed growth data to robustly include the break-crop(s) (the other crop(s) planted during rotation) in the DNDC or RothC modelling work.

Secondly, according to Angus et al.(2015), good rotation practices generally increase wheat yields by 0.5 to 1 t/ha.yr as a combined effect of disease control, pest control, weed control (such as black-grass in UK) and soil carbon/organic matter and nitrogen enrichment. In general, factors such as diseases, weeds and pests were not considered as the limiting factors in crop model simulations in this work. In other words, the potential yield increases benefited from disease, pest and weed control effects were already reflected in the model outputs. Undoubtedly, uncertainties remain in the effects of rotation on soil carbon and nitrogen contents. It is therefore suggested to conduct further researches to compare climate change mitigation potentials of each specific case, site-specific rotations might be necessary, and the impacts should be analysed by either by field trials or modelling approaches.

8.3.2.2 Approaches for estimating biomass carbon inputs to soil in RothC simulations

One of the required data inputs for the RothC model were the monthly biomass carbon inputs to soil. The Hillier's approach (Hillier et al. 2009) was adopted in this study, according to which the biomass carbon inputs were considered as a function of crop yields. However, knowledge is still evolving regarding the actual biomass carbon inputs to soil. There is an absence of a widely agreed approach to quantify this value, limited by insufficient site-measurements and availability of sufficiently granular spatially explicit data. This is especially the case for perennial crops such as *Miscanthus*, where the crop-growth cycle is generally up to, or more than, 20 years.

8.3.3 Limitations regarding the research scope

8.3.3.1 Integrating *Miscanthus* into cereal-dominated production system as buffer zones

The proposed integration of *Miscanthus* into wheat production systems where it replaces winter wheat on the sandy soils of a specified case study area, aimed to secure

LCB provision for bio-SA production whilst optimising terrestrial GHG emission balances during crop production phase. GHG emission reductions resulted mainly from three major components of feedstock production: i) sequestrating carbon into BGB and SOC pools on *Miscanthus* land; ii) reduced direct and indirect N_2O emissions during *Miscanthus* life cycle due to reduced nitrogen fertiliser application levels compared with wheat; iii) lower levels of fertiliser inputs and farming activities for *Miscanthus* compared with wheat.

However, the nutrient flow dynamics between *Miscanthus* land and adjacent land were not considered in this study. As suggested by Gopalakrishnan et al. (2012), by planting *Miscanthus* as buffer zone crop in areas immediately adjacent to wheat-producing fields with higher NO_3- leaching/run-off levels, the lost NO_3- could be captured and reutilised by *Miscanthus* crop. Additional GHG emissions could be avoided potentially through this enhanced nutrient use efficiency compared with the strategy studied in this work. Another similar strategy is to plant *Miscanthus* as riparian buffer strips adjacent to waterbodies to reduce potential aquatic pollutions. (Ferrarini et al. 2016) They suggested that bioenergy buffers were able to efficiently remove the incoming NO_3-N from groundwater by 60% to 80% in an Italian cases study. Other potential environmental benefits include reducing sediment and pesticides loss from crop fields, stabilising stream banks, and reducing bank erosion. (Bonin et al. 2012) Future works are suggested to investigate the feasibility of similar land use strategies under UK conditions and the associated GHG reduction potentials.

8.3.3.2 Comparing with other LCB-based value chains with robust sustainability methodologies

This work examined the climate change mitigation potential associated with the proposed LCB provision of succinic acid-based bioplastics (PBS) production system, compared with the 'business as usual' winter wheat production system. Other potential 'low-carbon' markets such as bio-ethanol production or electricity generation of the produced mixed LCB feedstocks were not considered or simulated in this study. As indicated in Section 8.2.2, in the cases where arable lands and biomass were locally limited resources, their deployment should be considered and determined based on a balanced evaluation of the ecosystem service provisioning and overall sustainability performance of each implementation scenario.

There are two potential significant areas for further work. First of all, the model-simulation approaches proposed in this study could be used to examine the performance regarding food production, energy provision and climate change mitigation potentials for specific bioenergy production scenarios. Then the comparison could be made at the level of the climate change mitigation potentials of different LCB value chains for this case study area. The second, as already indicated in Section 8.3.2, is that it is scientifically challenging but crucial to develop a robust and publicly acceptable integrated sustainability assessment methodology (preferably in the form of an integrated assessment tool), which could be used to test the overall sustainability performance of potential production scenarios.

