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A novel energy systems model to explore the role of land use and reforestation in achieving carbon mitigation targets: A Brazil case study

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Abstract

Due to its low global share of direct energy consumption and greenhouse gas emissions (1-2%), the implications of technological transitions in the agricultural and forestry sector on the energy system have been overlooked. This paper introduces the Agriculture and Land Use Sector module part of the ModUlar energy System Environment (MUSE), a novel energy system simulation model. The study presents a generalisable method that enables energy modellers to characterise agricultural technologies within an energy system modelling framework. Different mechanisation processes were characterised to simulate intensification/extensification transitions in the sector and its wider implications in the energy and land use system aiming at providing reliable non-energy outputs similarly to those found in dedicated land use models. Additionally, a forest growth model has been integrated to explore the role of reforestation alongside decarbonisation measures in the energy system in achieving carbon mitigation pathways. To illustrate the model's capabilities, Brazil is used as case study. Outputs suggest that by 2030 under a 2°C mitigation scenario, most of Brazil agricultural production would move from 'transitional' to 'modern' practices, improving productivity and reducing deforestation rates, at the expense of higher energy and fertiliser demand. By mid-century Brazil has the potential to liberate around 24.4 Mha of agricultural land, where large-scale reforestation could have the capacity to sequester around 5.6 GtCO₂, alleviating mitigation efforts in the energy system, especially reducing carbon capture and storage technology investments in the industry and power sector.

Keywords

Energy systems model; reforestation; agriculture; land-use; mechanisation; Brazil

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Nomenclature

Sets

$f \in \mathbf{F}$	set of fuel types
$r \in \mathbb{R}$	set of regions
$s \in S$	set of service type
<i>t</i> ∈ T	set of technology types

Parameters

а	regression coefficient a [-]
b	regression coefficient b [-]
a _i	average distance of data <i>i</i> to all the data observations within the cluster of which data <i>i</i> [-
b _i	lowest average distance of data i to all the data observations within the cluster of which
	data <i>i</i> is not a member [-]
$DM_{r,s}$	service demand in region r of service s [PJ]
$FD_{r,f}$	fuel demand in region r of fuel type $f[PJ]$
FE_{f}	emission factor for fuel f [tCO ₂ PJ ⁻¹]
$R_{E,r}$	actual emissions in region r [tCO ₂]
TS_s	technologies available for service type s [-]
X _i	data belonging to cluster C_k [-]
$\theta_{s,t}$	demand share of service s covered by technology type t [%]
$\gamma_{t,s}$	efficiency of technology t for service s [%]
μ_k	mean value of data assigned to cluster C_k [-]

Variables

cluster k [-]
fuel consumption in region r , of fuel type f by technology type t [PJ]
installed capacity in region r of technology type t [PJ year ⁻¹]
modelled emissions in region r [tCO ₂]
silhouette width of a data point <i>i</i> [-]
slack (emissions) for region r and fuel type $f[tCO_2]$
age of new forest [years]
difference in emissions in region r [tCO ₂]

Subscripts and Superscripts

agr	agriculture
сар	capita
mod	modern
mod_ren	modern renewable
trad	traditional
trans	transitional

Abbreviations

trad	traditional
trans	transitional
Abbreviat	ions
2DS	two-degree scenario
AB	above ground biomass
Ag&LU	agriculture and land use sector
ASM	average silhouette method
BAU	business as usual
BB	below ground biomass
BECCS	bioenergy with carbon capture and storage
С	carbon
CAPEX	capital costs
CCS	carbon capture and storage
DOM	dead organic matter
Ε	exponential
ESM	energy systems model
GDP	gross domestic product
ISM	integrated assessment model
L	linear
LL	log-log
MCA	market clearing algorithm
Mha	mega hectares
MUSE	ModUlar energy System Environment
NPV	net present value
OP	optimisation problem
OPEX	operational costs
PJ	petajoules
REF	reforestation
SL	semi-log
SOC	soil organic carbon

1. Introduction

It is expected that future climate change will severely disturb society and terrestrial ecosystems (Walther et al., 2002). Kang et al. (2009) investigated the negative effects of climate change on water availability and agricultural production and its wider implications on food and the environment. During the COP-21 conference, 195 country members have agreed to set up a plan to limit global warming to well below 2°C compared to pre-industrial levels (UN, 2015). Current estimations suggest that the remaining carbon budget for an increase of 2°C stands between 590–1,240 GtCO₂ (Rogelj et al., 2016), and with current annual emission rates (~40 GtCO₂ year⁻¹) there is a high probability that the budget will be depleted by mid-century. It is evident that strategies to reduce global greenhouse gas (GHG) emissions must be put in place rapidly.

In 2015, the agriculture, forestry and land use sector (AFOLU) demanded 8,142 PJ year⁻¹ of energy, with diesel (4,395 PJ year⁻¹) and electricity (2,120 PJ year⁻¹) responsible for almost three quarters of the global sector energy share (FAO, 2017; IEA, 2017). This represented 0.88 GtCO₂ year⁻¹ or 1.5-2.0% of global annual GHG emissions. However, if the whole food and agriculture supply chain is considered (including agrochemicals production and application, food transportation and processing, and land use dynamics), the sector is responsible for up to 30% of global emissions (Vermeulen et al., 2012). Therefore, introduction of modern technologies and practices in the sector is central to limiting global climate change (Woods et al., 2010).

Increasing food demands, land competition, unexpected climates, unsustainable bioenergy policies, and income inequality could have major implications for the sector's dynamics (Cirera and Masset, 2010). Rathmann et al. (2010) found that the emergence of large-scale dedicated energy crops has altered land use dynamics, switching from food-based towards biofuels-based production, subsequently impacting food prices in the short term. Nowadays, emerging economies are experiencing dynamic transitions within their energy systems and land use mainly due to high economic growth rates. Together with developed economies they are causing major disruptions over terrestrial emissions with high probability of being the main cause of global warming (IPCC, 2014b). Projections in agricultural commodities suggest that either intensification or land use expansion will be required to meet future demands (Baruah and Bora, 2008). Current average yield growth rates (<1.6% year⁻¹) might be insufficient to meet rising demands, where more land will be necessary to overcome production shortages, potentially causing environmental degradation (Ray et al., 2013).

1.1 Land management strategies for carbon mitigation

Several research regarding carbon neutral or carbon negative emission strategies in the AFOLU sector can be found in the literature (Minx et al., 2017). For example, large-scale bioenergy production and

utilisation has been identified as a promising measure to reduce fossil-fuel dependency and achieve carbon targets. Bioenergy crops, either for biofuels or power generation, have the capability of reducing emissions along the energy supply chain. In the literature, estimates of global bioenergy supply potential vary considerably. Past estimates of a global bioenergy supply potential of over 1000 EJ year⁻¹ (Smeets et al., 2007) have been considered too optimistic (Haberl et al., 2010). Recently more conservative estimates were given (lower than 400 EJ year⁻¹) (Deng et al., 2015). If only marginal and degraded lands were considered, the technical potential would be even lower than 200 EJ year⁻¹ (Nijsen et al., 2012). However, the extent of the benefit of bioenergy to the overall energy mix, is surrounded by many uncertainties related to its carbon life cycle. Added to this, there is not a universal method for the quantification of indirect land use change (iLUC) and the impacts of agrochemicals utilisation (Plevin et al., 2010).

The role of biomass and the associated emissions, become even more crucial, when climate change mitigation plans largely rely on combining bioenergy with carbon capture and storage (BECCS) (Azar et al., 2010). BECCS has been found to have the highest abatement potential in the power and industrial sectors. However, one of the main limitations for large-scale implementation is its current capital and operational costs. Although BECCS can be considered as a carbon negative strategy, the ecosystems and energy systems dynamics suggest its abatement potential might not be as large as anticipated (Muratori et al., 2016). Apart from evidence needed from operational CCS technologies as these have yet to be deployed at large-scale, the extensive use of bioenergy might lead to significant iLUC emissions and price pressure for other agricultural commodities due to land competition (Muratori et al., 2016).

There are other land management techniques that could play a role in carbon mitigation strategies as they directly affect the carbon cycle. Studies have shown that the carbon abatement potential of restoring degraded lands to their original state can have larger benefits than converting these marginal lands to agricultural production (Evans et al., 2015). Nevertheless, either the potential from reforestation/afforestation or energy crops to reduce GHG could be compromised by food security and other environmental goals. Smith et al. (2013) considered that consumption-based or demand side measures such as changing food diets, have a greater reduction land potential than supply side measures such as intervening in land management. In the last decades, optimal land use management, new technologies and genetically crop upgrading have allowed the sector to double its production without requiring extreme land expansion, allowing for degraded lands to be reforested (FAO, 2017; IPCC, 2014a). Measures such as biochar, soil carbon sequestration (SCS) and reforestation/afforestation recently have been broadly discussed in policy making due to its affordability and potential large-scale implementation (Minx et al., 2017). However, the

implementation of the aforementioned measures comes with high uncertainties in price, costs and risks, as few generalisable projects have reached maturity levels.

