

Implementing Land-use and Ecosystem Service Effects into An Integrated Bioenergy Value Chain Optimisation Framework

Miao Guo¹, Goetz M. Richter^{2†}, Robert A. Holland^{3†}, Felix Eigenbrod³, Gail Taylor³, Nilay Shah^{1*}

¹ *Department of Chemical Engineering, Imperial College London, London, SW7 2AZ UK,*

² *Rothamsted Research, West Common, Harpenden, Hertfordshire, AL5 2JQ, UK*

³ *Centre for Biological Sciences, University of Southampton, Highfield Campus, Southampton, SO17 1BJ, UK*

[†] *Equivalent contribution*

**corresponding author n.shah@imperial.ac.uk*

Abstract

This study presents a multi-objective optimisation model that is configured to account for a range of interrelated or conflicting questions with regard to the introduction of bioenergy systems. A spatial-temporal mixed integer linear programming model ETI-BVCM (Energy Technologies Institute - Bioenergy Value Chain Model) (ETI, 2015b; Geraldine Newton-Cross, 2015; Samsatli et al., 2015) was adopted and extended to incorporate resource-competing systems and effects on ecosystem services brought about by the land-use transitions in response to increasing bioenergy penetration over five decades. The extended model functionality allows exploration of the effects of constraining ecosystem services impacts on other system-wide performance measures such as cost or greenhouse gas emissions. The users can therefore constrain the overall model by metric indicators which quantify the changes of ecosystem services due to land use transitions. The model provides a decision-making tool for optimal design of bioenergy value chains supporting an economically and land-use efficient and environmentally sustainable UK energy system while still delivering multiple ecosystem services.

Keywords: optimisation, MILP, bioenergy supply chain, ecosystem services, food production, non-energy system

1. Introduction

A transition from the current fossil-based to a future bio-based carbon economy is expected to evolve progressively in the coming decades (Marquardt et al., 2010). Currently fossil fuels dominate world primary energy supply, meeting 80% of global energy demand (IEA, 2013). With projections that global energy demand will increase by 40% by 2035 (IEA, 2013) a pressing question is how this demand can be met while achieving an environmentally sustainable low carbon future. The energy sector is responsible for over 80% of the total greenhouse gas (GHG) emissions in the EU-28 (EEA, 2014) and approximately 83% of the UK GHG emissions in 2012 (DECC, 2014a). Bioenergy has been widely recognized as a strategic component for mitigating climate change (DECC, 2010; DECC et al., 2012) although the extent to which it is available in the future can vary depending on modelling assumption (Ekins et al., 2013; Helmut et al., 2013). This has triggered ambitious national/regional policy targets mandating the role of bioenergy within the overall energy portfolio

with an increasing focus on feedstock coming from non-food crops e.g. 2020 targets set in EU Renewable Energy Directive (RED) and EU new proposals (EuropeanParliament, 2015; EuropeanUnion, 2009). However, bioenergy is a complex system, which involves many interrelated or conflicting issues e.g. economic development vs. environmental and social sustainability, interaction between energy and non-energy sectors relying on the same resources and potentially the same productive lands (Cobuloglu & Buyuktahtakin, 2015; Čuček et al., 2012; van der Horst & Vermeulen, 2011). For the full potential of bioenergy to be exploited, a thorough understanding of the whole system and involved issues and opportunities must be developed for the environmental, social and economic consequences of key decisions enabling the identification of optimal pathways.

Landscapes generate a wide range of ecosystem services (ES) that provide benefits to human society (Mace et al., 2012; MillenniumEcosystemAssessment, 2005). These services fall into four broad categories that include - provisioning services such as food, animal feed, materials and energy; regulating and supporting services such as climate and water regulation and waste recycling; and cultural services such as recreational value and symbolic meaning. While the need to incorporate such ES into policy decisions at international, national and local scales is increasingly recognised (Daily & Matson, 2008; Gómez-Baggethun & Ruiz-Pérez, 2011), their value is often overlooked in real world land-use planning applications (Bateman et al., 2013). Land use transitions arising from increased production of bioenergy over coming decades have the potential to influence the provision of ES in both positive and negative ways (Holland et al., 2015; Milner et al., 2015). Such change will occur against a backdrop of ongoing global degradation of ecosystem services as highlighted by the Millennium Ecosystem Assessment (2005). Given their importance for human-wellbeing, their economic value and policy relevance, ES provide a useful framework to examine systems such as bioenergy (Gasparatos et al., 2011) and the associated environmental, social and economic implications of deployment strategies. The type, magnitude, and relative mix of services provided by ecosystems can vary with management interventions, where the ES trade-offs could occur at spatial and temporal scales (Rodriguez et al., 2006). A good example is the spatial-scale provisioning and regulating ES trade-offs arising from the land competition of bioenergy with the livestock sector, which has been recognised not only from a climate change (climate regulation ES) perspective but also in terms of agricultural household income source (food or energy provisioning ES) (Thornton & Gerber, 2010). The current study therefore sits at the nexus of a changing energy-food system over the coming decades and increased understanding of the importance of incorporating ecosystem services into land-use decisions.

There has been increasing research interests in modelling and optimisation of process industry supply chains since early 2000s as well as on bioenergy supply chains (Cucek et al., 2014; Elia & Floudas, 2014). Comprehensive reviews on biomass and bioenergy supply chain (SC) optimisation can be found in recent studies by De Meyer et al (2014), Cucek et al (2014), Yue et al (2014) and Samsatli et al (2015). As pointed out by Cucek et al (2014), most of the studies conducted on biorefinery SC focus on specific biofuel or limited production routes and are modelled as static

without considering dynamic behaviour. Recently, a comprehensive and flexible bioenergy pathway model ETI-BVCM addressed the research gap and considered multiple energy vectors and the future bioenergy mix and transition (ETI, 2015b; Geraldine Newton-Cross, 2015; Samsatli et al., 2015). At the same time, the optimisation studies in the field predominantly focus on economic feasibility or trade-offs between economic performance and GHGs for bioenergy SC design (Carnbero & Sowlati, 2014) although recent developments seek to incorporate a wider sustainability criteria. Zamboni et al. (2009) developed a multi-echelon corn-bioethanol SC optimisation model to simultaneously minimise well-to-tank GHG and economic cost. Mele et al.(2011) adopted a life cycle assessment (LCA) approach, combined with multi-objective optimisation model to consider the economic and environmental issues (e.g. global warming potential (GWP)) addressed from both mid-point and end-point perspectives. Čuček et al. (2012) introduced several environmental and social footprint indicators including a food-to-energy indicator measuring the mass-flow rate of food-intended crops converted into energy. El-Halwagi et al (2013) demonstrated a new approach to incorporate a safety matrix into the biorefinery optimisation framework. Gong and You (2014) presented a life cycle optimisation framework to simultaneously optimise the LCA functional unit based cost and GWP. Liu et al. (2014) developed a LCA-based biofuel SC optimisation model accounting for economic and two environmental objectives (fossil energy depletion and GWP). The review conducted by Yue et al (2014) discussed four layers (i.e. ecosystem, supply chain, process and molecule) concerned in bioenergy SC optimisation and highlighted the research needs to identify sustainable solutions to minimise adverse environmental impacts and maximise societal benefits. The lack of environmental and social sustainability concerns in bioenergy SC optimisation research was confirmed by De Meyer et al (2014), who reviewed studies between 1997 and 2012 with a focus on their modelling approach and objectives addressed. A comparatively few studies considered bioenergy deployment options while simultaneously incorporating system interaction or non-energy production into optimisation such as interaction of bioenergy with petroleum supply chains (D. J. Yue et al., 2014) and competition of food and biofuel supply chains (Cobuloglu & Buyuktahtakin, 2015; Cucek et al., 2014). The inclusion of such factors begins to explicitly acknowledge the value of ecosystem services e.g. food provisioning and the influence that they may exert on desirability of specific energy pathways.

The decision making should be supported by holistic and quantitative optimisation tools designed to consider conflicting objectives simultaneously and assessing the environmental and economic performance of bioenergy systems, considering the entire supply chain over the long-term. This study aims to bring ES into the multi-objective optimisation framework supporting bioenergy SC design and optimal land use for multiple systems (energy and non-energy use). Provisioning ES relating to food, livestock and energy production from dedicated and competing sources are considered quantitatively, as is the regulating service of stored carbon. A semi-quantitative approach to other ES is introduced (Holland et al., 2015; Milner et al., 2015) (ES categories given in Supplementary Information SI1). To our best knowledge, no publically available study has incorporated land-competing issues between bioenergy and non-energy (food) systems over time at

different land types and ecosystem services impacts due to land use transitions into such a spatially-explicit optimisation model.

2. Methodology

2.1 Problem statement

The underpinning concept is to integrate the effects of bioenergy penetration on ES and resource-competing systems (bioenergy vs. non-energy) within a comprehensive optimisation framework. This has been implemented by adopting and extending a spatial-temporal mixed integer linear programming (MILP) model - ETI-BVCM (ETI, 2015b; Geraldine Newton-Cross, 2015; Samsatli et al., 2015). MILP represents an effective mathematical modelling approach to solve complex optimisation tasks and identify the potential trade-offs between conflicting objectives, which can provide a better understanding of bioenergy systems and support decision-makers developing sustainable pathways towards bioenergy targets.

The ETI-BVCM model development was commissioned and funded by the UK's Energy Technologies Institute (ETI). This study is based on ETI-BVCM version 4.1.7. ETI-BVCM is a comprehensive and flexible toolkit for the whole-system optimisation of UK-based bioenergy value chains over the next five decades, supporting analysis and decision-making on optimal land use, biomass utilisation and different pathways for bioenergy production (ETI, 2015b). A model overview and a summary of the headline insights the ETI-BVCM model has generated to date have been addressed in details in the associated ETI papers (ETI, 2015b; Geraldine Newton-Cross, 2015; G. Newton-Cross & Evans, 2016). Mathematical formulations for ETI-BVCM can be found in (Samsatli et al., 2015).

The ETI-BVCM toolkit encompasses bioenergy systems considering biomass from diverse resources including domestic food crops, bioenergy crops, forest, organic and inorganic waste and imported biomass. It considers various pre-treatment and conversion technologies via biochemical, thermochemical and mechanical routes and uses inputs of yield models from feedstock resolved spatially for the UK (Hastings et al., 2014; Tallis et al., 2013). It is capable of analysing UK bioenergy supply chains at a grid resolution of $50\text{ km} \times 50\text{ km}$ and identifying the potential trade-off between GHG targets and cost optimal solutions for bioenergy value chain design over five decades (2010s-2050s). In this study, two terms for land cover classification are used i.e. land type, which refers to the non-cumulative areas linked to Corine land cover class, and land level, which denotes the cumulative areas. Land areas including arable lands, forestry lands, pasture lands and potential marginal lands, were considered in ETI-BVCM model and classified into four land type and four cumulative land levels according to the Corine land cover database (EuropeanCommission, 2009). As reported in (ETI, 2015b; Geraldine Newton-Cross, 2015; Samsatli et al., 2015), level 1 represents land type 1 i.e. arable land and heterogeneous agricultural areas; level 2 is defined as level 1 plus land type 2 (shrub and herbaceous vegetation association and open spaces with little or no vegetation); level 3 is the accumulation of level 2 and land type 3 (permanent crops and pasture

lands); level 4 is the accumulation of level 3 and land type 4 (forest and highly managed non-agricultural vegetated areas).