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Appendix

Appendix A Temperature, rainfall and Evaporation as inputs of RothC simulation

	Temperature (°C)	Rainfall （mm）	Evaporation （mm）
January	3.7	61	14.6
February	4.3	49	18.3
March	6	38	37
April	8.7	42	60
May	11.4	48	96
June	14.7	50	130
July	16.8	60	148
August	16.5	64	134
September	14.4	52	97
October	10.7	58	62
November	7.1	66	30
December	4.9	54	20

Appendix B Wheat grain and straw price (£/t) from AHDB database from Jun 15 to Jun 2018 (links: https://dairy.ahdb.org.uk/market-information/farm-expenses, accessed on 21 Nov 2018))

Date	Wheat grain	wheat straw	Date	Wheat grain	wheat straw
Jul-15	118.4	35	Apr-17	146.3	51
Aug-15	105.5	31	May-17	145.7	49
Sep-15	102	32	Jun-17	141.8	48
Oct-15	106.8	33	Jul-17	145.7	47
Nov-15	106.8	33	Aug-17	133	44
Dec-15	106.6	34	Sep-17	135.2	46
Jan-16	104.3	35	Oct-17	139.4	52
Feb-16	102	36	Nov-17	138.2	66
Mar-16	100.2	35	Dec-17	138.4	75
Apr-16	102.8	38	Jan-18	138.8	78
May-16	104	38	Feb-18	138.6	81
Jun-16	106	40	Mar-18	143.3	83
Jul-16	110	40	Apr-18	147.9	91
Aug-16	120	35	May-18	151	91
Sep-16	117.9	33	Jun-18	158.9	88
Oct-16	126.5	35			
Nov-16	134.2	38	Current	158.9	88
Dec-16	136	41	Lowest	100	31
Jan-17	139.4	44	Highest	159	91
Feb-17	144	50	Average	127	49
Mar-17	145.6	50			

Appendix C Background data for LCI of LCB feedstocks

			Winter wheat in SPBC	**Winter wheat in MPBC**	***Miscanthus* in SPBC**
Mass proportion			100%	4.98%	95.02%
Cultivation and harvesting	Seeds/rhizomes	kg/ha or p/ha	175	175	5921
	Ammonium nitrate	kg N / ha.a	205	209	60
	Ammonium sulphate	kg N / ha.a	0	0	0
	Calcium ammonium nitrate	kg N / ha.a	0	0	0
	Urea	kg N / ha.a	0	0	0
	Monoammonium phosphate	kg P_2O_5 / ha.a	0	0	0
	Diammonium phosphate	kg P_2O_5 / ha.a	0	0	0
	Single superphosphate	kg P_2O_5 / ha.a	0	0	0
	Triple superphosphate	kg P_2O_5 / ha.a	39	39	7.05
	Potassium chloride	kg K_2O / ha.a	48	48	0
	Potassium sulphate	kg K_2O / ha.a	0	0	105
	Calcium oxide	kg CaO / ha.a	0	0	175
	Total pesticides	kg / ha.a	1.03	1.03	1.15
	Manganese sulphate	kg / ha.a	0	0	5.6
	Total diesel consumption	kg / ha.a	**229.94**	**229.94**	**0.74**
Direct and Indirect N_2O Emission	N_2O emissions from soil	kg N/ha. a	0.71	0.73	0.25
	NO_3^- leaching	kg N/ha. a	66.03	60.32	58.24
	Indirect N_2O from NO_3^- leaching	kg N/ha. a	0.50	0.45	0.44
Emission from carbon stock change	ABG	kg C/ha.a	0.00	-2.69	29.052673
	BGB	kg C/ha.a	0.00	-0.62	-458.08
	SOC	kg C/ha.a	22.92	6.52	-920.6
	Deadwood	kg C/ha.a	0.00	0.00	0
	litter	kg C/ha.a	0.00	0.00	0
Loading at farm	Diesel consumption	kg / kg LCB	7.68E-04	7.68E-04	7.68E-04
Transport to storage and drying	Road transport round trip	km	50.00	50.00	50.00