1.2 Agriculture and land use in energy system models

For energy planning, energy system models (ESMs) are typically used to provide insights into technological implementation, often alongside socio-economic and environmental implications (Riahi et al., 2017). In recent years, most of ESM research has been focused in investigating decarbonisation pathways in different sectors. For instance, for the industry, Bataille et al. (2018) analysed the sector's technical potential to reduce GHG emissions from energy intensive processes aiming at reaching Paris agreement targets. Similarly, Griffin et al. (2018) analysed the potential to reduce energy demand and GHG emissions from the UK pulp and paper industry by investigating different energy sources and technologies. For buildings, García Kerdan et al. (2017) used an exergy-based stock model to calculate the potential of different low carbon technologies to reach sectoral emission targets in the UK while Sachs et al. (2019) implemented a novel agent-based model within an bottom-up ESM aiming at characterising different type of investors and understand their role in regional and national large-scale decarbonisation efforts. In the transport sector, Dhar et al. (2018) used the MARKAL ESM to study transition decarbonisation pathways in the Indian passenger and freight subsectors while Siskos et al. (2018) used PRIMES ESM to understand the implications of delaying decarbonisation in the European Union (EU) transport sector. In addition to the demand sectors, power sector decarbonisation has been widely investigated. Recently, Kefford et al. (2018) studied the challenge of early decommissioning of fossil-based power plants to reach carbon reduction targets. Outputs show that this would create more than US\$ 500 billion worth of stranded assets only in the USA, China, EU and India.

On the other hand, due to the low global share of direct energy use in agriculture (IEA, 2017), ESMs have overlooked the implications of decarbonisation policies in the agricultural and forestry sector and its wider implications in the energy system. Similar to other sectors, agricultural production can be modelled as a collection of discrete physical processes, as presented in Walker (1984). Jones et al. (2017) provided an extended summary of agricultural systems models, demonstrating their multidisciplinarity and the importance in decision-making. Some research groups have provided links between energy and land use models (Wise et al., 2014); however, the AFOLU sector still lacks a comprehensive technological representation in ESMs. One of the most common approaches to assess the implications of the technological changes in agriculture onto the energy systems are based on using a soft-link between energy and land use models.

IMAGE (IMAGE-contributors, 2019), considered as an ecological-environmental modelling framework, has been soft-linked to TIMER (Bert J.M. de Vries et al., 2001) to assess energy supply and demand. The energy model provides a limited representation of the agriculture sector (represented

as "Other" sectors), where it uses structural elasticity to determine the sectoral energy demand. Moreover, the details of the agricultural sector is modelled using a third model, the agro-economic model MAGNET (G.B. Woltjer et al., 2014), which is a computable general equilibrium (CGE) model connected via a soft-link to IMAGE. Although it has the strength of modelling prices of production factors, resource availability and technological progress, energy demand is not accounted for.

MAgPIE (Dietrich J et al., 2018) is a popular global agricultural and land use allocation model, which is connected to the grid-based dynamic vegetation model LPJmL (Schaphoff et al., 2018). The model is able to forecast the demand of agricultural commodities based on regional economic conditions, modelling technological development, production, spatially explicit yields and land use. To account for energy demand and supply, a soft-link has been done with REMIND (Luderer et al., 2015), a global energy system multi-regional optimisation model. The model uses 'constant elasticity of substitution approach' (CES) to model future competition of technologies. Although the tool has the capacity to model several technologies in the energy sector, there is a lack of agricultural technologies representation.

GLOBIOM is a recursive-dynamic partial-equilibrium agriculture and land use model (Krey et al., 2016) that is able to represent land use competition including a spatially explicitly bottom-up representation of the agricultural, forestry and bioenergy sector. The model has been soft linked to MESSAGE (Krey et al., 2016), a linear programming (LP) partial equilibrium energy model that aims to assess the role of different types of bioenergy sources in the wider energy system. One of the limitations of MESSAGE is that only distinguishes between three types of energy end-uses: transport, buildings and industry, leaving the agricultural sector with a limited representation in the energy system.

GCAM (Calvin et al., 2019) has been able to integrate the energy sector along natural ecosystems and terrestrial carbon cycles models, dividing the world into 151 agro-ecological regions. The model uses sharing logit models to account for land use decisions with the possibility of using multiple management types for different crops, allowing the model to simulated price-based intensification in the sector. GCAM has been able to include multiple agricultural management practices, which enables to calculate intensification rates endogenously. However, the energy module lacks explicit agricultural technologies characterisation, limiting its capability to relate energy demand and land use implications from specific technological uptake.

On one hand, soft-linking between energy and land use models have the capacity to address deeper sustainability dimensions, different systemic effects and precise biophysical interactions. On the other hand, soft-links could provoke a fragile internal model coherence and added complexity, where land

demand is usually modelled using economic approaches, with limited accounting for the impact of technological uptake. Additionally, these complex models might have high computational requirements. Novel approaches are necessary to overcome this long-standing limitation, aiming to create robust models without the need to soft-link independent models.

In general, there are two main limitations in the development of agricultural models in ESMs: 1) a scarcity of energy and technological data, and 2) inadequate knowledge systems that effectively communicate model results to decision makers (Jones et al., 2017). As novel technologies in agriculture and changes in carbon taxes can easily impact land use allocation and energy consumption (Wise et al., 2009), novel models are required to gain insight into future energy, economic and environmental interactions.

To the best of authors' knowledge there is still a lack of an integrated modelling approach which can describe the interactions between the deployment of mechanisation in agriculture and the rest of the energy and land use system. The novelty of this study is to present a newly developed agricultural energy system model and to provide a generalisable methodological framework capable of characterising agricultural processes that eventually would be useful for energy and land use assessment in ESMs. Thus, the objective of the paper is twofold. Firstly, to describe the "Agriculture and Land Use" (Ag&LU) framework embedded within the MUSE energy system model, by proposing an alternative method to model agricultural technology productivity and future uptake based on mechanisation levels. The model intends to reduce complexity while still capturing major indicators such as intensification and land use. Secondly, using Brazil as a case study, the model is tested to determine the dynamics and interconnections between the land use and the energy system, exploring the role of agriculture and reforestation alongside the country's energy system in reaching carbon mitigation targets.

This paper is organized as follows. First, the methodology and the development of the MUSE-Ag&LU global model is presented. Next, the case study is presented alongside the proposed modelling scenarios. Following, the paper will show the obtained results, followed by discussions considering the combined role of agriculture, land use and the energy system in achieving mitigation pathways. Finally, conclusions and suggestions for future work are presented.

2. Material and methods

2.1 The MUSE model and the Ag&LU model structure

The ModUlar energy systems Simulation Environment (MUSE) is a new bottom-up integrated assessment model, implemented in Python, aiming to explore plausible long-term decarbonisation scenarios of energy systems (Giarola et al., 2019). MUSE is a partial-equilibrium simulation model with microeconomic foundations. The equilibrium is reached when supply and demand of commodities is attained in the market clearing algorithm (MCA). The global model considers demand, conversion and supply sectors, with a disaggregation of 28 regions. An overview of MUSE simulation environment can be found in Appendix A, while a detailed representation of the regions can be found in supplementary data S.1.

Specifically, the MUSE-Ag&LU model, is a technology-rich bottom-up agricultural model that simulates energy demand and land use requirements in the medium and long-term (up to 2030/2050 or 2100). It aims to produce a time series of fuel demand, agrochemicals demand, land use, and emissions in order to meet four general agricultural services: a) crops, b) meat-based products, c) forestry products and d) bioenergy. Similar to other demand modules in MUSE, the Ag&LU model dynamically exchanges a set of variables with the MCA by sending information regarding fuel demand and emissions per region, time period and timeslice. Figure 1 illustrates a generic iteration in a generic time-period and time-slice.



Figure 1. Ag&LU model integration into MUSE and data flow with the MCA

2.2 Simulation workflow

The Ag&LU module dynamically exchanges a set of variables with the MCA of MUSE to determine the fuel demand in every region per time period and timeslice. The simulation is based in a two-step approach.