The non-energy systems incorporated in the extended ETI-BVCM model include food and industrial timber (e.g. roundwood) production and demand, which could compete with the bioenergy system due to their dependence on the same biomass resources and land demands (Fig 1). The economics of the system investigated focus on biomass cultivation, conversion technology, capacity assignment, logistics and transport networks (Shah, 2004).

The model was extended in this work to account for a range of ES and the impacts on ES induced by the land use transitions to the production of bioenergy and other products such as food and timber. Land use intensity (LUI, tonne C/ha) was introduced into the model as a performance indicator for supporting ES to represent the primary production efficiency per unit available land. The model is configured to account for annually harvested biomass extracted for socioeconomic use in multiple systems, which leads to an efficient land use system and supports sustainable development of bioenergy and non-energy markets. LUI along with GHGs is evaluated using a life cycle approach to take into account the impacts of the entire bioenergy supply network on carbon regulating and supporting ES. Other impacts of land use transitions on ES are assessed using the matrix approach described by Holland et al (2015) (section 2.2.4 and Table 3). The research objective of this study is to extend the ETI-BVCM modelling framework to investigate the bioenergy system configuration to deliver optimal value chains best supporting an economically efficient, low-GHG and land-use efficient UK energy system while maximising the ES benefits and limiting the detrimental effects on ES to ensure UK food security and sustainable development of the non-energy resource market.

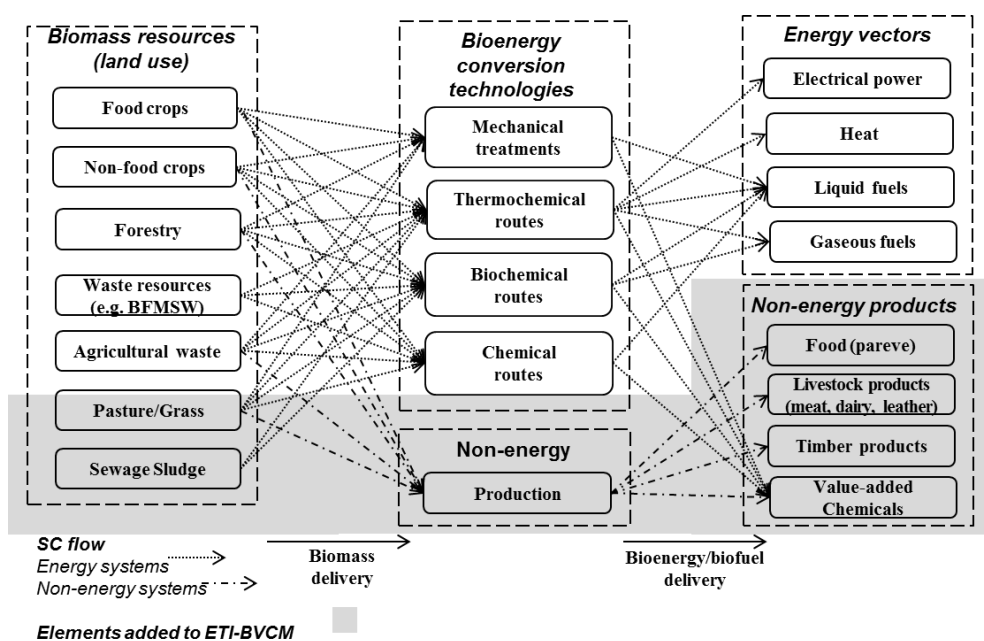


Figure 1 Bioenergy supply chains and non-energy systems (Notes: BFMSW=biodegradable fraction municipal solid waste)

2.2 Model formulation

The multi-objective MILP model ETI-BVCM (ETI, 2015b; Samsatli et al., 2015) was extended and formulated to account for non-energy systems, and ecosystem services (sections 2.2.1-2.2.5 & Table 1).

2.2.1 Objective function

ETI-BVCM adopted a multi-objective optimisation approach in which the objective function was formulated as a weighted sum of costs & revenues, GHG emissions, energy production and exergy production. By providing weights, the user could either minimise the total discounted costs, minimise the total GHGs or maximize energy/exergy production or supply chain profit within land availability constraints (Samsatli et al., 2015). In this study, the objective function is to minimise the total economic and GHG impacts of a bioenergy supply chain (Eq. (1)) where the weighting factor for GHGs is the market price for traded carbon (C) emissions.

$$Obj = \sum_d \sum_{kpi} (TSCI_{kpi,d} Weight F_{kpi,d}) \quad \forall kpi \in KPI, d \in D \quad (1)$$

2.2.2 Land constraints

The total areas allocated at each cumulative land level for bioenergy and non-energy resources are upper-bounded by the land availability ($MaxA_{c,al,d}$) in each cell at selected cumulative land level and the user-defined parameters for land allocation (Eq. (2), (3) and (4)). The area at each land type for energy and non-energy systems are constrained by the maximum available areas ($MaxA_{c,al,d} - MaxA_{c,al-1,d}$) for biomass plantation at a given land type (al) in each cell (c) and each decade (d) and user-defined land allocation parameters (Eq. (5)).

$$\sum_{al \leq \theta_{r,d}} \sum_r \sum_c (A1_{r,c,al,d} + A2_{r,c,al,d}) \leq \sum_c MaxA_{c,al,d} \gamma_{al,d} \quad \forall r \in B \cup FT, c \in C, al \in AL, d \in D \quad (2)$$

$$\sum_{al \leq \theta_{r,d}} \sum_{r \in B} A1_{r,c,al,d} \leq MaxA_{c,al,d} \alpha_{al,d} \quad \forall r \in B, c \in C, al \in AL, d \in D \quad (3)$$

$$\sum_{al \leq \theta_{r,d}} \sum_{r \in FT} A2_{r,c,al,d} \leq MaxA_{c,al,d} \beta_{al,d} \quad \forall r \in FT, c \in C, al \in AL, d \in D \quad (4)$$

$$\sum_{r \in B \cup (FT - FR)} (A1_{r,c,al,d} + A2_{r,c,al,d}) \Big|_{al \leq \theta_{r,d}} + \sum_{fr} A2_{fr,c,al,d} \Big|_{al = \mu_{fr,d}} \leq (MaxA_{c,al,d} - MaxA_{c,al-1,d}) \gamma_{al,d} \quad c \in C, al \in AL, d \in D \quad (5)$$

2.2.3 Non-energy system constraints

2.2.3.1 Soil bound livestock production

The livestock and derived products considered in the model mainly include – 1) cattle and calves and their derived beef and veal products; 2) pigs and pig meat; 3) sheep and lamb as well as their derived meat (and dairy); 4) poultry and poultry meat; 5) milk and other dairy (e.g. cheese) and 6)

hen eggs. The animal feed in general can be classified into two categories – 1) processed animal feed i.e. compound feed including cereal crops (e.g. wheat, maize, barley) cereal by-products, sugarbeet pulp and molasses, oilseed rape cake and meal; 2) pasture and wood lands including hay and silage derived from pasture, permanent grassland, rotational grassland (i.e. intensive grassland), extensive grassland for rough grazing and woodland for grazing.

The total livestock population in the UK is accounted for in the model, including the proportion of each livestock population ($1 - \varepsilon_{lr,d}^{min}$) raised for future breeding as well as the remaining population ($\varepsilon_{lr,d}^{min}$) raised for satisfying direct food demands (Eq. (6) and Eq. (10), respectively).

In the model, the UK livestock population is classified into two categories according to their feeding material - fodder-fed population (i.e. livestock fed with high proportion of processed feed and the silage derived from arable crops and residues as well as co-products from ethanol production) and forage-fed population (i.e. livestock mainly consuming biomass directly by grazing and hay or silage derived from grassland).

The pasture and woodland demand for forage-fed livestock feeding are further classified into four categories according to their soil quality and management (Armstrong et al., 2003; DEFRA, 2014; UKAgriculture, 2014), which are linked to Corine land types incorporated in BVCM model.

- “Rotational grassland” consists of grassland which is re-sown every few years (≤ 5 year) as part of the intensive grassland and/or an arable crop rotation (ley arable or grass ley). Its main usage is silage and forage for forage-fed cattle and dairy livestock. This category is linked to land type 1 (arable land and heterogeneous agricultural areas).
- “Permanent grassland” (or pasture) represents the grassland maintained perpetually without re-seeding and the grassland over five years old. Its usage is dominated by non-dairy young cattle and other grazing animals. This category is linked to land type 3 (permanent crops and pasture lands).
- “Rough grazing grassland” includes un-cultivated grassland that is found on the mountains, hills, moors and heaths of the UK. Its primary usage is assumed for sheep grazing. This category is linked to land type 2 (shrub and herbaceous vegetation association and open spaces with little or no vegetation).
- Woodland for livestock grazing is directly linked to land type 4 (forest and artificial non-agricultural vegetated areas). This is a minor fraction linked to rare breeds and natural habitat conservation.

To facilitate the aggregation of livestock groups with different species and ages, a Livestock Unit (LU) is introduced as a reference, which defines the grazing equivalent of one adult dairy cow producing 3000 kg of milk annually, without additional concentrated feed (Eurostat, 2013). Thus the land demand associated with each land type for livestock directly grazing is determined by the annualised stocking rate (LU/ha/y) in each cell for each livestock population and demand for forage-fed livestock population, whereas the land demand at each land type to provide fodder feed is determined by the annual crop yield (ton/ha), the annualised feeding rate (ton/LU/y) and total

demand for fodder-fed livestock population. Stocking rates are extremely variable with type of land quality, livestock type, temporal and spatial pattern of grazing regimes. Spatially explicit stocking rates at the regional/county scale have been under investigation in the UK for various regions e.g. map developed for Scotland (Matthews et al., 2012). The livestock sector along with food and other non-energy systems (e.g. winter wheat food demand, bio-chemical demand) have been incorporated into the extended BVCM model.