Offloading & Loading at storage	Diesel consumption	kg / kg LCB	1.54E-03	1.54E-03	1.54E-03
Transport to plant	Road transport round trip	km	50.00	50.00	50.00
Offloading at plant	Diesel consumption	kg / kg LCB	7.68E-04	7.68E-04	7.68E-04
Other data	Timeframe	Years	30	30	30
	Wheat Grain+Straw/ *Miscanthus* Yield	kg / ha.yr	10010.00	10130.00	12750.00
	Harvest area	ha	396400.00	366200.00	30200.00
	Wheat grain yield	Kg/ha	7730.00	7820.00	NA
	Wheat straw yield	Kg/ha	2280.00	2310.00	NA
	Wheat grain price	£/kg	0.13	0.13	NA
	Wheat straw price	£/kg	0.05	0.05	NA
	Wheat grain energy content	MJ/kg	16.50	16.50	NA
	Wheat straw energy content	MJ/kg	17.60	17.60	NA
	Grain HI		0.53	0.53	NA

Appendix D Background data sources for LCI of plastics end-products (based on Patel. 2018)

Process or material	Data Sources	Notes
Corn stover to Bio-SA	Cok et al. 2014	Blank box Economic allocation; exclude biogenic carbon embedded in plastics.
Wheat straw	Previous section in this thesis	Baseline climate condition
Miscanthus	Previous section in this thesis	Baseline climate condition
LCB pretreatment	Villegas et al., cited in Patel et al. 2018	SE and OS; with biogas production from co-products
Succinic acid production from Dextrose or C6	Cok et al., cited in Patel et al. 2018	
Bio-BDO production from starch-based and LCB-based Bio-SA	Novamont group, cited in Patel et al.,2018	
PBS polymerisation	PlasticsEurope, cited in Patel et al. 2018	
PP production	EcoInvent 3, cited in Patel et al. 2018	Granulate RER
PET production	EcoInvent 3, cited in Patel et al. 2018	Granulate, amorphous, RER
PE production	EcoInvent 3, cited in Patel et al. 2018	Low-density polyethylene, granulate RER
PP extrusion and thermoforming for trays	Sharpark, cited in Patel et al. 2018	
PET extrusion and thermoforming for trays	Sharpark, cited in Patel et al. 2018	
PBS extrusion and thermoforming for trays	Sharpark, cited in Patel et al. 2018	PET extrusion and thermoforming adjusted for lower melting point of PBS Assume 99% material efficiency with scrap incinerated.
Extrusion for films	EcoInvent 3, cited in Patel et al. 2018	Extrusion, plastic fi lm RER. Assume 97.7% material efficiency with scrap incinerated.
Transport by lorry	EcoInvent 3	Transport, freight, lorry >32 metric tonne, EURO3 RER
Incineration of plastics (PP)	EcoInvent 3, cited in Patel et al. 2018	Waste polypropylene CH, treatment of, municipal incineration
Incineration of plastics (PET)	EcoInvent 3, cited in Patel et al. 2018	Waste polyethylene terephthalate CH, treatment of, municipal incineration
Incineration of plastics (PE)	EcoInvent 3, cited in Patel et al. 2018	Waste polyethylene CH, treatment of, municipal incineration
Incineration of plastics (pb-PBS)	EcoInvent 3, cited in Patel et al. 2018	Waste plastics, mixture CH, treatment of, municipal incineration
Collection of PE agricultural film	EcoInvent 3, cited in Patel et al. 2018	Baling CH, processing, without plastics wrapping impacts
Incineration of PE agricultural film	Briassoulis et al., cited in Patel et al. 2018	

Hear credits from MSWI	EcoInvent 3, cited in Patel et al. 2018	Heat, central or small scale, natural gas-fired boiler, Europe without Switzerland, at boiler condensing modulating <100 kW
Electricity	EcoInvent 3, cited in Patel et al. 2018	Electricity, medium voltage in Europe, ENTSO. Also used as electricity credit for MSWI
Industrial composting	EcoInvent 3, cited in Patel et al. 2018	Biowaste CH, treatment of, composting
Carbon balance of industrial compost	Hermann *et al.*, cited in Patel et al.2018	
Degradation of PBS films on agricultural field	Yeung et al., cited in Patel et al. 2018	
Moss peat replacement	EcoInvent 3, cited in Patel et al. 2018	Peat Moss, RoW, peat moss production, horticultural use