2.2.1 Service demand forecast

In a first step, the MUSE-Ag&LU model projects demand by energy content of each agricultural services. As the aim of the study is to present a methodological framework that could be easily generalisable to any agricultural commodity categorisation, for the purpose of this study and to keep the model computationally tractable and to reduce computational burden, commodities have been aggregated by the following four general agricultural services

- **Crops** have been modelled by aggregating the six major agricultural crops by global production: rice, wheat, maize, soybean, sugarcane and potatoes.
- Meat-based products: beef, pig, poultry and sheep.

- Forestry products: round wood and wood fuel.
- **Bioenergy**: miscanthus, switchgrass, agricultural and meat-based residues, and forestry residues.

Service demands are derived from regression analysis defined from exogenously given macrodrivers (gross domestic product (GDP) and population). As agricultural data usually is collected in units of mass or volume (kg, tonnes, m³), these have been converted into energy units by applying the energy content value of each specific agricultural product. Food, forestry products and bioenergy demands are based on regional diets and past consumption trends (1970-2015). Data on GDP and population has been taken from the World_Bank (2017). A set of regression models have been tested, as proposed in the literature by Cirera and Masset (2010) and Tilman et al. (2011). In this study, similarly to van Ruijven et al. (2016) approach, optimal fit for the demand of agricultural products has been identified. The models tested are reported in the eqs. 1-4.

$$Linear(L): C = a + b * GDP_{pc}$$
(1)

$$Exponential(E): C = a * e^{b*GDP_{pc}}$$
(2)

$$Semi - log (SL): C = a + b * ln(GDP_{pc})$$
(3)

$$Log - log (LL) : lnC = a + b * ln(GDP_{pc})$$
(4)

In which *a* and *b* are constants estimated in the regression and would serve as an input to MUSE. In agreement with similar studies such as Cirera and Masset (2010) which described the relationship between food consumption and income and Bodirsky et al. (2015) which analysed the functional relationships between income and food demand, the log-log function or Engel's curve (eq. 4) has been identified as the most appropriate to estimate the demand for agricultural services. The outputs demonstrates that as per capita income increases, population demand for agricultural products would increase; however, the increase is under-proportional with income. In the case of food products, high income economies usually show to have reach a per capita saturation level and, in some cases, even a decrease in demand for meat-based products, subsequently switching to vegetable-based diets. The data and obtained regression coefficients by region and agricultural commodity can be found in the supplementary data (S.1).

For the case of bioenergy, the model endogenously calculates the necessary production based on demands from the rest of the sectors (industry, buildings, power, refinery, etc). In this way, dynamic supply curves are built for every iteration and time period until convergence is reached (Figure 2).



Figure 2. Endogenous bioenergy demand calculation in MUSE-Ag&LU

2.2.2 Modelling technology investment

As a second step, to model investment decisions and operating strategies, a merit order approach based on Net Present Value (NPV) is used to define technology market share and fuel mix. To represent the future state of the sector, the model selects technologies based on capital and operational costs, technology efficiency and environmental impact. Finally, the model ranks the technologies and decides which ones to operate in order to meet the demand of service. Depending on the technologies which are operating, the model calculates: fuel and agro-chemicals demand, the running operating costs (OPEX), environmental performance (GHG emissions), energy and residual crop supply and land use, per region, time period and timeslice. At the next iteration, the model will receive updated fuel and carbon prices from the MCA and will repeat the simulation.

As illustrated in Figure 3, the simulation is broken up into several distinct mutually exclusive interactions. In this way, the model determines the necessary technological uptake, where appropriate actions such as dispatch, technological investment and land management is applied for each iteration.



Figure 3. Flow chart of MUSE-Ag&LU simulation algorithm

2.3 Definition of agricultural technologies

The main challenge in developing the model has been the characterisation of comprehensive processes that relate energy demand, agricultural production and land use. In this study, the proposed approach is based in associating specific technological processes based on mechanisation or intensification levels (Figure 4).



Figure 4. Basic representation of different mechanisation levels combining agricultural technology, fuel share, production and land use demand.

According to the European Commission (EC, 2019), the input intensity of an agricultural process can be defined as the level of inputs used per unit of factor of production. Overall, the intensity or mechanisation level of an agricultural process is the result of the combination of different inputs such as energy, fertiliser, technology efficiency and land use practices. Intensification or the uptake of higher mechanisation levels represents technological change through the adoption of non-human/nonanimal sources of power to undertake agricultural operations (Diao et al., 2014). For example, the

European Environment Agency (EEA, 2005) uses different mechanisation indicators (IRENA No. 15) to study agricultural intensification/extensification related to average expenditure, stocking rates and yields. The indicator has been applied to describe an increase in farm input intensity in different regions. The demand for farm mechanisation emerges at the point when it becomes cost-effective for farmers to use it over other available options. To characterise agricultural technologies in MUSE, a pre-processing six step approach combining qualitative and quantitative methods is proposed. Figure 5 presents the framework, detailed in sections 2.3.1 and 2.3.2.



Figure 5. Framework to characterise agricultural processes based on qualitative and quantitative approaches

2.3.1 Qualitative characterisation (Steps 1-3)

Without considering any economic or biophysical implication on yields, the qualitative method proposed by Opio et al. (2013) has been extended by integrating inferential statistics. As Step 1, data on total production by country has been collected for the main agricultural commodities (crops, meat, and forestry products) and converted into energy units. Following, land use demands have been obtained for each agricultural commodity per region (FAO, 2017). After aggregating total production and land use demand per type of commodity, it is possible to obtain yields in energy units per area (PJ Mha⁻¹). Distributions for each agricultural product on a global scale is shown in Figure 6 (Step 2).



Figure 6. Distribution (bars) and the fitted probability distribution (lines) of global yields for different agricultural commodities. Source: FAO (2017).

These outputs have been used to get a first qualitative definition of mechanisation levels depending on empirically observed yields (Step 3). In this case, as detailed in Table 1, three different levels of mechanisation have been defined using the quartiles calculated from the distributions. This technological classification is similar to mechanisation levels defined by the Food and Agriculture Organization (FAO, 2000) (*traditional, transitional, and modern*) and by IRENA (EEA, 2005) (*low level, intermediate level, and high level*).

Mechanisation level		Yields	Qualitative description		
		(Quartile)	Quantative description		
an Landanal		Below the	Represents the original method of farming that developed through		
		1 st quartile	the interaction of social and environmental systems with a minimum		
			amount of mechanised equipment. Minimum energy inputs are		
			characterised by the use of biomass, kerosene, coal and low		
			integration of electricity.		
			e.g. Traditional cropping countries: Nicaragua, Cameroon, Haiti		
			(FAO, 2017).		
2.	Transitional or	Between	Represents the introduction of mechanisation in more parts of the		
	Intermediate level	the 1 st and	agricultural production chain. Tractors, tilling machines, mechanical		
	level	3 rd	heating/drying and irrigation using mainly electricity and other		
		quartiles	traditional fossil fuels such as diesel and gas are considered in this		
			process. The use of fertilizers and agrochemicals is common.		
			e.g. Transitional cropping countries: India, Russia, Brazil (FAO,		
			2017).		
an Illah lanal		Above the	Describes a wide type of production practices employed by some		
	or High level	3 rd	developed countries. Apart from a fully mechanised supply chain, it		
		quartile	makes use of technologically advanced equipment with higher		
			energy demands for machinery, farm overhead, water irrigation, and		
			fertilizers.		
			e.g. Modern cropping countries: United States, Netherlands, Japan		
			(FAO, 2017).		
3.1	. Modern-	Above the	Same as 'Modern' but assumes that the process' energy inputs are		
	Renewable ^{\$}	3 rd	based on 'renewable' sources such as biodiesel, bioelectricity and		
		quartile	other biomass sources combined with more sustainable agricultural		
			practices (micro-fertilisation)		

Table 1. Qualitative description of mechanisation levels in MUSE-Ag&LU model

^S An additional mechanisation level has been created representing a full renewable-based modern technology (with similar technology efficiency and yields as 'Modern').

2.3.2 Quantitative characterisation (Steps 4-6)

To quantitatively represent the proposed mechanisation levels, inputs on energy, land demand, and agrochemicals need to be assigned. However, as FAO (2017) and IEA (2017) balances do not provide comprehensive land or energy data separated by specific agricultural products or processes, a bottom-up approach cannot be followed. Therefore, a hybrid approach using big data analysis has been selected. As Li et al. (2019) suggests, the application of big data techniques has the potential to reduce blind spots in ESMs, such as the presented problem of characterising agriculture technologies.

First, to provide fuel share and land demand for each mechanisation process per agricultural product, a cluster analysis has been implemented by locating countries with similar energy input/output ratios and yields per agricultural product (Step 4). Similar to Conforti and Giampietro (1997), the non-hierarchical method approach, based on the separation of clusters at different levels of distance between observations, has been used to get a first subjective assessment for crops, meat and forestry products. Although several economic, social, environmental and biophysical indices can impact agricultural productivity, it has been decided to perform the cluster analysis based on yields and GDP agricultural share (% GDP_{agr}), as population income (GDP_{cap}) might not provide an adequate insight into the agricultural mechanisation development in a country.