2.2.3.2 Constraint formulation

To achieve the optimal design of bioenergy value chains whilst minimizing the damages on provisioning ES (or even mitigating ES) to ensure UK food security and sustainable non-energy product supply, two constraints (Eq.(6) and Eq.(10)) are introduced to limit the maximum amount of biomass resources to be used for bioenergy production. As stated in Eq. (6), UK local demand for food or non-energy products (Dr) should be met by import and local production, which is determined by the conversion efficiency, area and annual biomass yield (Eq.(7), Eq.(8)(9)). The concept of conversion factor $Con_{r,p,c,d}$ is explained in Table 2, where a negative conversion factor indicates the consumption rate of resource r for non-energy technology (p); a positive conversion factor represents the production factor of resource (r) in a given technology (p). Decision variable $PT_{p,c,d}$ determines the productivity of each non-energy technology (p) in cell (c), decade (d). To further achieve the domestic food security and sustainability development of non-energy provisioning ES, a certain fraction (security factor as a user-defined parameter) of UK demand for food and other non-energy products need to be met by local production (Eq.(10)).

$$\sum_c (Im_{r,c,d} + Pr_{r,c,d} \varepsilon_{r,d}^{min} |_{r \in LR}) \geq D_{r,d} \quad \forall r \in DR, c \in C, d \in D \quad (6)$$

$$Pr_{r,c,d} = \sum_p Con_{r,p,c,d} PT_{p,c,d} \quad \text{if } Con_{r,p,c,d} > 0 \quad \forall r \in DR, c \in C, d \in D, p \in P \quad (7)$$

$$-\sum_p Con_{r,p,c,d} PT_{p,c,d} = \sum_{al \leq \theta_{r,d}} A2_{r,c,al,d} Yield_{r,c,s,d} \quad \text{if } Con_{r,p,c,d} < 0 \quad \forall r \in (FT - FR), al \in AL, c \in C, d \in D, s \in S, p \in P \quad (8)$$

$$-\sum_{p \in PL} Con_{r,p,c,d} PT_{p,c,d} = A2_{r,c,al,d} |_{al = \mu_{fr,d}} \quad \text{if } Con_{r,p,c,d} < 0 \quad \forall r \in FR, al \in AL, c \in C, d \in D, p \in PL \quad (9)$$

$$\sum_c Pr_{r,c,d} \varepsilon_{r,d}^{min} |_{r \in LR} \geq D_{r,d} SecF_{r,d} \quad \forall r \in DR, c \in C, d \in D \quad (10)$$

2.2.4 Ecosystem services impacts

The variable $ESI_{epi,d}$ represents the change of ES brought about by land use transitions in response to bioenergy system development in each decade (d), which is constrained by the user-defined maximum allowed relative change to ES (Eq.(11)). As presented in Eq. (12), the decadal impacts on ES caused by the land transition to these uses can be semi-quantified by introducing land use transition factors $ESIF_{r,al,epi}$. The impact matrix of land transition is being developed under this project research agenda to assess the ES impacts of land use change associated with a biomass

production system. The principles for developing such a matrix which identifies the direction and magnitude of the changes in ES impacts of new land use patterns have been addressed in (Holland et al., 2015; Milner et al., 2015) and through the ETI-funded ELUM project (ETI, 2015a). Work is ongoing to refine this matrix to match land types specified in the BVCM, and to consider spatial provision of services. In the current study we present scores based on an approximate cross-walking between land categories used in the studies of (Holland et al., 2015; Milner et al., 2015) and the BVCM land classes.

Each land use ES change factor is divided into seven impact levels with indicator scores assigned (not spatially explicit, ESIF scores given in Table 3). A negative score (-1,-2,-3) indicates that the land use transition would likely have a negative effect on the ES whereas a positive (1, 2, 3) or a neutral score (0) represent positive effects or little/no impacts on ES for any given land-use transition. $TR_{r,c,al,d}$ denotes the transitions from areas of a reference cropping system to bioenergy feedstock (r) production at each land type (al), cell (c) due to bioenergy penetration in each decade (d). As given by Eq. (13) decision variable $Tr_{r,c,al,d}$ is dependent on the difference in dedicated areas at each land type (al) for bioenergy feedstock production at the end of each decade (d) compared with the previous decade ($d-1$). A negative land use transition value indicates land use change from a bioenergy to non-energy cropping system whereas a positive value implies land transition from non-energy to bioenergy system use. Therefore, not only the land transition to bioenergy use (positive $Tr_{r,c,al,d}$) coupled with positive influences on a given epi could bring the beneficial effects (positive $ESI_{epi,d}$) but also avoidance of negative ES impacts of bioenergy cropping system (negative $ESIF_{r,al,epi}$) by moving land use towards non-energy systems (negative $Tr_{r,c,al,d}$) could potentially lead to an environmentally beneficial system (Table 3). Note that (i) the key contribution here is the modelling framework and (ii) the results obtained in certain ES categories are sensitive to input data which suffer from paucity, hence the semi-quantitative approach; however, a spatially-explicit quantitative approach is being developed under this research agenda to map out the bioenergy impacts on biodiversity and wider ES in the UK over multiple time periods.

$$ESI_{epi,d} \geq MinESI_{epi,d} \quad \forall epi \in EPI, d \in D \quad (11)$$

$$ESI_{epi,d} = \sum_{r \in B} \sum_c \sum_{al} TR_{r,c,al,d} ESIF_{r,al,epi} \quad \forall r \in B, c \in C, al \in AL, d \in D, epi \in EPI \quad (12)$$

$$Tr_{r,c,al,d} = (A1_{r,c,al,d} - A1_{r,c,al,d-1}) \Big|_{al \leq \theta_{r,d}} \quad \forall r \in B, c \in C, al \in AL, d \in D \quad (13)$$

2.2.5 Land use intensity

LUI (tonne C/ha) formulated in Eq. (14) was introduced into the model - it is calculated after the model is solved. NPP is referred to as the net primary production of an ecosystem in terms of carbon fixation rate, quantified as the net amount of carbon assimilated in a given period by vegetation (Krausmann et al., 2013; Zhuang et al., 2013). $NPPh_{r,c,s,d}$ represents the biomass extracted for further socioeconomic use and includes harvested crops, consumed crop residues, fuel wood and

industrial roundwood as well as forage (including biomass directly consumed by livestock by grazing and biomass indirectly consumed through harvest for production of hay & silage). $NPPh_{r,c,s,d}$ involves above-ground harvested biomass for economic use and the used above-ground residues, which generally can be derived from Eq. (15). The parameters $Fabv_r$, HI_r , $Blos_r$, Fh_r , Rc_r can be obtained from publically available data sources e.g. (Zhuang et al., 2013). $NPP_{r,c,s,d}$ represents the difference between gross primary production (GPP describes the rate at which the plant produces useful chemical energy and is defined as the total amount of carbon fixed by photosynthesis) and plant respiration, and can be projected by using well-validated process-based simulation models e.g. NASA-CASA model, DeNitrification-DeComposition (DNDC). In this project, NPP will be linked to spatially resolved maps of biomass production and yield.

$$LUI_d = \frac{\sum_{r \in B \cup FT} \sum_c \sum_{al} NPPh_{r,c,s,d} (A1_{r,c,al,d} + A2_{r,c,al,d})}{\sum_c \sum_{al} MaxA_{c,al,d}} \quad (14)$$

$$NPPh_{r,c,s,d} = NPP_{r,c,s,d} \cdot Fabv_r \cdot HI_r \cdot (1 - Blos_r) \cdot (1 + Fh_r \cdot Rc_r) \quad (15)$$

Table 1 Nomenclature for extended ETI-BVCM model

Indices and sets	
$r \in R$	resources (biomass, non-energy resources e.g. water, sugar and energy carriers e.g. electricity, biofuel)
$b \in B \subseteq R$	biomass resources used for bioenergy system
$ft \in FT \subseteq R$	biomass resources for non-energy systems including timber resources, food crops, forage/fodder (including grassland/woodland biomass directly consumed by livestock by grazing and biomass indirectly consumed through harvest for production of compound feed, hay & silage)
$fr \in FR \subseteq FT$	forage feed i.e. grazed pastureland (including hay and stillage derived from grassland) and woodland
$dr \in DR \subseteq R$	non-energy demand products produced from biomass resource e.g. wheat flour, livestock
$lr \in LR \subseteq DR$	livestock including fodder-fed and forage-fed livestock
$s \in S$	scenarios e.g. low/medium carbon concentration scenarios based on UK Climate Projections 2009
$d \in D$	decades {2010s, 2020s, 2030s, 2040s, 2050s}
$c \in C$	UK grid cells {1, 2, ..., 157}
$al \in AL$	land types {'1': "arable land and heterogeneous agricultural areas", '2': "shrub and herbaceous vegetation association and open spaces with little or no vegetation", '3': "permanent crops and pasture lands", '4': "forest and artificial non-agricultural vegetated area"} This set also represents the cumulative land levels - level 1 represents land type 1; level 2 is defined as level 1 plus land type 2; level 3 is the accumulation of level 2 and land type 3; level 4 is the accumulation of level 3 and land type 4.
$p \in P$	non-energy production technology (including livestock feeding)
$pl \in PL \subseteq P$	livestock production by consuming forage/fodder
$kpi \in KPI$	key performance indicators including the cost, CO ₂ and other GHGs
$epi \in EPI$	ecosystem service performance indicators e.g. biodiversity, water quality and soil quality
Parameters	
$MinESI_{epi,d}$	Maximum allowed change to regulating/supporting ES or minimum food/timber/energy provisioning ES (indicator epi) in decade d
$WeightF_{kpi,d}$	Weighting factor for key performance indicator kpi in decade d; in the case of GHGs, market price for traded C emissions may be applied (£/kg CO ₂ equivalence)
$ESIF_{r,al,epi}$	Impacts on ecosystem service (indicator epi) due to new land use transition patterns for cultivation of biomass resource r on land type al for bioenergy system development (unit:

	per ha)
$Yield_{r,c,s,d}$	Maximum yield (oven dry weight) of resource r in cell c under scenario s in decade d (odt/ha/y)
$MaxA_{c,al,d}$	Maximum available lands for biomass plantation in cell c at cumulative land level al in decade d (ha)
$\alpha_{al,d}$	Fraction of area allocated for biomass cultivation for bioenergy system at cumulative land level al in decade d
$\beta_{al,d}$	Fraction of total area allocated for biomass cultivation for non-energy systems at cumulative land level al in decade d
$\gamma_{al,d}$	Fraction of total area allocated for total biomass cultivation for energy and non-energy systems at land type/level al in decade d
$D_{r,s,d}$	Annual demand of resource r under scenario s in decade d for non-energy system (timber, food etc.) (unit resource/y)
$SecF_{r,d}$	Security factor to ensure a certain fraction of resource r demand for provisioning ecosystem services (e.g. food, timber) to be met by local production in decade d
$\theta_{r,d}$	Cumulative land level restriction for biomass resources r in each decade d
$\mu_{fr,d}$	Land type restriction for forage biomass fr in each decade d;
$\epsilon_{lr,d}^{min}$	Proportion of livestock population to be slaughtered or consumed for food production
$Con_{r,p,c,d}$	Conversion factor for resource r under non-energy production technology p in cell c in decade d; a negative conversion factor indicates the consumption factor of resource r in p; a positive conversion factor indicates the production factor of resource r in p (unit resource)
$NPPh_{r,c,s,d}$	Harvested net primary production (NPP) of biomass r in cell c under scenario s in decade d for socioeconomic use (t C/ha)
$NPP_{r,c,s,d}$	Net primary production of biomass r in cell c under scenario s in decade d (t C/ha)
$Fabv_r$	Proportion of aboveground biomass for resource r
HI_r	Harvest index of biomass resource r, measuring the proportion of total aboveground biomass allocated to economic yield of crop
$Blos_r$	Proportion of biomass loss or return for resource r
Fh_r	Harvest factor for resource r representing the ratio of available above-ground residues to above-ground economic yield of harvested biomass
Rc_r	Recover rate of biomass r refers to the ratio of used above-ground residues to available above-ground residues