Appendix E Fates of biogenic carbon embedded in plastics end-products for different end-of-life treatment options (Yeung et al., unpublished)

Treatment option and product	Fates of embedded carbon and avoided electricity /heat/ Moss peat	Proportion	Unit
Incineration (PP, PE, PET,PBS)	Proportion of C released	99%	%
	Electricity recovery	0.12	MJ / MJ waste
	Heat recovery	0.3	MJ / MJ waste
Composting (PBS)	% mass converted to compost at composting facility	60%	%
	% C released quickly after application to land	35%	%
	% C contributing to humus	5%	%
	Moss peat replaced by compost	0.79	kg / kg compost
Field Biodegradation (PBS)	% C contributing to humus	5%	%
	Proportion of C released	95%	

Appendix F RothC preliminary run results: Monthly biomass carbon inputs needed to reach NATMAP soil organic carbon content prior to the start of simulation

SERIES_NAME	t C/ha/month	SERIES_NAME	t C/ha/month
ABERFORD	0.2736	FROME	0.2014
AGNEY	0.2798	HOLME MOOR	0.363
BLACKWOOD	0.2951	HOLDERNESS	0.241
BRICKFIELD	0.2913	HUNSTANTON	0.2343
BROCKHURST	0.2429	ISLEHAM	0.5518
BURLINGHAM	0.1696	KEXBY	0.2951
BLACKTOFT	0.2629	METHWOLD	0.216
BISHAMPTON	0.2335	MILTON	0.2499
CONWAY	0.2893	NEWCHURCH	0.331
COOMBE	0.3681	NEWPORT	0.1689
CRANNYMOOR	0.5789	RAGDALE	0.2525
CURDRIDGE	0.1638	RIVINGTON	0.2333
CARSTENS	0.2164	ROMNEY	0.2591
CANNAMORE	0.2716	RUSKINGTON	0.2341
DENCHWORTH	0.2595	SALOP	0.2814
DOWNHOLLAND	0.7265	SESSAY	0.367
DUNKESWICK	0.2915	TATHWELL	0.1847
ELLERBECK	0.2523	WHIMPLE	0.2539
ENBORNE	0.2962	WICK	0.2201
EVERINGHAM	0.2527	WICKHAM	0.2715
EVESHAM	0.2751	WIGTON MOOR	0.2657
FLADBURY	0.3612	WORCESTER	0.2073
FOGGATHORPE	0.2515	WALLASEA	0.3239
FLINT	0.2429		