To reduce the total number of heterogeneous agricultural levels to be introduced into the model, *kmeans clustering* has been applied to categorise factors levels into groups with similar adoption preferences. To define the clusters, a minimisation problem based on the Hartigan-Wong algorithm (Hartigan and Wong, 1979) aiming to reduce the within-cluster variation is performed:

$$W(C_k) = \sum_{x_i \in C_k} (X_i - \mu_k)^2$$
(5)

where C_k is cluster k, X_i is a data belonging to cluster C_k , and μ_k is the mean value of data assigned to cluster C_k . In this study, the desired number of groups has been set to three, as per the number of mechanisation levels defined in section 2.3.1. Later, the *Average Silhouette Method* (ASM) (Rousseeuw, 1987) is used to locate and justify the optimal number of clusters. The silhouette width of a data point *i* can be defined as follows:

$$S_i = \frac{b_i - a_i}{\max(b_i, a_i)} \tag{6}$$

where a_i is the average distance of data *i* to all the data observations within the cluster of which data *i* is a member, b_i is the lowest average distance of data *i* to all the data observations within the cluster of which data *i* is **not** a member. High average values (close to 1.0) indicate that values are well clustered. Graphically, the optimal number of clusters *k* is located where the function S_i is maximised. Figure 7 presents the outputs obtained for crops, meat and forestry products at a global scale. Global data used for the analysis as well as countries' abbreviations can be found in supplementary data S.2.



Figure 7. Cluster analysis (left) and silhouette scores (right) for agricultural commodities: crops, meat and forestry products

Figure 7 illustrates the different clusters and the distance between them per agricultural product. The cluster results for crops demonstrate three very distinct groups:

- **Cluster#1** (green), is represented by low- and medium-income economies (with low-medium GDP share from agriculture) with medium yields that could be considered as mainly having transitional agricultural processes for crop production.
- **Cluster #2** (red), is represented by low income economies with high GDP share from agriculture that have the lowest yields and could be considered as mainly having a traditional mechanised sector. In these countries, some medium productivity levels are due to favourable geographical and climatic conditions.
- **Cluster #3** (blue) is represented by high-income economies (with low GDP share from agriculture) and could be considered as highly mechanised with high levels of productivity.

For meat, the clusters classification follows a similar outcome, as meat production mainly depends on external man-based inputs such as machinery, energy inputs and farm quality.

- Cluster #1 (blue) is represented by low-income economies with low yields, which can be categorised as traditional farming.
- **Cluster #2** (red) is represented by medium-income economies with average production levels (transitional farming).
- Cluster #3 (green) is represented by industrialised economies with high yield meat production (modern farming).

Forestry products follow a similar grouping as cropping due to the effect of local geographical conditions in productivity levels. The ASM outputs seem to agree with the predefined number of groups (k=3). However, for the case of forestry, the optimal number of clusters has been found at four, as cluster 1 could be separated into two smaller clusters. To keep consistency of mechanisation levels among agricultural services, three levels have been kept as the graph demonstrates that k=3 has the second highest ASM width value.

Inputs bounds

After grouping countries accordingly to MUSE regions, data on energy, fertiliser and land demand per unit product has been aggregated and probability distributions have been assigned to characterise those specific groups (Step 5). Therefore, for each mechanisation level and agricultural product, fuel share, agrochemicals demand, and yields have been defined with lower and upper bounds. For the case of energy crops, the data obtained from typical crops has been used. The mean values for fuel (PJ/PJ), emissions (CO_{2eq} PJ⁻¹) and yields (Mha PJ⁻¹) per unit product outlined by mechanisation level, agricultural product and region can be found in the supplementary data (S.3).

Installed capacities (technology calibration)

Finally, it is necessary to calculate the total installed capacities by mechanisation level and by agricultural product (Step 6). In ESMs, accounting for the base-year technological installed capacity is important as it provides a mean to calibrate the model and understand whether the modelling assumptions are correct. For this, an optimisation problem (OP), based on integer linear programming (ILP) implemented in GAMS (GAMS Development Corporation, 2013) has been proposed considering that only data on total sectoral energy demand and emissions by region are available. It is important to mention that the proposed OP is used for calibration purposes, which means that it is built on the purpose of defining the stock of every single technology in the sector at the beginning of the simulation. Considering the uncertainty in the data available, it was concluded that is more effective to constrain the demand for agricultural products and the energy consumption of the sector, closing the remaining degree of freedom minimising the gap between actual emissions and estimated emission values by region. This is achieved by providing a series of lower and upper bounds for parameters such as energy demand by fuel type, fuel share, and technology efficiency. Depending on the region's economic development and on its agricultural share of GDP, a share of each mechanisation level is assumed. As such, every country and region could have some mechanisation level, to greater or lesser extent. In this study, the assumed bounds for mechanisation share by type of economy are shown in Table 2.

Type of Economies	Traditional θ_{trad}	Transitional θ_{tran}	$\substack{ \textbf{Modern} \\ \boldsymbol{\theta}_{mod} }$	Modern Renewable θ_{mod_ren}
Least Developed (%GDP _{agr} share > 0.16)	50-70%	10-20%	10-20%	1-2%
<i>Emerging</i> $(0.02 < \% GDP_{agr} share < 0.16)$	10-20%	50-70%	10-20%	3-5%
Developed (%GDP _{agr} share < 0.02)	10-20%	10-20%	50-70%	5-10%

 Table 2. Mechanisation share lower and upper bounds assumptions for different type of economies

Along upper and lower bounds in other input parameters, the OP is formulated as follows.

• Objective function:

The objective function is defined to minimise the difference between modelled emissions from real emissions in the sector:

$$\min Z = \sum_{r} |\Delta E_r| + \sum_{r,f} |sl_{r,f} * FE_f|$$
⁽⁷⁾

where ΔE_r is the difference in emissions, while $sl_{r,f}$ represents the aggregation of all calculated slack variables (for feasibility purposes) and FE_f is the emission factor for fuel type f.

Emissions Difference

The difference in emissions (ΔE_r) is obtained by:

$$\Delta E_r = R_{E,r} - M_{E,r} \tag{8}$$

where $R_{E,r}$ represent the real emissions in region r (obtained from FAO or IEA), and $M_{E,r}$ is the modelled emissions in region r given by the model.

Emissions of the Model

The modelled emissions are calculated as follows:

$$M_{E,r} = \sum_{f,t} CN_{r,f,t} * FE_f \tag{9}$$

where $CN_{r,f,t}$ is the fuel consumption for region *r* and technology *t*, and FE_f is the emission factor for fuel type *f*.

• Constraints

The OP is subject to the following quality and inequality constrains:

Mass Balance

First, the mass balance must be satisfied for every region, technology and agricultural service:

$$\sum_{t \in TS_s} CP_{r,t} > DM_{r,s} \qquad \forall t \in TS_s$$
⁽¹⁰⁾

where *CP* refers to installed capacity, *DM* to service demand, *r* refers to region, *t* to technology mechanisation level, *s* to service type and TS_s are the technology mechanisation levels available for service *s*.

Service Demand

The demand per service must be met by the sum of the share of production per mechanisation levels:

$$DM_s = \sum_t \theta_{s,t} \tag{11}$$

where θ refers to the demand share covered by technology mechanisation level *t*.

Mechanisation level share

The share of production per mechanisation level ($\theta_{s,t}$) is obtained by dividing the demand met by specific mechanisation level over the total demand for service *s*:

$$\theta_{s,t} = \frac{DM_{s,t}}{\sum_{t \in TS_s} DM_s} \qquad \forall t \in TS_s$$
⁽¹²⁾

The share sum of mechanisation levels per service is constrained by the following equality:

$$\sum_{t} \theta_{s,t} = \theta_{s,trad} + \theta_{s,tran} + \theta_{s,mod} + \theta_{s,mod_ren} = 1$$
(13)

Fuel Balance

The capacity per region and technology $(CP_{r,t})$ is calculated from the total fuel consumption by technology (PJ) multiplied by the technology yield or efficiency (PJ/PJ) :

$$CP_{r,t} = \sum_{f} CN_{r,f,t} * \gamma_{t,s} \qquad \forall t \in TS_s$$
(14)

where f refers to fuel type, $CN_{r,f,t}$ to fuel consumption per region and technology, and γ to efficiency of technology t for service s.