Continuous variables

$TSCI_{kpi,d}$	Total impacts caused by whole bioenergy supply chain in decade d expressed as key performance indicator kpi (including cost and GHGs), consisting of the decadal impacts caused by crop production, infrastructure/capital, technology operation, resource import and storage, resource purchase, transport, carbon transport, waste disposal, credits brought by carbon capture and storage, carbon sequestration by long rotation forestry and offset by by-products
$ESI_{epi,d}$	Ecosystem services impacts of bioenergy supply chain in terms of indicator epi in decade d
$TR_{r,c,al,d}$	Area expansion/contraction of biomass r in cell c, at land type al in decade d to represent the land use transition (ha)
$A1_{r,c,al,d}$	Areas dedicated for cultivation of resource r for bioenergy system in cell c, at land type al in decade d (ha, non-negative)
$A2_{r,c,al,d}$	Areas dedicated for cultivation of resource r for non-energy systems in cell c, at land type al in decade d (ha, non-negative)
$Im_{r,c,d}$	Import rate of resource r for non-energy systems in cell c in decade d (unit output/y)
$Pr_{r,c,d}$	Production rate of resource r for non-energy systems in cell c in decade d (unit output/y)
$PT_{p,c,d}$	Productivity of non-energy technology p in cell c, in decade d (unit output/y)
LUI_d	Land use intensity - harvested NPP for cultivation of given biomass feedstock per unit available land in decade d (t C/ha)

Table 2 Illustrative example for production of food and non-energy resources

Examples - food resources (arable crops and livestock) and non-energy resources		
Set of non-energy production P	$Con_{r,p,c,d}$ for input r	$Con_{r,p,c,d}$ for output r
Forage-fed cattle by grazing	Permanent Grass -0.5 ha	Dairy Cattle 1 LU
Forage-fed cattle by rough grazing	Woodland -10 ha	Cattle 1 LU
Fodder-fed cattle by compound feed	Wheat - 0.83tonne	Cattle 1 LU
Milk production	Rotation grass -1 ha	Milk 10450L
Wheat flour	Wheat -1 tonne	Wheat flour 0.9 ton
Timber products	Forest -1 tonne	Timber product 0.8 ton

Table 3 Land transition matrix score and ecosystem services impacts

ES impact level	Likely strong negative	Likely negative	Likely weakly negative	No impact	Likely weakly positive	Likely positive	Likely strongly positive
ESIF scores (per ha)	-3	-2	-1	0	1	2	3
Direction of change of ecosystem services impacts brought about by land use transition towards bioenergy production system (note positive indicates an improvement)							
$ESIF_{r,al,epi}^a$	$TR_{r,c,al,d}^b$			$ESI_{epi,d}^c$			
+	+			+			
+	-			-			
-	+			-			
-	-			+			

Notes: a) positive and negative $ESIF_{r,al,epi}$ values indicate beneficial and damaging effects respectively of transitioning to a bioenergy crop; b) positive $TR_{r,c,al,d}$ means land use transition towards bioenergy feedstock whereas negative $TR_{r,c,al,d}$ suggests land use transition from energy to non-energy systems; c) positive or negative $ESI_{epi,d}$ represents the resulted benefits or detrimental impacts on ES respectively of the actual transition.

3. Results and discussion

To demonstrate the model concept i.e. the trade-off between livestock and bioenergy provisioning ES as well as the effects of constraining ES impacts on other system-wide performance indicators two illustrative case studies are presented based on the representative rather than actual data. Please note that these case studies only aim to illustrate the concept and functionality of the extended model but not intend to give any indicative information or insight for policy recommendation. The extended BVCM model was solved in AIMMS 3.14 using CPLEX 12.6 solver on a 3.4GHz 16GB RAM computer.

3.1 Case study on resource-competing systems – transport biofuel vs. livestock

3.1.1 UK livestock overview and case study assumptions

The livestock sector is a complex system. The total population dominated by cattle, sheep, lamb, pig and poultry in the UK are presented in Fig 2, where goats, farmed deer and horses are negligible. According to the statistics (1985-2014), overall more than 70% of UK domestic supply of animal products is met by home-fed production (Fig 3). The UK cattle populations declined from 13.03 to 9.84 million heads between 1985 to 2014 (DEFRA, 2015a). This equates to 3.39-3.75 million beef

and dairy breeding heads plus 0.77-0.92 million other above 2-year old female cattle (not breeding) and 2.87-3.09 million younger female heads (<2 years) as well as 2.74-3.03 million male cattle. The majority of ruminant livestock utilises grassland for much of the year. Typically, dairy and breeding cattle are housed for approximately 24 weeks over the winter period (Jerram et al., 2001). Whilst cattle are a large consumer of fodder they also consume composite or compound animal feed (especially for dairy cows) which is produced mainly from UK cereal and their by-products supplemented with soya/oilseed rape cake and meal.

In the UK, 100% of milk supply was met by domestic production (Fig 3); there was a significant increase in the efficiency per dairy cow (average yield 4872 to 7916 L/y) and a decline in the dairy herd (3213-1850 thousand head) from 1985 to 2014 (DEFRA, 2015a). The total dairy population can be classified into three types (Table 4) - 1) cows at grass which are predominantly grass-based and operating at lower yield levels; 2) composite category, which is fed and housed with a mixed approach but operated at maximum use of farm labour; and 3) high-output cows which are housed for most of the year with intensive inputs (AHDB, 2014). Based on the analysis given in the Supplementary Information, it is assumed that the proportion of the three dairy farm classification in DairyCo's Milkbench+ Evidence Report (AHDB, 2014) is representative of the UK dairy industry structure. The average grass-feeding period and non-forage feeding rate for each dairy farm classification are given in Table 4.

To estimate stocking rates, all forage-fed livestock groups (species and ages) are converted to a consistent reference livestock unit (LU) using the coefficients listed in Table 5. The derived stocking rates vary significantly with land quality (grassland type), livestock type, temporal and spatial pattern of grazing regimes. More detailed information about the livestock sector and overview of the average stocking rate linked to each land category (without accounting for spatially-explicit livestock density) is given in Supplementary Information (SI2).

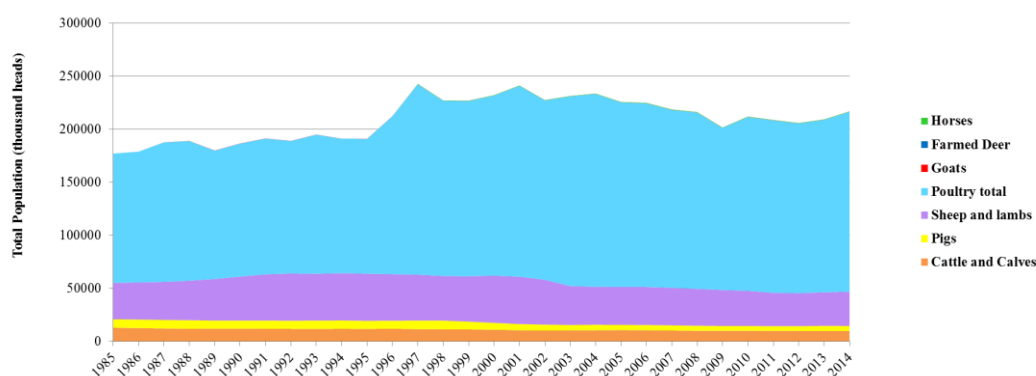


Figure 2 Total livestock population in the UK (DEFRA, 2015a)

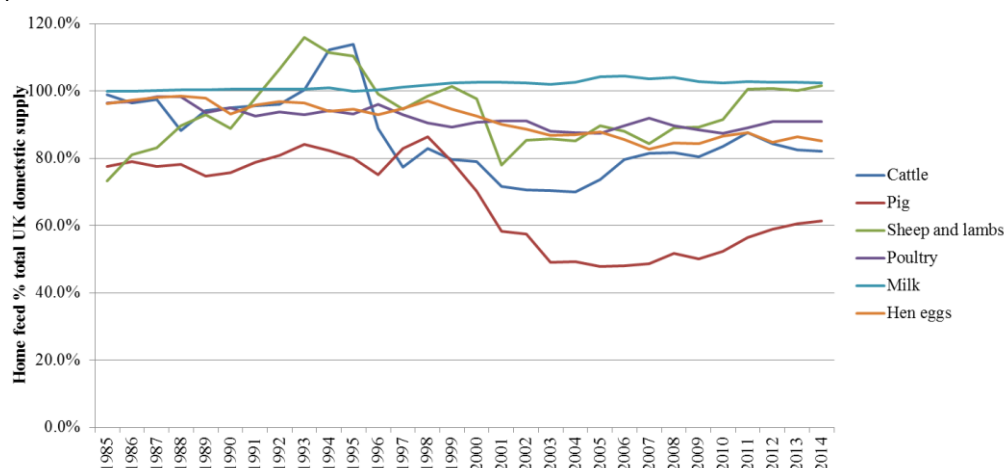


Figure 3 Contribution of the home-fed production to the total domestic supply in the UK (DEFRA, 2015a)

Table 4 UK dairy farming system (AHDB, 2014)^a

Dairy System	Grass based	Composite	High input/output
Non-forage feed (kg/cow)	1326	2745	2853
Grass-feed (weeks/year)	35 (67%)	26 (50%)	22 (42%)
Wheat fraction as non-forage (t/cow/y) ^b	0.385	0.796	0.827
Number of farms	120	130	72
Average herd size (head) ^c	168	185	266
Average milk yield (litres/cow/y)	5890	7885	8619
UK dairy population included in AHDB survey (%) ^d	0.90%	1.07%	0.85%

Notes: a. It is assumed that DairyCo's Milkbench+ Evidence Report is representative of the UK dairy industry with total 13265 farms in 2013 (AHDB, 2014); b. the feeding rate for wheat is assumed based on the feeding rate of compound/blend fodder feeding for dairy cows and the share of the wheat in raw compound feeding materials (average 29% from 1997-2014)(AHDB, 2014; Defra, 2015b); c. UK average herd size has been increasing from 89 in 2002 to currently about 128 in 2013 and herd size varies by region (AHDB, 2014); d. total dairy cattle population of 1.78 million heads (AHDB, 2014).

Table 5 The livestock unit coefficient (Eurostat, 2013)

Cattle	Under 1 year old	0.400
	1 - 2 years old	0.700
	Male, 2 years old and over	1.000
	Heifers, 2 years old and over	0.800
	Dairy cows	1.000
	Other cows, 2 years old and over	0.800
Sheep and goats		0.100
Horse		0.800

Pigs	Piglets having a live weight of under 20 kg	0.027
	Breeding sows weighing 50 kg and over	0.500
	Other pigs	0.300
Poultry	Broilers	0.007
	Laying hens	0.014
	Ostriches	0.350
	Other poultry	0.030

3.1.2 Case study for 2G transport fuel vs. cattle population

The extended ETI-BVCM model was applied to a UK advanced biofuel case study with the EU RED target of a 10% share of renewables in the transport sector by 2020 (equivalent to an annual minimum transport fuel demand of 164 PJ (Murray & Cluzel, 2014)) and a cap of 7% on the contribution from food crops (EuropeanParliament, 2015). Thus, in this case study a 3% share of UK transport fuel is assumed to be met by UK domestic production of 2G biofuel by 2020, including biomethanol, biodiesel and bioethanol derived from Miscanthus and short rotation coppiced (SRC) willow via biochemical and thermochemical routes. It is assumed that the total UK transport fuel demands in the coming decades (2030s-2050s) will remain constant whereas UK local 2G biofuel production will contribute 6%, 8% of 10% share of the market for the 2030s, 2040s 2050s, respectively. The market prices for traded C emissions in five decades were assumed as £23.2/t CO₂ (2010s) £45.5/t CO₂ (2020s), £99.5/t CO₂ (2030s), £164.5/t CO₂ (2040s), and £230.7/t CO₂ (2050s), respectively where a discount rate of 3.5% is applied to discount the C price back to 2010. The objective function of this case study is to achieve trade-off between minimised biofuel supply chain cost and minimised GHG emissions simultaneously meeting the ES constraints on soil quality. An illustrative land transition impact matrix is given in Table 8, the assumed transition factors $ESIF_{r,al, soil\ quality}$ for cultivation of biomass resources on four land types are used in this case study. Minimum required soil quality ES ($MinESI_{epi,d}$) for each decade is assumed as 1000. In addition, there is no land constraint assumed at each land level in this case study ($\alpha_{al,d}, \beta_{al,d}, \gamma_{al,d}$ assumed as 1). The spatially resolved maps of biomass production and yield were derived from outputs of process-based models for arable crops, e.g. winter wheat (Richter & Semenov, 2005) or sugar beet (Richter et al., 2006). Output from these scenario simulations was used to generate empirical (meta-) models to estimate of regional resource distribution dependent on UK climate projections (UKCP09) and European Soil Data Base. Respective empirical correction factors were applied to account for yield gap, technological progress and carbon fertilisation effect. For perennial crops alternative routes were taken to derive yield maps either by empirical or process modelling for Miscanthus (Hastings et al., 2009; Richter et al., 2008) and willow (Tallis et al., 2013).