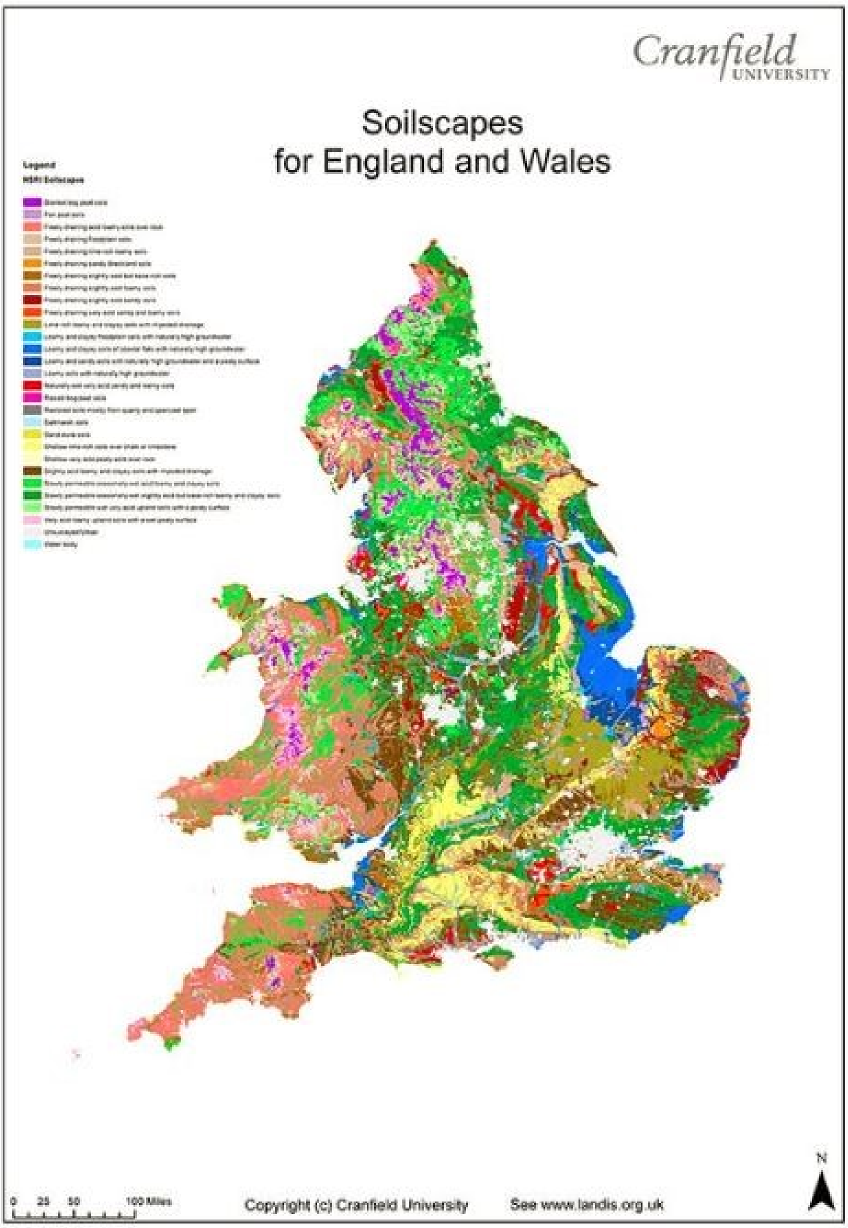
Appendix G Monthly biomass carbon inputs calculate basing on Hillier's approach and STAMINA simulated winter wheat yield outputs

SERIES_NAME	**DMY**	**Annual C input**	**Monthly C input**	**SERIES_NAME**	**DMY**	**Annual C input**	**Monthly C input**
	t/ha	t C/ha/year	t C/ha/month		t/ha	t C/ha/year	t C/ha/month
ABERFORD	7.14	3.20	0.2667	FROME	6.77	3.17	0.2640
AGNEY	6.86	3.18	0.2647	HOLME MOOR	6.36	3.13	0.2609
BLACKWOOD	6.43	3.14	0.2614	HOLDERNESS	6.52	3.15	0.2622
BRICKFIELD	6.50	3.14	0.2620	HUNSTANTON	6.74	3.17	0.2638
BROCKHURST	6.60	3.15	0.2628	ISLEHAM	6.81	3.17	0.2644
BURLINGHAM	6.48	3.14	0.2619	KEXBY	6.18	3.11	0.2594
BLACKTOFT	6.92	3.18	0.2652	METHWOLD	6.84	3.17	0.2645
BISHAMPTON	6.40	3.13	0.2612	MILTON	6.76	3.17	0.2640
CONWAY	6.82	3.17	0.2644	NEWCHURCH	6.83	3.17	0.2645
COOMBE	6.80	3.17	0.2643	NEWPORT	6.46	3.14	0.2617
CRANNYMOOR	6.27	3.12	**0.2601**	RAGDALE	6.41	3.14	0.2613
CURDRIDGE	6.67	3.16	0.2633	RIVINGTON	6.70	3.16	0.2635
CARSTENS	6.81	3.17	0.2643	ROMNEY	6.97	3.19	0.2655
CANNAMORE	6.58	3.15	0.2626	RUSKINGTON	6.82	3.17	0.2644
DENCHWORTH	6.53	3.15	0.2622	SALOP	6.48	3.14	0.2618
DOWNHOLLAND	6.98	3.19	0.2656	SESSAY	6.76	3.17	0.2640
DUNKESWICK	6.54	3.15	0.2623	TATHWELL	6.77	3.17	0.2641
ELLERBECK	6.80	3.17	0.2643	WHIMPLE	6.70	3.16	0.2636
ENBORNE	6.69	3.16	0.2635	WICK	6.36	3.13	0.2609
EVERINGHAM	6.24	3.12	0.2599	WICKHAM	6.63	3.16	0.2630
EVESHAM	6.55	3.15	0.2624	WIGTON MOOR	6.71	3.16	0.2636
FLADBURY	6.82	3.17	0.2645	WORCESTER	6.51	3.14	0.2621
FOGGATHORPE	6.47	3.14	0.2618	WALLASEA	6.86	3.18	0.2648
FLINT	6.45	3.14	0.2616				