Fuel Constraint

The sum of fuel consumption by region and technology $(CN_{r,f,t})$ is constrained by the total fuel demand in the region:

$$\sum_{t} CN_{r,f,t} < \left(FD_{r,f} + sl_{r,f}\right) \tag{15}$$

where $FD_{r,f}$ is fuel demand f in region r, and $sl_{r,f}$ is a slack variable added to make the problem feasible and fulfil the fuel constraints.

By solving the OP, all structural alternatives are evaluated, and the best solution can be identified. Following, the energy share must be adjusted to reflect the natural variations across regions, showcasing natural factors such as soil fertility, climate, and water availability. The GAMS source code and the obtained technologies installed capacities can be found in the supplementary data S.4 and S.5 respectively. The case study section will show the application of the OP in a single region.

2.4 Fertiliser demand and non-CO₂ emissions

A similar approach has been followed to assign nutrient input and related emissions for each mechanisation level that accurately represents real farming practices and fertiliser inputs. Levels of fertiliser per ton of production have been obtained from FAO (2017) and USDA (2017). The methodology to determine these inputs requires information concerning country crop production (FAO, 2017), its nutrient consumption (USDA, 2017), and the yield associated with each mechanisation level defined in the previous section. Similarly, methane (CH₄) emissions (mainly from livestock management) are considered due to their significance in the agricultural sectors contribution to global GHG releases. For calibration purposes, the study from Pimentel (2009) which provided several baseline estimates of such levels has been used.

2.5 Economic costs of mechanisation

For the economic characterisation of each mechanisation level, data on costs and return estimates from USDA (2017) has been collected. These figures have been converted into USD per hectare using historic yield data (FAO, 2017) and then to USD per PJ year⁻¹ to obtain unit price for installed capacity. For illustration purposes, data on maize crops has been plotted against yields (Figure 8), and by locating the mechanisation level according to the yield, the capital, fixed and variable costs are assigned.



Figure 8 Costs per planted maize energy content, USD2010 PJ year⁻¹. Data: USDA (2017)

2.6 Land use and related emissions

After the model calculates the required technologies to cover the agricultural demands, specific land requirements are obtained. These land values are then aggregated to obtain a final demand per land type, region, period and time slice. Table 3 shows the eight different land types modelled in MUSE.

Table 3 Land types simulated in MUSE-Ag&LU		
Land type	Description	
Cropland	• land suitable for or used for the cultivation of crops.	
Pasture land	land typically used for grazing livestock	
Forestry products	land for silviculture activities	
Energy crops	 land dedicated exclusively for bioenergy crops 	
Natural forest	land for primary and secondary forest	
Non-arable land	• land which is unsuitable for arable farming (desert, ice, tundra, rock)	
Urban/Infrastructure	land for human settlements	
Available	• cleared land potentially available for other agricultural commodities	

If the current land available to meet the demand of a certain service (e.g. crops or meat) is not sufficient at a specific simulation period, this might become available either via a land use change through deforestation (e.g. forest land converted to pasture), or via a change in the destination of other land types that were liberated due to either service demand reduction or intensification. Table 4 shows the possible land use changes in the model. However, if there is no land available to cover the required demand or polices that limit deforestation are in place, the model will endogenously increase yields by increasing investment in higher yields mechanisation levels.

Table 4. Possible changes in land use modelled in MUSE-Ag&LU		
Land Source	Possible Land Destination	
Cropland	Available, Pasture, Forestry Land, Energy crops	
Pasture	Available, Cropland, Forestry Land, Bioenergy	
Forestry Products	• Available, Cropland, Pasture, Energy crops	
Energy crops	• Available, Cropland, Pasture, Forestry Products	
Natural Forest	Cropland, Pasture, Forestry Products	
Available	Natural Forest, Cropland, Pasture, Forestry Land, Energy crops	

Regarding land use emissions, the calculation is based on the IPCC Tier 1 approach (IPCC, 2006) outlined in Appendix B.

2.6.1 Reforestation model

A simple reforestation module has been integrated into MUSE-Ag&LU to assess its potential role alongside the energy system in reaching emission targets. In past years, several models have been designed aiming at understanding the potential role of reforestation in mitigation pathways. For instance, Silver et al. (2000) analysed the carbon sequestration potential of tropical reforestation considering the impact of previous agricultural land (crops or pasture), identifying different sequestration rates. Kraxner et al. (2003) developed a forest growth model in temperate regions to illustrate the potential of reforestation and bioenergy with CCS (BECCS) to permanently remove large amounts of carbon from the atmosphere. Similarly, Evans et al. (2015) calculated carbon sequestration potentials from biofuel production and reforestation on marginal lands. Albanito et al. (2016) integrated a spatial production allocation model and the IPCC Tier 1 method to assess carbon potential implications of switching land from food production to either energy crops or regenerated forest. Dwivedi et al. (2016) designed a forest growth model to analyse the carbon abatement of reforestation under different carbon markets. Krause et al. (2017) investigated optimal sequestration rates considering BECSS and afforestation in combination by accounting for diverse land biophysical properties such as nitrogen cycles, carbon dynamics between carbon pools and surface albedo. Most of reforestation studies have calculated that sustainable carbon management from forest is valued at around \$25-50 tCO₂⁻¹, while industrial CCS costs are estimated at around \$100-\$160 tCO₂⁻¹ (Ni et al., 2016).

In MUSE-Ag&LU, biomass growth models simulating reforestation taking place on marginal or abandoned land over a 100 year period have been developed. Biomass accumulation is modelled for aboveground biomass and carbon accumulation for soil, considering the tropical rainforest region as case study. To develop the models, most of the data has been obtained from Silver et al. (2000). Table 5 shows the growth models used in MUSE. These are related to tree age and differentiate between agriculture and pasture land as previous land use.

 Table 5. Forest biomass growth functions modelled in MUSE-Ag&LU. Source: Silver et al.

 (2000)

Previous land	Previous land Model		
	Biomass (above ground) in kg		
Pasture	-0.03* tree _{age} ² + 3.48* tree _{age} + 13.69	0.44	
Agriculture	-0.03* tree _{age} ² + 4.09* tree _{age} + 10.49	0.84	
Soil Organic Carbon			
Pasture	$18.31*\ln(\text{tree}_{\text{age}}) + 1.73$	0.66	

	Agriculture	$10.88*\ln(\text{tree}_{age}) + 31.24$	0.22
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Based on data from Ribeiro et al. (2015), the belowground biomass pool has been added by developing a relationship with the aboveground biomass pool. Then, an average carbon concentration in aboveground and belowground of 44.5% and 37.8% respectively has been assumed. Figure 9 illustrates CO_2 uptake models for the three carbon pools, assuming that new forest reaches a carbon saturation point at roughly after 50 years (Silver et al, 2000).



Figure 9 Total CO₂ accumulation by carbon pool after reforestation in different land types

For the economic evaluation of reforestation projects, land acquisition costs, operational costs, management, maintenance and supplements application costs have been obtained from Guitart and Rodriguez (2010). After adjusting them for inflation, cost of investments have been defined as follows: CAPEX as US\$ 5,524 ha⁻¹ and OPEX as US\$ 51.7 ha⁻¹. A discount rate of 5% is used as it is a common value for terrestrial carbon studies (Sullivan et al., 2005).

2.7 Summary: Model's Inputs/Outputs

To summarise the methodology section, Table 6 presents a summary of all the inputs to and outputs from the model in a generic iteration.