In this case study, the whole UK cattle population is taken into account to demonstrate the model functionality. The total cattle population of 9905 thousand head is equivalent to 7058.6 thousand LU in 2010s (average data of 2011-2014), which includes all age groups to meet 100% UK milk consumption and about 84% beef demand (DEFRA, 2015a). The latest statistics for dairy system

structure and milk production was used in this case study to represent the current technology and practice in dairy industry. It is assumed that cattle for breeding and meat demands are forage-based whilst feeding of dairy cattle is met by a combination of composite fodder and forage. The land demands for winter wheat for compound fodder are examined in this case study implementing a feeding rate for each dairy farm class based on non-forage and wheat share (Table 4). To demonstrate the model functionality, the scenario was simplified by adopting a country-level average stocking rate for each grassland type across the UK. However, such average stocking rates are not representative of the different livestock density across the UK. Key assumptions for 2010s are given in Table 6 whereas the annual total cattle population in the following decades (2020s-2050s) were assumed to follow the historical trend over the time period of 1980-2014 ($Population (head/y) = -98.765 \times decade + 208241.615$) (DEFRA, 2015a) with herd structure and feeding regime unchanged (Fig 4). This assumption may represent a very low demand scenario for future cattle-derived food products (e.g. beef and veal, milk and cheese).

As the optimal configuration presented in Table 7 and Fig 5A, the total areas allocated for cattle feeding (intensive and permanent grassland, woodland and winter wheat plantation) over five decades (2010s-2050s) vary between 1.54 to 2.87 million ha, accounting for 6.9%-12.9% of total UK lands, where the intensive and permanent grassland predominates. Permanent grassland sites are located in 21-49 cells across the UK (Fig 7) occupying 5.2% -8.7% of total available UK lands over five decades. On the contrary to the decreasing trends of land occupation by cattle feeding, an increase in land allocation for 2G biofuel production is observed with shifting from 2010s to 2050s (Fig 5A). A dramatic change in land allocation for Miscanthus and rough grazing throughout five decades is noticeable (Table 7). Such changes can be explained by the fact that the model outputs only represent the cost and GHG optimal solutions for each decade without accounting for any additional costs caused by such land transitions (e.g. infrastructure re-establishment due to transition). The identified optimal configurations for biofuel supply chain design between 2010s-2050s are presented in Fig 5B, which involve the deployment of pyrolysis and hydro-treating technology (upgraded biocrude oil) as well as gasification and catalytic conversion (bio-methanol) from SRC willow and Miscanthus. Taking into account the carbon trading values, the economic impacts for the entire 2G biofuel supply chain are the dominant contributor towards the objective function (Fig 6B), where the costs for biorefineries are driving factors. Over five decades, the operational and capital costs at biofuel production stage vary between 1569.6 and 3392.3 million pounds, causing 88.4-93.6% of the decadal economic impacts (Fig 6A). The total contributions of the crop production stage and natural gas purchase range between 6.1% and 12% whereas only negligible costs occur at transport stage (Fig 6A).

This illustrative case study demonstrates the underpinning concept of the extended model i.e. to integrate resource-competing systems such as livestock into bioenergy supply chain optimisation model and to examine the optimal land allocation strategies for sustaining two provisioning ES (bioenergy and livestock production). However, this illustrative case study adopted assumptions

(e.g. decadal total cattle population) and illustrative data (e.g. land transition ES score, average stocking rates), thus the derived pathways and optimal solutions (e.g. the non-realistic area allocation for the biofuel production) should not be considered as policy-recommendation. Currently, for grassland, spatially explicit productivity is approximated by using country-level average stocking rates and land availability thus the derived forage feed maps are not representative. In the future, a process model based on the Lingra approach (Schapendonk et al., 1998) will be used to predict productivity of different grassland types in the UK. A wider range of compound feeding material as well as other livestock population (e.g. sheep, lamb, pig and poultry) will be investigated in future studies, where multi-scenarios with actual data will be modelled.

Table 6 Key parameters for UK cattle population

Cattle population (lr)	Annual demand $D_{r,d} _{d=1}$	Feeding resource (ft)	Land type restriction for feeding resource $\mu_{fr,d}$	Stocking rate or feeding rate ($Con_{r,p,c,d}$ for input r)
Dairy breeding herd (≥ 2 year) grass-based	Population: 573897 LU Milk 3380251636L	Rotational grass	Level 1	1.8LU/ha/y
		Wheat	Level 1	0.385 t/LU/y
Dairy breeding herd (≥ 2 year) composite	Population 684634 LU Milk 5398336936 L	Rotational grass	Level 1	1.8LU/ha/y
		wheat	Level 1	0.796 t/LU/y
Dairy breeding herd (≥ 2 year) high-output	Population 545202 LU Milk 4699094976 L	Rotational grass	Level 1	1.8LU/ha/y
		Wheat	Level 1	0.827 t/LU/y
Female breeding beef herd (≥ 2 year)	Population 1306733 LU	Rotational grass	Level 1	2.5 LU/ha/y
Other Female cattle and male cattle (≥ 2 year)	Population 1108394 LU	Rough grazing grass	Level 2	0.25LU/ha/y
		Permanent grass	Level 3	2 LU/ha/y
		Woodland	Level 4	0.1LU/ha/y
Younger female and male cattle (< 2 year)	Population 2839743 LU	Permanent grass	Level 3	2 LU/ha/y

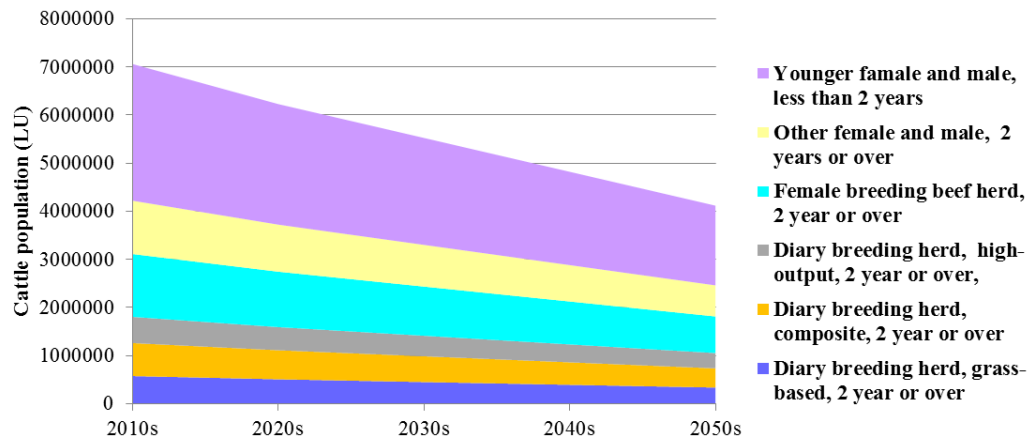


Figure 4 Assumed decadal cattle population in the UK

Table 7 Land allocation for transport fuel and cattle feeding in the UK in optimal configuration

Area allocation $A_{2,r,c,al,d}$	Land type	2010s	2020s	2030s	2040s	2050s
Forage and fodder feeding resources for cattle (unit: ha)						
Winter wheat	1	1.59E+05	1.47E+05	1.02E+05	7.19E+04	6.96E+04
Rotation grass	1	5.23E+05	4.61E+05	4.09E+05	3.57E+05	3.05E+05
Rough grazing grass	2	2.43E+05	2.64E+04	2.15E+05	9.42E+04	0.00E+00
Permanent grassland	3	1.94E+06	1.74E+06	1.52E+06	1.34E+06	1.15E+06
Woodland	4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.40E+04
Biomass for transport biofuel production (unit: ha)						
SRC willow	1	4.35E+03	1.13E+04	5.20E+04	6.47E+04	6.35E+04
	2	8.38E+05	1.33E+06	2.14E+06	2.27E+06	2.42E+06
	3	2.40E+04	1.07E+05	1.72E+05	3.66E+05	5.00E+05
	4	8.12E+04	1.36E+05	1.93E+05	2.28E+05	3.12E+05
Miscanthus	1	0.00E+00	1.20E+04	0.00E+00	0.00E+00	0.00E+00
	2	0.00E+00	1.38E+05	0.00E+00	0.00E+00	0.00E+00
	3	0.00E+00	4.98E+04	0.00E+00	0.00E+00	0.00E+00
	4	0.00E+00	4.35E+04	0.00E+00	0.00E+00	0.00E+00

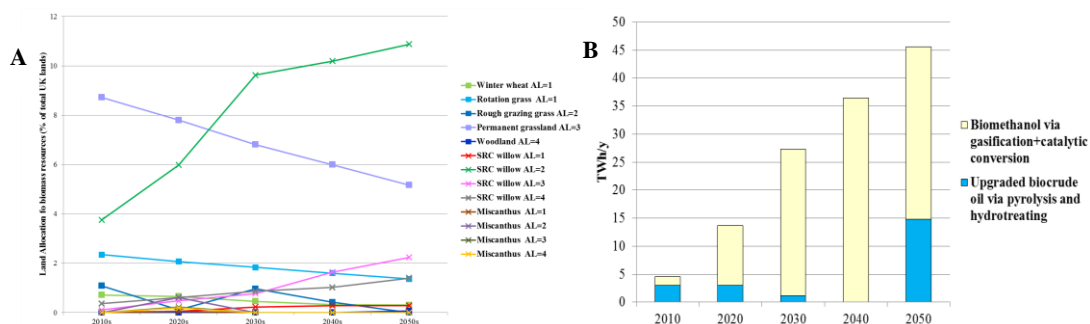


Figure 5 Land allocation (% total UK lands) for 2G biofuel and cattle feeding at each land type *al* (A) and annual 2G transport biofuel energy production (B) in optimal configuration