Appendix H Monthly biomass carbon inputs calculate basing on Hillier's approach and STAMINA simulated Miscanthus yield outputs on selected soils

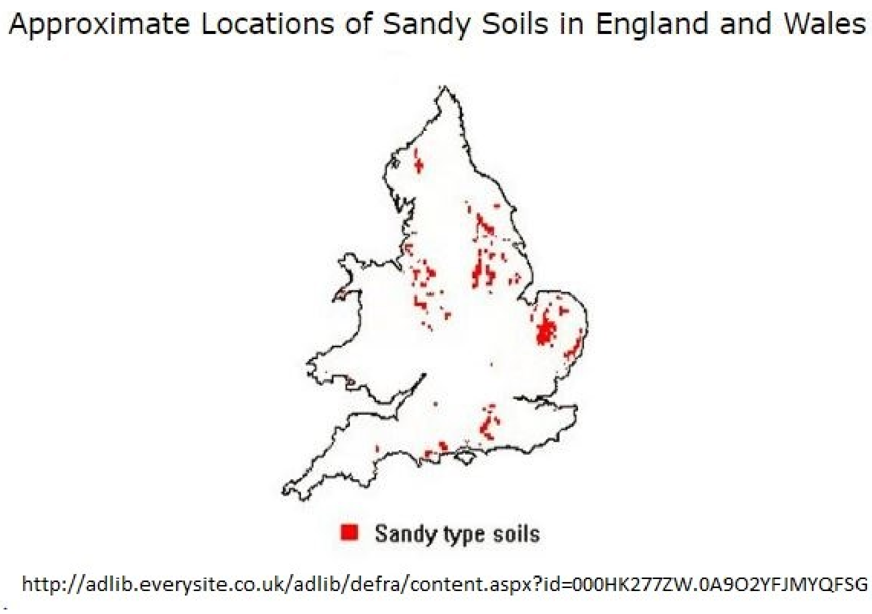
SERIES_NAME	DMY	Annual C input	Monthly C input
	t/ha	t C/ha/year	t C/ha/month
CRANNYMOOR	11.09	6.55	0.5460
EVERINGHAM	10.67	6.52	0.5435
HOLME MOOR	11.25	6.56	0.5468
KEXBY	10.50	6.51	0.5425

Appendix I UK Soil Observatory: Soilscapes for England and Wales



Map legend

Key	NSRI Soilscapes
	Blanket bog peat soils
	Fen peat soils
	Freely draining, acid, loamy soils over rock
	Freely draining, floodplain soils
	Freely draining, lime rich, loamy soils
	Freely draining, sandy Breckland soils
	Freely draining, slightly acid but base rich soils
	Freely draining, slightly acid, loamy soils
	Freely draining, slightly acid, sandy soils
	Freely draining, very acid, sandy and loamy soils
	Lime rich, loamy and clayey soils with impeded drainage
	Loamy and clayey floodplain soils with naturally high groundwater
	Loamy and clayey soils of coastal flats with naturally high groundwater
	Loamy and sandy soils with naturally high groundwater and a peaty surface
	Loamy soils with naturally high groundwater
	Naturally wet, very acid, sandy and loamy soils
	Raised bog peat soils
	Restored soils, mostly from quarry and opencast spoil
	Saltmarsh soils
	Sand dune soils
	Shallow, lime rich soils over chalk or limestone
	Shallow, very acid, peaty soils over rock
	Slightly acid, loamy and clayey soils with impeded drainage
	Slowly permeable, seasonally wet, acid, loamy and clayey soils
	Slowly pearmable, seasonally wet, slightly acid but base rich loamy and clayey soils
	Slowly pearmable, wet, very acid, upland soils with a peaty surface
	Very acid, loamy, upland soils with a wet peaty surface
	Unsurveyed/urban
	Water body



http://adlib.everysite.co.uk/adlib/defra/content.aspx?id=000HK277ZW.0A9O2YFJMYQFSG

Appendix K UK Corine Land Cover of map