_	-
MUSE-Ag&LU Key Inputs	MUSE-Ag&LU Key Outputs
-Techno-economic characterisation for each agriculture	-Agricultural mechanisation index detail by time
technology (mechanisation level) in each time period	slice, technology type and region.
and region.	• Fuel demand by source (PJ)
• Energy input by source (PJ/PJ)	• Agricultural commodity production
• Conversion efficiency (%)	(crops, meat and forestry products) (PJ)
• Energy emissions (ktCO ₂ /PJ)	• Energy crop production (miscanthus,
• Agrochemicals emissions (N fertiliser) (ktCO _{2eq}	switchgrass) and other bioenergy residues
/PJ)	outputs (agricultural residues, meat-based
• Methane emissions (ktCO _{2eq} /PJ)	residues, forestry residues) (PJ).
• Yields (Mha/PJ)	• Aggregated demand of agrochemicals (kt)
• Land use type demand (-)	• Land use demand by agricultural
• Unit capital and operational cost (\$USD/PJ)	commodity and aggregated land demand
• Existing stock for the model base year per region	by land (Mha)
by technology type, including their retirement	• Aggregated emissions due to direct energy
profile (PJ year ⁻¹)	use and land use change (kt)
-Policy framework and fiscal regimes.	• Aggregate CAPEX and OPEX of new
-Macro-economic drivers' projections (e.g. GDP _{cap} ,	installed technologies (mechanisation)
population, urbanisation).	(\$USD), and retirement in capacity terms
	by time period, technology type and
 Unit capital and operational cost (\$USD/PJ) Existing stock for the model base year per region by technology type, including their retirement profile (PJ year⁻¹) Policy framework and fiscal regimes. Macro-economic drivers' projections (e.g. GDP_{cap}, 	 commodity and aggregated land demand by land (Mha) Aggregated emissions due to direct energy use and land use change (kt) Aggregate CAPEX and OPEX of new installed technologies (mechanisation) (\$USD), and retirement in capacity terms

Table 6. Exchange data flow for the MUSE-Ag&LU model

3 Case study and description of scenarios

To illustrate the model capabilities, Brazil is used as a case study. The model is capable to simulate the energy and land use systems, projecting different emissions pathways depending on user-defined policy assumptions. To model the Brazilian energy system, data from the Energy Research Company (EPE, 2017) has been the main source for calibration and validation. Supported with historical statistics from the *International Energy Agency* (IEA, 2017), service demands for each end-use has been projected. For agriculture, forestry and land use, data from the Brazilian Geographic and Statistics Institute (IBGE, 2018) and FAO (2017) is used. Land demand for different Brazilian forest separated by biome as well as areas for silviculture has been obtained from the Ministry of Environment (MME, 2018), while data for sugarcane crops from the Sugarcane Union Industry (UNICA, 2018).

region

3.1 Agriculture demand projection

To project service demands in agriculture, eq. 4 is used. Figure 10 shows correlated data for average daily crop and meat intake with household income for Brazil^{*}. This data has been regressed to project demand for 2050 by using IIASA SSP2[†] scenario data on GDP and population (Fricko et al., 2017).



Figure 10. Relation in the consumption of food and average income per capita in Brazil (1970-2010) and projections to 2050. Source: FAO (FAO, 2017).

3.2 Technology characterisation and land use representation

Brazil, with average yields of 10.49 PJ Mha⁻¹ for crops, 1.16 PJ Mha⁻¹ for meat-based, and 7.66 PJ Mha⁻¹ for forestry (FAO, 2017), can be found mainly with transitional mechanisation levels across all the agricultural services. This could also be explained by the share of agricultural production to the national GDP, which stands at 4.3% (FAO, 2017), thus being considered an emerging economy according to the classification presented in Table 2.

By applying the optimisation problem (equations 7-15), installed capacity and fuel input per unit of service (PJ) for each agricultural service has been obtained. The OP model minimises modelled emission against actual emissions from energy use, which stand at about 23.4 MtCO₂ year⁻¹ (FAO, 2017). The obtained installed capacity alongside the technoeconomic parameters are presented in Appendix C (Table C.1).

^{*} Same function has been used to regress forestry products.

[†] The SSP2 narrative describes a middle-of-the-road development in mitigation and adaptation

To account for carbon emissions and sequestration potential from land use, carbon densities are taken from the IPCC (2006) and other studies (Miteva et al., 2014; Opio et al., 2013; Sallustio et al., 2015). These are characterised for each land use category in Table 7.

Land type	Above Ground (tC ha ⁻¹)	Below Ground (tC ha ⁻¹)	Dead Organic Matter (tC ha ⁻¹)	Soil Organic Carbon ^{&} (tC ha ⁻¹)	Total (tC ha ⁻¹)
Cropland	10.0	5.4	1.0	53.1	69.5
Pasture	7.6	1.1	0	78.9	87.6
Forestry prod. ⁺	62.0	12.8	1.8	42.0	118.6
Bioenergy *	16.0	14.3	1.0	33.5	64.8
Forest**	78.2	28.9	5.2	44.0	156.3
Non- arable	-	-	-	-	0
Urban	-	-	- 🖌	-	0

Table 7. Estimated average C values for each land use and carbon pool (IPCC, 2006; MMA,2017)

[&]Estimations from the topsoil layer (0-20 cm in depth)

*Sugarcane, considering an average productivity (yield) of 60 t/ha

⁺Eucalyptus plantation

** Average values considering all six biomes have been considered (Amazonia, Caatinga, Cerrado, Mata Atlántica, Pampa and Pantanal).

A split sample validation approach has been performed. Values on energy use, emissions, and land use have been calibrated using 2010 as base year. This year has been selected because of the existence and reliability of data for all the sectors as well as being a year without significant political, economic or environmental circumstances. A model validation has been performed using 2015 data on agricultural commodity demand and fuel consumption.

3.3 Scenarios

Three scenarios between 2015 and 2050 based on the SSP2 (Fricko et al., 2017) are modelled:

Scenario 1 – Business as Usual (BAU): Explores a scenario where there is a lack of a carbon emission reduction target and current energy and land use policies are assumed. For example, power sector expansion plans (ANEEL, 2018), gasoline/ethanol blending mandates and oil and natural gas extraction rates (ANP, 2019)are modelled accordingly to current government plans and policies. Other main assumptions are related to agricultural productivity (FAO, 2017) and land use expansion (e.g. sugarcane expansion) (UNICA, 2018). Agricultural yields are kept to baseline values while new land for agricultural use is not constrained, therefore deforestation could take place.

Scenario $2 - 2^{\circ}C$ without reforestation (2DS-REF): Based on research from Rochedo et al. (2018), this scenario contemplates a carbon budget for the period 2015-2050. This budget, which considers Brazil's solely contribution to reach Paris agreement targets has been obtained by running several

global integrated assessment models (IAM). Originally, the authors have suggested an average carbon budget of around 24 GtCO₂ (considering land and energy emissions only); however, in this study a budget of 35 GtCO₂ has been considered, as the model also contemplates non-CO₂ emissions from agriculture. A full range of technologies for decarbonising the energy sector are available. For instance, it is assumed electrification in most of the sectors by reducing costs on solar and wind power (Elshurafa et al., 2018), electric vehicles (Soares M.C. Borba et al., 2012) and efficient air conditioning systems (air source heat pumps) (Fortes et al., 2018) as well as limiting extraction of fossil fuels by 2030. Additionally, it is assumed agricultural sector intensification (e.g. from an average of 1.0 to 1.7 cattle heads per hectare (EPE, 2016)) and constraints in forest deforestation after 2030 (MAPA, 2009). in this scenario, it is considered that liberated agricultural land remains abandoned throughout the analysed period.

Scenario 3 – 2°C with reforestation (2DS+REF): Similar to Scenario 2, but abandoned agricultural land is subject to a reforestation process.

4 Results and Discussions

4.1 Agriculture intensification: mechanisation share, energy use and emissions

Figure 11 shows agricultural mechanisation share projections considering aggregated service demands (crops, meat, forestry products and bioenergy) for each analysed scenario. In the base year, agricultural production has the following mechanisation share: traditional: 13%, transitional: 56%, and modern: 31%. Compared to the agro-environmental index (intensification – extensification) used by the European Commission (EC, 2019), the Brazilian base year mechanisation share is similar to current practices in Central European countries such as the Czech Republic and Poland. By 2050, the share of modern mechanisation would reach 54% in a BAU scenario and up to 63% (2DS+REF) in a carbon constrained pathway. This would represent similar production of today's Denmark (60%) and Germany (61%); however, still below to Belgium (77%) and the Netherlands (88%). Also, for both carbon constrained scenarios, a higher share of renewable-based modern mechanisation is expected. In Appendix D (Figure D.1), mechanisation share separated by agricultural service (crops, meat, forestry products and bioenergy) is illustrated.



Figure 11. Share of different agricultural mechanisation levels for each scenario

Figure 12 illustrates the projected total agricultural energy demand by fuel as well as the direct energyrelated emissions. In the base year, the sector demands around 540 PJ year⁻¹, reaching 1,349, 1,447 and 1,477 PJ year⁻¹ for BAU, 2DS-REF and 2DS+REF respectively. The main difference is the highest share of renewable sources in the 2DS scenarios. Agricultural residues, biogas and biodiesel will represent around 17-20% (251-288 PJ year⁻¹), while in the BAU these would reach 11% (158 PJ year⁻¹) of the energy mix. However, diesel and electricity will still be the predominant energy sources (71-78%).



Figure 12. Energy demand projections by fuel and energy-related emissions for both scenarios

In the base year, the energy use per hectare stands at 1.7 PJ ha⁻¹, which is comparable to the lowest agricultural energy users in the European Union (Rumania and Bulgaria: 1.6 PJ ha⁻¹ and Greece: 2.1 PJ ha⁻¹). By 2050, the model suggest that this metric will increase to 3.6 PJ ha⁻¹ in BAU, 4.8 PJ ha⁻¹ in 2DS-REF and 5.0 PJ ha⁻¹ in 2DS+REF. These values will be similar to current energy use in Spain (4.1 PJ ha⁻¹), Sweden (4.6 PJ ha⁻¹) and Hungary (5.1 PJ ha⁻¹), and just below the current EU average index (5.4 PJ ha⁻¹).