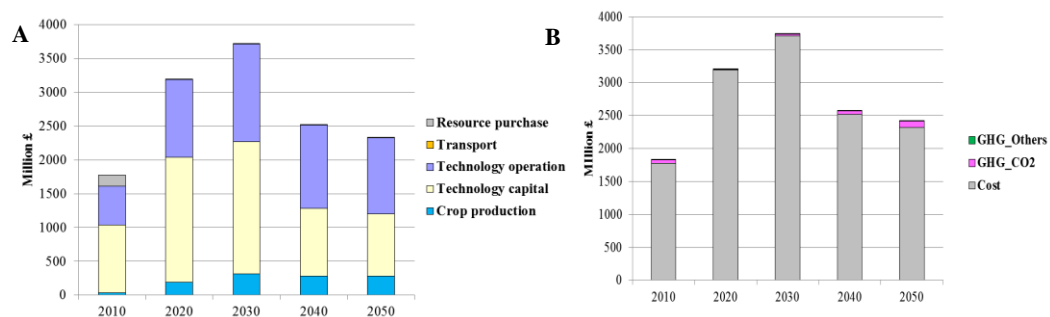


Figure 6 Decadal cost (A) and system performance (B) of optimal transport biofuel supply chain

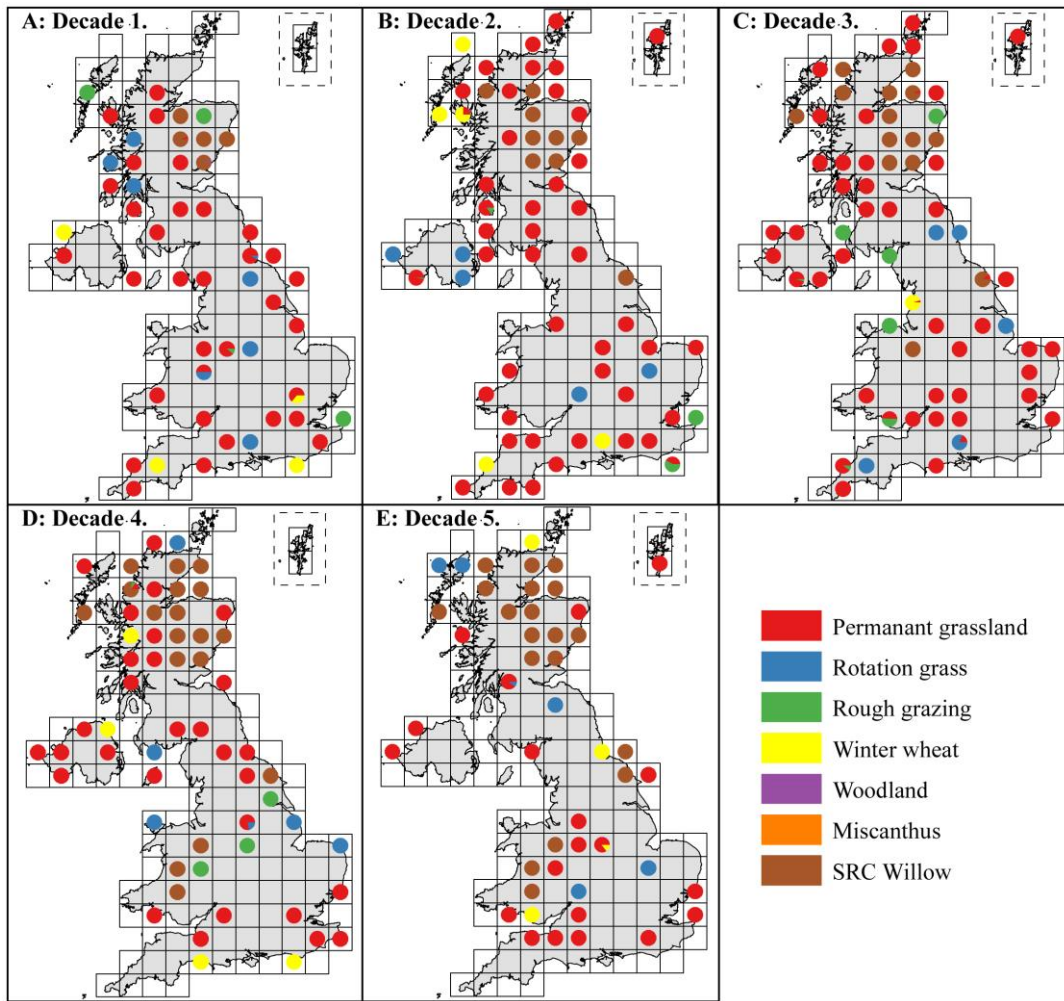


Figure 7 Land allocation configurations for bioenergy and non-energy systems over five decades (A 2010s; B 2020s; C 2030s; D 2040s; E 2050s). Notes: Pie charts indicate the share of biomass in each cell but not represent the allocated land areas proportional to the total areas of each cell.

3.2 Case study for UK transport biofuel sector – application of ES matrix

The extended ETI-BVCM model has been applied to a case study with the EU RED target of a 10% share of renewables in the UK transport sector by 2020 (equivalent to an annual minimum transport fuel demand of 164 PJ (Murray & Cluzel, 2014)), where 6% share was assumed to be met by local production in the UK. The latest statistical data were used to represent current renewable transport fuel demand (annual transport fuel supply of 45.6 PJ) (DECC, 2014b). In this case study, transport fuels including bioethanol, biodiesel, bio-butanol, biocrude oil and biomethanol derived from first generation crops (1G including winter wheat, sugarbeet) and second generation feedstock (2G including SRC willow, Miscanthus, short/long rotation forest (SRF/LRF)) via biochemical and thermochemical routes were modelled. The market price for traded C emissions and annual winter wheat demand in 2020s were assumed as £34.45/t CO₂ and 13,926,000 t/y (2013-2014 annual domestic consumption (HGCA, 2014)) respectively. A land transition impact matrix for ecosystem service performance indicator (*epi*) biodiversity is shown in Table 8, where assumed transition factors $ESIF_{r,al,biodiversity}$ for cultivation of biomass resources on four land types are given.

The effects on system-wide performance measures (cost and GHGs) for 2020 scenario by constraining biodiversity ES is shown in Fig 8 (configurations 1 to 18). Example 1 considers economic and environmental (GHG, biodiversity) performances whereas in example 2 the objective function is to minimise the total cost of bioenergy supply chains where the impacts of SC on ES are constrained. Along the curve from configuration 1 to configuration 18, the SC costs increase by approximately 19% with shifting the lower bound for SC impacts (maximum allowed damage on ES moves within a range of -10,000,000 and +10,000,000, negative and positive values indicate negative and beneficial effects on ES respectively). With the shift from an positive to negative aggregate score, a significant reduction in land use for 1G biomass and an increase in land utilization for cultivating 2G feedstock for bioenergy demand are projected (from configuration 1 to 18 in Figs 9A, 9B). Particularly from configuration 14 to 18, all the bioenergy production is met by 2G feedstock including Miscanthus, willow and forest (SRF/LRF). The total UK land allocation for bioenergy system in examples 1 and 2 varies within the range of 15- 25% and 12-20%, respectively whereas winter wheat food production accounts for 9.3-9.6% of total available UK lands across all configurations for 2020s. However these data should be interpreted with caution; it should be recognised that such high land demands for biofuel production represent merely the ‘technical potential’ and should not be interpreted as policy recommendations until the illustrative ES scores adopted in the scenarios are further validated.

Example 1, configuration 13 is given below to illustrate the insight the extended optimisation modelling framework could provide for strategic design of bioenergy supply chains in 2020s. The optimal configuration is presented in Fig 12A where 2G biofuel technologies are deployed and upgraded biocrude oil derived from SRC willow and Miscanthus represents the dominant transport fuel, accounting for 97 % total fuel production in 2020s (Fig 12A). As presented in Fig 11, the optimal locations (cells) of over 30 biorefinery facilities are projected to be close to the biomass cultivation sites (Fig 10B, 10C). The total dedicated areas for SRC willow and Miscanthus are

2,619,521 ha and 1,285,715 ha, respectively covering 11.8% and 5.8% of total UK available land areas (including all land types in 157 cells) (Figs 10 B and C). Local winter wheat production is the only supply to meet the UK domestic wheat food demand. Wheat cultivation sites are located in 64 cells across UK with total allocated areas of 2,085,049 ha, accounting for 9.4% of total available lands in the UK (Fig 10A). As presented in Fig 12B, nearly 90% of the decadal costs for transport biofuel SC are attributed to the biofuel production (operation and capital) stage. 2G biomass cultivation contributes approximately 13% whereas the share of transport is negligible.

This case study illustrates the extended model functionality, which accounts for ES impacts of land use transition in response to bioenergy penetration and allows exploration of the effects on system-wide performance measures (e.g. cost and GHG profiles) by constraining maximum acceptable level of impacts on ES (here, biodiversity). In the current study, only a semi-quantified matrix (based on evidence from the literature) was introduced as a synthetic measure to assess the change in ES as a consequence of land use transition associated with biomass production systems. To contribute to the development of bioenergy policy a spatially-explicit quantitative approach based on a range of provisioning (e.g. crop and livestock production), regulating (e.g. soil quality, water quality), and cultural (e.g. recreation) services is being developed for implementation into future versions of the model.

Table 8 Illustrative land use transition matrix score – impacts of new land use patterns on ES ^a

Land type ^b	$ESIF_{r,al, soil\ quality}$ (per ha)		$ESIF_{r,al, biodiversity}$ (per ha)				
	Miscanthus	SRC willow	Miscanthus	SRC willow	SRF	LRF	1G
1	+1	+1	+2	+3	+3	+3	0
2	+3	+2	+1	+1	+2	+2	-1
3	-1	-1	-1	-1	+1	+1	-2
4	-2	-2	-2	-2	0	0	-3

Notes:

a. The matrix score of ecosystem services indicators as implications of land use transition is being developed based on evidence from the literature, using the approach addressed by Holland et al. (2015) and Milner et al (2015). Here the matrix scores for biodiversity and soil quality are given for illustrative purpose

b Land type 1 = arable land and heterogeneous agricultural areas; land type 2=shrub and herbaceous vegetation association and open spaces with little or no vegetation; land type 3=permanent crops and pasture lands; land type 4 =forest and artificial non-agricultural vegetated areas

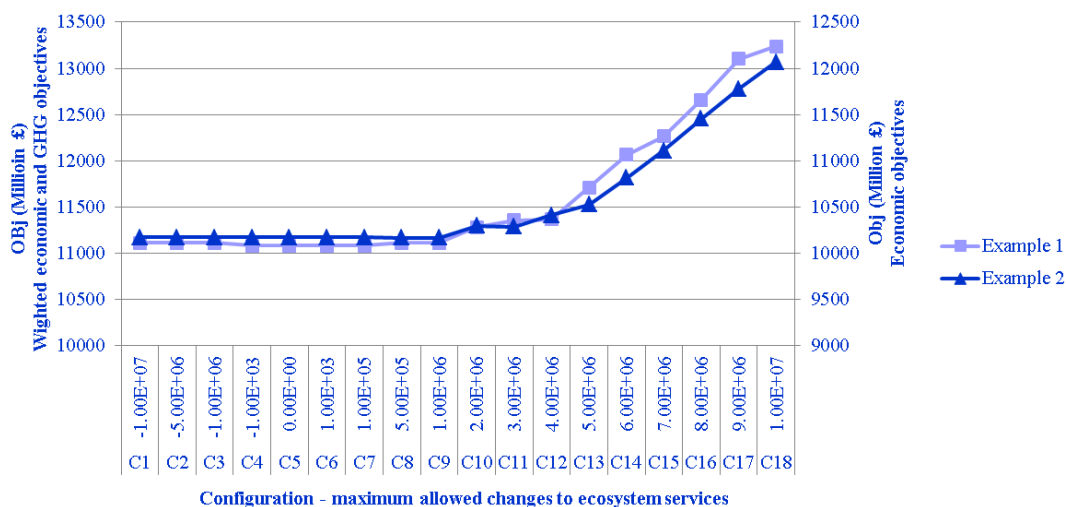


Figure 8 The effects of constraining biodiversity ES on system-wide performance (cost and GHGs)