Direct energy-related emissions will reach between 29.5-30.3 MtCO₂ year⁻¹; however, most of the sectoral emissions will come from CH₄ and N₂O. Today's agricultural emissions (excluding energy use) stand at 451 MtCO2_{eq} year⁻¹ (FAO, 2017). CH₄ from enteric fermentation and N₂O from manure

management are responsible for 58% and 23% of the total emissions respectively, while 5% is related to N_2O due to synthetic fertiliser application. In the BAU scenario, is expected an increase of 47% by 2050, reaching a total of 659 MtCO_{2eq} year⁻¹. This value will be lower for the 2DS scenarios, reaching around 627-634 MtCO_{2eq} year⁻¹. Figure 13 illustrates the projected CO_{2eq} emissions (including energy) from the agricultural sector for each modelled scenario.



Figure 13 CO₂, CH₄ and N₂O (CO_{2eq}) emissions in each scenario

4.2 Land use demand and emissions

Figure 14 shows land use patterns for each scenarios. The amount of land devoted to growing all agricultural services increases by a concurrent decrease in other lands such as forest.





In the BAU scenario, it is expected that total agricultural land would grow from 302 to 375 Mha, while for the 2DS-REF agricultural land demand will be reduced to 301 Mha, and 294 Mha in 2DS+REF. In all three scenarios, due to a demand increase in meat-based products, pasture land would constantly increase until 2030, reaching 259 Mha for BAU, 209 Mha for 2DS-REF and 201 Mha for 2DS+REF. After 2030, pasture land would keep increasing in the BAU scenario, while for both 2DS scenarios, a peak demand would have been reached, liberating land at an average rate of 0.6% year⁻¹ due to intensification in livestock production. On the other hand, crop land will constantly increase in all scenarios until the end of the simulation period at an annual rate of 0.8% year⁻¹ between 2015 and 2030. However, in the 2DS+REF, growth rates will slow down to 0.3% year⁻¹ reaching 94 Mha by 2050, compared to 99 Mha in 2DS-REF and 100 Mha in BAU. Bioenergy land reaches a higher demand in 2DS scenarios, as larger requirements for energy crops are found; nevertheless, due to sector intensification, after 2040, bioenergy land will stabilise at around 12 Mha. The results show that compared to BAU, 2DS+REF could save around 57 Mha of forest by 2050 while also adding 24.4 of new forest land.

Figure 15 illustrates the projected land CO₂ flux for each scenario. As the simulation progresses in the BAU scenario, the carbon stock losses 13 GtCO₂, reducing the 2015 national carbon stock from 340 GtCO₂ to 327 GtCO₂ by 2050, which represent the depletion of 37% of the carbon budget. The main carbon losses come from soil organic carbon (SOC) pools from pasture land and the above-ground biomass from deforested lands. For the 2DS-REF scenario, carbon stock gets reduced to 336 GtCO₂ (9 GtCO₂ or 26% of the budget), while for the 2DS+REF, as soon as land becomes available (2030), new forest starts absorbing carbon at a rate of 0.09 GtCO₂ year⁻¹. The rate increases in the following periods, reaching a peak sequestration rate of 0.52 GtCO₂ year⁻¹ in 2040, to then stabilise around 0.40 GtCO₂ year⁻¹ by 2050. The higher rates in 2040 are due larger availability of former pasture land combined with higher sequestration rates of new forests plantations. By 2050, the total land carbon stock would reach 344 GtCO₂, almost recovering carbon stock values to base year levels.



4.3 Sectoral emissions

4.3.1 Measures in the energy system and the role of land use

Figure 16 presents Brazil emissions trajectory separated by land use, (non-energy) agriculture and the energy systems. In Appendix E, detailed emissions by sector in the energy system (Figure E.1) as well as the power sector energy mix (Figure E.2) is shown.

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Figure 16 Total emissions projections by source for each scenarios

In the BAU scenario, minimum decarbonisation measures are enforced in the energy sector. Thus, from current emissions of 0.47 GtCO₂ year⁻¹, the energy sector reaches 0.78 GtCO₂ year⁻¹ by 2050, with the industry and transport sectors as major contributors (0.29 and 0.28 GtCO₂ year⁻¹ respectively). For the 2DS scenarios cross sectoral efficiency measures are introduced to reduce national emissions. In both 2DS scenarios, higher electrification is expected as illustrated in the power system in Figure E.2. While the BAU reaches an installed capacity of 239 GW, the 2DS-REF and 2DS+REF reach 271 GW and 270 GW respectively. In all three scenarios, hydropower remains as the main source (44-49%), reaching between 117-120 GW installed capacity. In both 2DS scenarios, more biomass and natural gas will be necessary to cover the extra demand; however, this will be in combination with carbon capture and storage (CCS). Gas with CCS would have an installed capacity of around 42 GW (16% of the total installed capacity) while BECSS would be about 18 GW (7%); however, in the 2DS-REF, more investments in renewable sources such as on onshore wind farms would be required to further reduce sectoral emissions.

For the rest of the sectors, in the 2DS-REF, higher decarbonisation efforts would be necessary in buildings, transport, and industry. It is expected that in the building sector, 42% of the lighting demand will be covered by LEDs, while air and ground source heat pumps (ASHP and GSHP) would cover 49 % of the cooling installed capacity. In the transport sector, battery cars will cover 46% of the passenger demand, decommissioning some of the gasoline-ethanol flex fuel options. The industry sector would require the highest decarbonisation levels, as 98% of the production would require CCS (with special focus in the cement, iron and steel subsectors). When reforestation is considered (2DS+REF), the sectors are not as pressured to reduce its emissions. For example, although LED in buildings will also represent 42% of the artificial lighting capacity, heat pumps will reduce its share to 38%. Similarly, electric cars will cover 39% of passenger demand, while CCS in industry will cover 86% of the production. The carbon price in the 2DS-REF scenario has been calculated at US\$ 1,480 tCO₂⁻¹, higher than the US\$ 856 tCO₂⁻¹ from 2DS+REF.

4.3.2 Investments in industrial CCS and reforestation

Figure 17 shows the required CCS investments per sector for both 2DS scenarios. Most of the investment in the energy and land sector takes place after 2030, when both 2DS scenarios already depleted 20-21 GtCO₂ (60% of the 35 GtCO₂ budget). Is after 2030, when high CCS investments in the industry, refinery and power arise. For the 2DS-REF, it takes 10 years and US\$ 949 billion in CCS for the energy sector to reach negative emissions. However, to reach mitigation targets by 2050, an additional US\$ 1,659 billion would be required, sequestering around 1.6 GtCO₂ by 2050. For the 2DS+REF, similar investments in industrial CCS are made by 2040 (US\$ 942 billion). However, an

initial investment of US\$ 159 billion is made for reforestation between 2030 and 2040. This has two effects in the 2DS+REF energy system: i) delays negative carbon emissions in the energy sector until 2045, and ii) reduces investments in CCS between 2040 and 2050 by 31%, saving US\$ 506 billion. Moreover, the combination of CCS and reforestation sequesters 3.9 GtCO₂ between 2040 and 2050, achieving carbon targets at a lower cost. In this scenario, 86.9% of the total investment will be made in the industry, while reforestation would only require 10.5 % or US\$ 237 billion, resulting in an average sequestration cost of US\$ 47.8 tCO_2^{-1} .





4.4 Discussion

For emerging economies such as Brazil, if crop, pasture, forestry and bioenergy production is to be increased by 2050, intensifying agriculture would be fundamental to achieve carbon mitigation goals with minimum effects on deforestation and crop competition.

While a BAU scenario, where no intensification is triggered, has projected agricultural lands to reach almost half of the country's total land (375 Mha), 2DS scenarios constrained this expansion to about 300 Mha. To validate this outputs, MUSE values have been compared against those from the GLOBIOM-Brazil model published in an INPE-UNEP report (INPE, 2015). In their BAU scenario, the report has projected an increase in agricultural area (crops, pasture, planted forest and bioenergy) from 278 Mha in 2010 to 334 Mha by 2050, which lies in between with the analysed scenarios. The main differences are found in the demand patterns from pasture land. While both models agree that around 2030, pasture land would reach a peak in demand, the 2DS scenarios have projected a higher land liberation rate until 2050, reaching as low as 194 Mha by 2050 in the 2DS+REF. GLOBIOM have projected a slower intensification reaching 208 Mha. Land productivity could also incentivise producers to further expand production to new lands; however, these land use dynamics are difficult to predict in presence of different stakeholders. Lastly, agricultural land abandonment, such as those

simulated in BAU and 2DS-REF, could have negative effects on biodiversity and increase its susceptibility to climate-driven natural disasters.