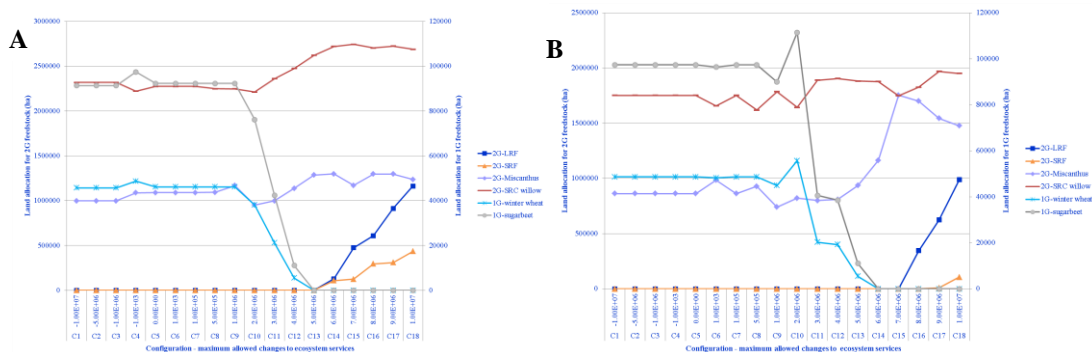


Figure 9 The effects of constraining biodiversity ES on land allocation for 1G and 2G feedstocks for 2020s scenario (A: example 1; B: example 2)

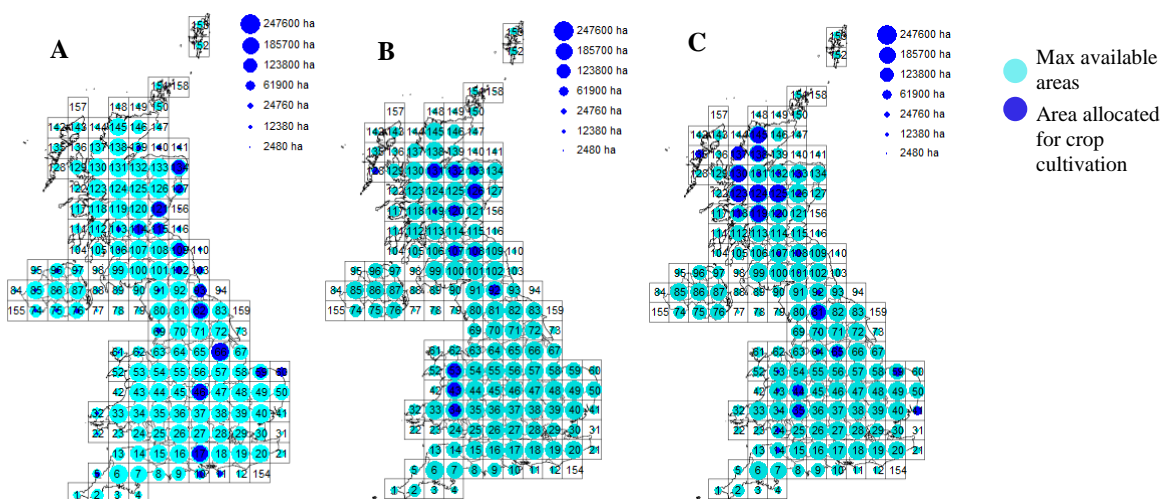


Figure 10 Optimal UK biomass supply network configuration for 2020s scenario (A winter wheat crop production for food system; B Miscanthus biomass production for bioenergy system; C SRC willow biomass production for bioenergy system)

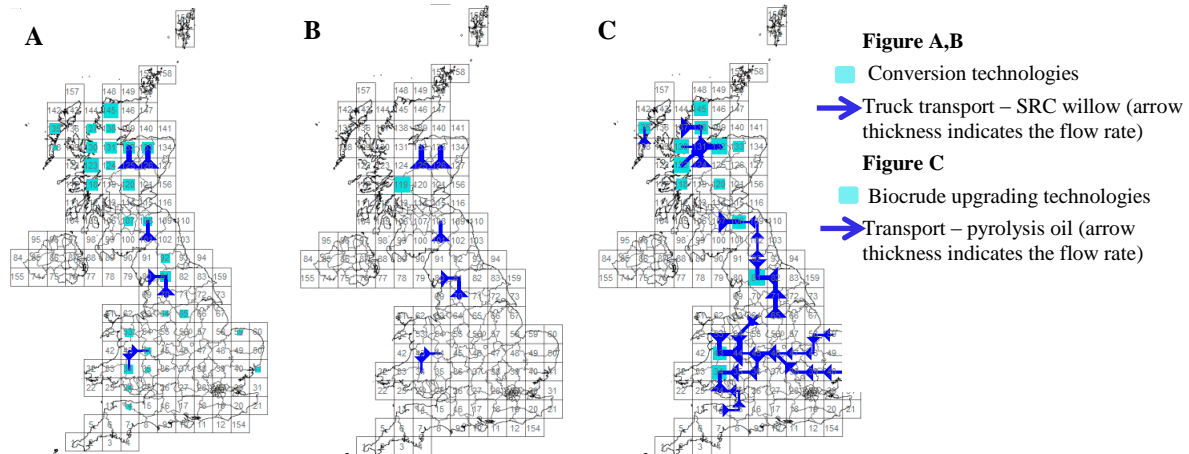


Figure 11 Optimal UK transport biofuel supply chain network configuration for 2020s scenario (A pyrolysis; B gasification & catalytic conversion of syngas to methanol; C pyrolysis oil upgrading)

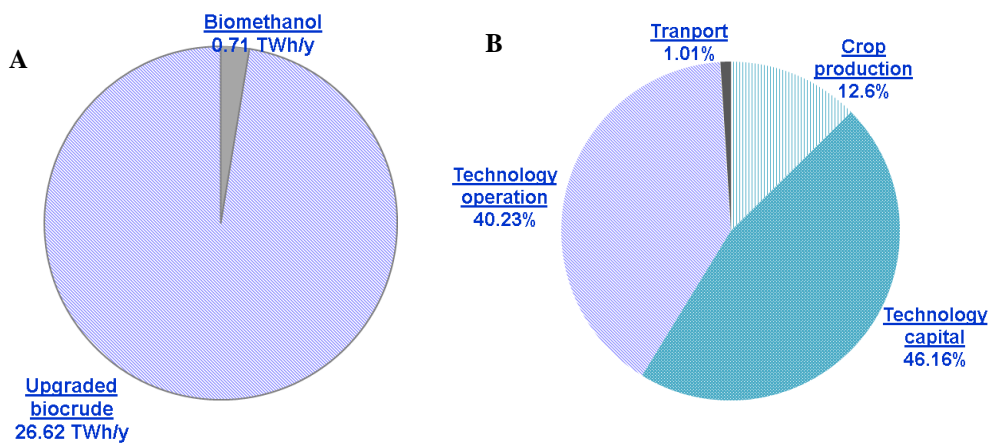


Figure 12 Annual energy production (A) and total cost of optimal transport biofuel supply chain (B) for 2020s

4. Conclusion

A multi-objective bioenergy supply chain optimisation model - ETI-BVCM - is extended to account for interrelated and conflicting issues in bioenergy supply chain design. Our research contributes to the field by proposing a modelling framework which considers land-competition across different land types and sectors (e.g. bioenergy vs. livestock sectors) and accounts for ecosystem service changes due to changes in land use. This enables users to evaluate land use transitions over multiple time periods using a spatially-explicit optimisation model for multiple systems and across the whole value chain. Within this methodologically focussed paper, we use a number of quantitative and semi-quantitative indicators of ecosystem services, focussing on provisioning (e.g. bioenergy, livestock) and biodiversity. These were intended to be illustrative of the influence that incorporating such measure has on the identification of promising value chains.

Future work will focus on development of models and these indicators. This will include process-based biogeochemistry and crop models (including a Lingra-based grassland model that differentiates management intensity), and spatially-explicit quantitative indicators for a range of provisioning, regulating and cultural ecosystem services. From this it will be possible to further extend the optimisation model to incorporate realistic understanding of the spatio-temporal dynamics of the system furthering our understanding of the implications of bioenergy supply chains. With such data, policy options can be explored based on multiple scenarios, with varying assumptions for UK non-energy and bioenergy demand, to identify decadal pathways and optimal land allocation for meeting UK multiple ecosystem services.

With the proposed modelling approaches, this research highlights the valuable insights the extended optimisation modelling framework can provide for strategic design of bioenergy supply chains. By explicitly accounting for competing demands for land, and the influence of transitions to alternate land uses, it is possible to explore routes which best support an economically viable, land-use efficient and environmentally sustainable UK energy system.

Acknowledgements

This study is based on the research supported by the Engineering and Physical Sciences Research Council UK through the SUPERGEN Bioenergy Hub. We would like to thank all participants in consortium project Bioenergy value chains: Whole systems analysis and optimisation (EP/K036734/1). We gratefully acknowledge the Energy Technologies Institute for commissioning and funding the development of the BVCM toolkit and providing a licence for using and modifying the ETI-BVCM tool, particularly thank to Dr Geraldine Newton-Cross for her support throughout the project. We also would like to acknowledge Dr Geraldine Newton-Cross and Hannah Evans for their very insightful comments on our work and this manuscript. Research on developing the underlying SRC willow feedstock supply model in the laboratory of GT was supported by grants from The Institute For Life Sciences and the Software Sustainability Institute, alongside NERC funded project Carbo-BioCrop (NE/H010742/1). We also wish to acknowledge the key developers of the ETI-BVCM formulation and model Dr Nouri Samsatli and Dr Sheila Samsatli from Imperial College London, Fabio Montemurro and Richard Taylor from E4Tech.

References

- AHDB. (2014). Dairy Statistics An Insider Guide 2014. In. Agriculture and Horticulture Development Board Diary.
- Armstrong, H. M., Poulson, L., Connolly, T., & Peace, A. (2003). A survey of cattle-grazed woodlands in Britain. In: UK Forest Research.
- Bateman, I. J., Harwood, A. R., Mace, G. M., Watson, R. T., Abson, D. J., Andrews, B., Binner, A., Crowe, A., Day, B. H., Dugdale, S., Fezzi, C., Foden, J., Hadley, D., Haines-Young, R., Hulme, M., Kontoleon, A., Lovett, A. A., Munday, P., Pascual, U., Paterson, J., Perino, G., Sen, A., Siriwardena, G., van Soest, D., & Termansen, M. (2013). Bringing Ecosystem

- Services into Economic Decision-Making: Land Use in the United Kingdom. *Science*, 341, 45-50.
- Carnbero, C., & Sowlati, T. (2014). Assessment and optimization of forest biomass supply chains from economic, social and environmental perspectives - A review of literature. *Renewable & Sustainable Energy Reviews*, 36, 62-73.
- Cobuloglu, H. I., & Buyuktahtakin, I. E. (2015). Food vs. biofuel: An optimization approach to the spatio-temporal analysis of land-use competition and environmental impacts. *Applied Energy*, 140, 418-434.
- Cucek, L., Martin, M., Grossmann, I. E., & Kravanja, Z. (2014). Multi-period synthesis of optimally integrated biomass and bioenergy supply network. *Computers & Chemical Engineering*, 66, 57-70.
- Čuček, L., Varbanov, P. S., Klemeš, J. J., & Kravanja, Z. (2012). Total footprints-based multi-criteria optimisation of regional biomass energy supply chains. *Energy*, 44, 135-145.
- Daily, G. C., & Matson, P. A. (2008). Ecosystem services: From theory to implementation. *Proceedings of the National Academy of Sciences of the United States of America*, 105, 9455-9456.
- De Meyer, A., Cattrysse, D., Rasinmaki, J., & Van Orshoven, J. (2014). Methods to optimise the design and management of biomass-for-bioenergy supply chains: A review. *Renewable & Sustainable Energy Reviews*, 31, 657-670.
- DECC. (2010). 2050 pathways analysis. In: Department of Energy & Climate Change.
- DECC. (2014a). 2012 UK Greenhouse Gas Emissions, Final Figures In: Department of Energy and Climate Change.
- DECC. (2014b). Digest of United Kingdom energy statistics (DUKES). In: Department of Energy & Climate Change.
- DECC, Defra, & DFT. (2012). UK Bioenergy Strategy. In D. f. T. Department of Energy and Climate Change, Department of Energy and Climate Change (Ed.). Department of Energy and Climate Change.
- DEFRA. (2014). Farming Statistics Final Land Use, Livestock Populations and Agricultural Workforce. In (JUNE 2014 ed.): Department for Environmental Food and Rural Affairs.
- DEFRA. (2015a). Agriculture in the United Kingdom data sets. In: Department for Environment, Food & Rural Affairs.
- Defra. (2015b). Animal Feed Production Statistics. In: Department for Environment, Food & Rural Affairs.
- EEA. (2014). EEA greenhouse gas - data viewer. In: The European Environment Agency.
- Ekins, P., Keppo, I., Skea, J., Strachan, N., Usher, W., & Anandarajah, G. (2013). The UK Energy System in 2050: Comparing Low-Carbon, Resilient Scenarios. In: UKERC.
- El-Halwagi, A. M., Rosas, C., Ponce-Ortega, J. M., Jiménez-Gutiérrez, A., Mannan, M. S., & El-Halwagi, M. M. (2013). Multiobjective optimization of biorefineries with economic and safety objectives. *AIChE Journal*, 59, 2427-2434.
- Elia, J. A., & Floudas, C. A. (2014). Energy Supply Chain Optimization of Hybrid Feedstock Processes: A Review. *Annual Review of Chemical and Biomolecular Engineering*, Vol 5, 5, 147-179.
- ETI. (2015a). Ecosystem Land-Use Modelling (ELUM) In: Energy Technologies Institute.
- ETI. (2015b). Overview of the ETI's Bioenergy Value Chain Model (BVCM) capabilities. In: Energy Technologies Institute.
- EuropeanCommission. (2009). CORINE Land Cover Map for 2006 In: European Environmental Agency.
- EuropeanParliament. (2015). Fuel quality directive and renewable energy directive. In E. Parliament (Ed.). European Biofuels Technology Platform.
- EuropeanUnion. (2009). Directive 2009/28/EC of the European Parliament and of the Council; In: The European Parliament and the Council of the European Union.
- Eurostat. (2013). Livestock unit coefficients. In: European statistics.
- Gasparatos, A., Stromberg, P., & Takeuchi, K. (2011). Biofuels, ecosystem services and human wellbeing: Putting biofuels in the ecosystem services narrative. *Agriculture, Ecosystems & Environment*, 142, 111-128.
- Gómez-Baggethun, E., & Ruiz-Pérez, M. (2011). Economic valuation and the commodification of ecosystem services. *Progress in Physical Geography*, 35, 613-628.

- Gong, J., & You, F. (2014). Global optimization for sustainable design and synthesis of algae processing network for CO₂ mitigation and biofuel production using life cycle optimization. *AIChE Journal*, 60, 3195-3210.
- Hastings, A., Clifton-Brown, J., Wattenbach, M., Mitchell, C. P., & Smith, P. (2009). The development of MISCANFOR, a new *Miscanthus* crop growth model: towards more robust yield predictions under different climatic and soil conditions. *Global Change Biology Bioenergy*, 1, 154-170.
- Hastings, A., Tallis, M. J., Casella, E., Matthews, R. W., Henshall, P. A., Milner, S., Smith, P., & Taylor, G. (2014). The technical potential of Great Britain to produce ligno-cellulosic biomass for bioenergy in current and future climates. *Global Change Biology Bioenergy*, 6, 108-122.
- Helmut, H., Karl-Heinz, E., Fridolin, K., Steve, R., Timothy, D. S., & Smith, W. K. (2013). Bioenergy: how much can we expect for 2050? *Environmental Research Letters*, 8, 031004.
- HGCA. (2014). UK cereals supply and demand. In: HGCA.
- Holland, R. A., Eigenbrod, F., Muggeridge, A., Brown, G., Clarke, D., & Taylor, G. (2015). A synthesis of the ecosystem services impact of second generation bioenergy crop production. *Renewable and Sustainable Energy Reviews*, 46, 30-40.
- IEA. (2013). Resources to Reserves 2013. In: International Energy Agency.
- Jerram, R., Jefferson, R., & Backshall, J. (2001). Chapter 7 Meadows And Enclosed Pasture In The upland management handbook. Natural England
- Krausmann, F., Erb, K. H., Gingrich, S., Haberl, H., Bondeau, A., Gaube, V., Lauk, C., Plutzer, C., & Searchinger, T. D. (2013). Global human appropriation of net primary production doubled in the 20th century. *Proceedings of the National Academy of Sciences of the United States of America*, 110, 10324-10329.
- Liu, Z. X., Qiu, T., & Chen, B. Z. (2014). A study of the LCA based biofuel supply chain multi-objective optimization model with multi-conversion paths in China. *Applied Energy*, 126, 221-234.
- Mace, G. M., Norris, K., & Fitter, A. H. (2012). Biodiversity and ecosystem services: a multilayered relationship. *Trends in Ecology & Evolution*, 27, 19-26.
- Marquardt, W., Harwardt, A., Hechinger, M., Kraemer, K., Viell, J., & Voll, A. (2010). The biorenewables opportunity - toward next generation process and product systems. *AIChE Journal*, 56, 2228-2235.
- Matthews, K., Miller, D., & Buchan, K. (2012). Stocking Rates of Land Capability for Agriculture Classes. In. The Scottish Government The James Hutton Institute.
- Mele, F. D., Kostin, A. M., Guillén-Gosálbez, G., & Jiménez, L. (2011). Multiobjective Model for More Sustainable Fuel Supply Chains. A Case Study of the Sugar Cane Industry in Argentina. *Industrial & Engineering Chemistry Research*, 50, 4939-4958.
- MillenniumEcosystemAssessment. (2005). *Ecosystems and Human Well-being: Synthesis*. In. Island Press, Washington, DC.
- Milner, S., Holland, R. A., Lovett, A., Sunnenberg, G., Hastings, A., Smith, P., Wang, S., & Taylor, G. (2015). Potential impacts on ecosystem services of land use transitions to second-generation bioenergy crops in GB. *Global Change Biology Bioenergy*, n/a-n/a.
- Murray, J., & Cluzel, C. (2014). Fuels Roadmap for 2020 and beyond - implications for future strategy. In (Vol. 2014): Low Carbon Vehicle Partnership.
- Newton-Cross, G. (2015). Bioenergy Insights into the future UK Bioenergy Sector, gained using the ETI's Bioenergy Value Chain Model (BVCM). In. Energy Technologies Institute.
- Newton-Cross, G., & Evans, H. (2016). Delivering greenhouse gas emission savings through UK bioenergy value chains. In. Loughborough, UK: Energy Technologies Institute.
- Richter, G. M., Qi, A., Semenov, M. A., & Jaggard, K. W. (2006). Modelling the variability of UK sugar beet yields under climate change and husbandry adaptations. *Soil Use and Management*, 22, 39-47.
- Richter, G. M., Riche, A. B., Dailey, A. G., Gezan, S. A., & Powlson, D. S. (2008). Is UK biofuel supply from *Miscanthus* water-limited? *Soil Use and Management*, 24, 235-245.
- Richter, G. M., & Semenov, M. A. (2005). Modelling impacts of climate change on wheat yields in England and Wales: assessing drought risks. *Agricultural Systems*, 84, 77-97.

- Rodriguez, J. P., Beard, T. D., Bennett, E. M., Cumming, G. S., Cork, S. J., Agard, J., Dobson, A. P., & Peterson, G. D. (2006). Trade-offs across space, time, and ecosystem services. *Ecology and Society*, 11, 14.
- Samsatli, S., Samsatli, N. J., & Shah, N. (2015). BVCM: A comprehensive and flexible toolkit for whole system biomass value chain analysis and optimisation – Mathematical formulation. *Applied Energy*, 147, 131-160.
- Schapendonk, A. H. C. M., Stol, W., van Kraalingen, D. W. G., & Bouman, B. A. M. (1998). LINGRA, a sink/source model to simulate grassland productivity in Europe. *European Journal of Agronomy*, 9, 87-100.
- Shah, N. (2004). Process industry supply chains: Advances and challenges. In A. P. BarbosaPovoa & H. Matos (Eds.), *European Symposium on Computer-Aided Process Engineering - 14* (Vol. 18, pp. 123-138). Amsterdam: Elsevier Science Bv.
- Tallis, M. J., Casella, E., Henshall, P. A., Aylott, M. J., Randle, T. J., Morison, J. I. L., & Taylor, G. (2013). Development and evaluation of ForestGrowth-SRC a process-based model for short rotation coppice yield and spatial supply reveals poplar uses water more efficiently than willow. *Global Change Biology Bioenergy*, 5, 53-66.
- Thornton, P., & Gerber, P. (2010). Climate change and the growth of the livestock sector in developing countries. *Mitigation and Adaptation Strategies for Global Change*, 15, 169-184.
- UKAgriculture. (2014). Grassland in the UK - an introduction. In.
- van der Horst, D., & Vermeulen, S. (2011). Spatial scale and social impacts of biofuel production. *Biomass and Bioenergy*, 35, 2435-2443.
- Yue, D., You, F., & Snyder, S. W. (2014). Biomass-to-bioenergy and biofuel supply chain optimization: Overview, key issues and challenges. *Computers & Chemical Engineering*, 66, 36-56.
- Yue, D. J., You, F. Q., & Snyder, S. W. (2014). Biomass-to-bioenergy and biofuel supply chain optimization: Overview, key issues and challenges. *Computers & Chemical Engineering*, 66, 36-56.
- Zamboni, A., Bezzo, F., & Shah, N. (2009). Spatially Explicit Static Model for the Strategic Design of Future Bioethanol Production Systems. 2. Multi-Objective Environmental Optimization. *Energy & Fuels*, 23, 5134-5143.
- Zhuang, Q. L., Qin, Z. C., & Chen, M. (2013). Biofuel, land and water: maize, switchgrass or Miscanthus? *Environmental Research Letters*, 8, 6.