Modern technologies have the capacity to increase productivity by having higher yields and conversion efficiencies. The study shows that agricultural emissions, mainly CH_4 and N_2O from enteric fermentation, manure management and fertiliser use will be difficult to reduce, as intensification would come with larger amounts of embodied emissions. In both 2DS scenarios, emissions from agriculture would reach 0.63 GtCO₂ year⁻¹, offsetting carbon sequestration rates from the energy and land use sector. These emissions can lead to a higher pressure on the environment, as the uncontrolled increase in fertiliser utilisation increases the risk of nutrient contamination into water bodies and soil. Appropriate land management practices are necessary to sustain soil fertility as well as appropriate management on livestock and manure left on pastures. In this sense, biogas production from agricultural residues and manure have the capacity to reduce methane emissions in agriculture, with potential to inject biomethane into the Brazilian gas grid.

Careful decarbonisation of different sectors combined with appropriate land use management and forest recovery have the potential to support more sustainable policies. Reforestation could have an important role in reaching decarbonisation targets. As demonstrated in 2DS+REF, a policy to incentivise large-scale reforestation would result in the possibility to sequester large amount of carbon at a lower cost. However, for this to take place, the agriculture sector needs to intensify its production rapidly while reducing direct and indirect deforestation. In both 2DS scenarios, BECCS can only make a limited contribution to carbon mitigation goals, as bioenergy expansion in the first 15 years of the analysed period (2015-2030) would provoke indirect land use emissions by moving crop and pasture production to the agricultural frontier. Afterwards, when land becomes available, bioenergy starts competing with reforestation, where current uncertainties and high prices of BECCS limits its wider implementation in the energy system.

The proposed method can be generalised to other regions. The minimum data requirement is represented by two data types: national average agricultural productivity by commodity and sectoral energy use/emissions; which is available from international organisations (FAO, IEA). However, for a more reliable and feasible application other type of data is desirable such as spatial representation of agricultural productivity per type of commodity as well as detailed data of energy consumption per unit production for specific agricultural technologies. Ideally, these data would come at a sub-regional level; nevertheless, as sub-regional data might be difficult to obtain, data sources mainly from local governmental and non-governmental organisations need to be investigated.

5 Conclusion and future research

The agriculture and land use sector is set to face some of its toughest challenges in the coming decades, not only due to increasing food demand but also rising pressures on bioenergy cultivation and the effects of climate change. Agricultural decarbonisation pathways are not widely discussed in energy modelling due to its small share in direct energy use and related emissions. Additionally, modellers have faced the challenges in modelling agricultural technology diffusion in ESMs. The sector is of greater importance in the wider energy and land use system and its understanding is vital in achieving decarbonisation targets.

This paper has presented MUSE-Ag&LU, a new modelling framework that combines both energy and land use simulation without the necessity of soft-linking separate complex models. The developed modelling approach based on mechanisation levels, can explicitly track agricultural technology diffusion, simulating energy use, agrochemical demands and its implication in land use and energy and non-energy emissions. In previous research, the definition of mechanisation levels has been merely qualitative. In this study, the main focus has been to provide a quantitative approach based on inferential statistics, cluster analysis and optimisation. The approach has proved to be an effective tool when comprehensive data is not available for agricultural services and technologies.

To test the technology characterisation framework as well as the MUSE-Ag&LU model, the Brazil case study explored the complex relationship between agriculture, deforestation and the energy system under three scenarios. For both 2DS scenarios, agricultural modernisation has been essential to reduce indiscriminate land expansions. Moreover, if the abandoned land could be used to regenerate the natural landscape, this could help the country to reach carbon mitigation pathways while alleviating decarbonisation efforts and reducing investments in the rest of the economy.

The obtained results have shown that the presented framework has the capability to inform policy makers by showing the agricultural, forestry and land use landscape within the energy systems context.

This raises pertinent policy questions not only for Brazil, but globally, coupling both energy system development ambitions alongside agriculture and land use change concerns. Outputs have shown the importance of reforestation not only as a significant carbon sequestration process but also to reduce investments in CCS projects in the power and industry sectors as well as lowering decarbonisation efforts in the rest of the sectors. Nevertheless, detailed accounting of energy use in every sector as well as appropriate accounting of nitrous oxide and methane emissions from supply chain is necessary to provide an integrated view of the energy systems and the cross-sectoral effects of land use change.

Some limitations exist in the model and the selected methodology. The main one refers to decision uncertainty which involves the subjective choice by the modellers for representing agriculture technologies by mechanisation levels instead of explicit technologies. Some information could be lost as mechanisation levels have a fixed fuel share demand. Moreover, although the global model is characterised by several regions (28), in the presented case study where a single region is modelled, intraregional interactions have not been considered, meaning that the effect of trade is not accounted for. Additionally, land use and land use change processes are subject to large uncertainties. Brazil's ecosystem is diverse and carbon stocks per hectare might vary among regions and depth. Also, the selected land use calculation methodology (IPCC Tier 1 approach) does not consider explicit change between lands, where carbon pools' dynamics are specific to land use conversion (e.g. tree growth rates, dead matter oxidation, etc.).

For future research, the model would be expanded to characterise different crops, pasture, silviculture, and bioenergy products in different regions. Also, the model will be able to model more realistic dynamics in the land use, by simulating time delays between land use changes (e.g. forest to crops, pasture to bioenergy) and reforestation growth. Finally, the effect of trade (within and between regions) will be considered as this could have major implications in local production and resource utilisation.

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Appendix A. MUSE - ModUlar energy systems Simulation Environment

MUSE is a bottom-up technology-rich global model of the whole energy system (i.e. including demand, conversion and supply sectors), with a disaggregation into 28 geopolitical regions and a time slice disaggregation which varies depending on the sector. The MUSE general framework is illustrated in Figure A.1. MUSE follows a simulation approach coupled with an imperfect foresight to model the real-world decision making of investors as realistically as possible. This framework allows sectorspecific modelling and thus the use of the most appropriate methodology for each energy sectors. The main focus lies on an accurate description of the investment and operational decision making in each sector, where a variety of methods are implemented ranging from merit-order simulation methods to agent-based modelling. This is distinct in that most models either use a central planning approach to suggest optimal energy system changes, or use a single investment metric across the economy. The focus on the investors view within the modelling results in an arguably more realistic presentation of the energy market transition compared with the normative pathways from optimisation models. Besides giving a new perspective on the energy system transitions, MUSE is designed to enable transparent and flexible analysis of all sectors of the energy market as a whole or separately. It includes all sources of CO₂ emissions and shows the complex relationships within the energy system among technology, economics, and impact on the environment. The energy equilibrium of MUSE is given by the market clearing algorithm (MCA) which connects all parts of the model and is responsible for the information flow between all sectors. The solution algorithm of MUSE is given by an inner loop for each time period and an outer loop for the simulation horizon (e.g. 2050 or 2100). The MCA iterates between sector modules until price and quantity of each energy commodity converge. MUSE includes supply sectors, conversion (power and refinery) and demand sectors (residential, commercial, transport, industry, and agriculture). One of the main characteristics is its modular flexibility allowing representation of the specific drivers to technological investments and operation in each energy sector.



Figure A.1 Schematic representation of the MUSE Framework

Appendix B. Estimation of the land carbon stock and emissions

Regarding land use emissions, the calculation is based on the IPCC Tier 1 simplified approach (IPCC, 2006). This approach is a non-spatially method, which calculates net changes in land use categories over a period in time. The IPCC considers emissions and removals of CO₂, based on changes in ecosystem carbon (C) stocks for each land use category[‡]. Four carbon pools have been quantified to determine the LUC: i) above ground biomass, ii) below ground biomass, iii) dead organic matter (DOM), and iv) soil organic carbon (SOC). To calculate carbon stock changes in any pool the stock-difference method has been used. The method calculates the difference of carbon stocks per pool for a given land at two points of time:

$$\Delta C_l = \frac{(C_{l,t2} - C_{l,t1})}{(t_2 - t_1)} \tag{B.1}$$

where ΔC_l is the change between periods in carbon stocks in the pool *l*, $C_{l,t1}$ is the carbon stock at time 1 and $C_{l,t2}$ is the carbon stock at time 2. To account for period carbon stock changes per land type, the following formula is used:

[‡] Changes in C stock categories are converted to units of CO_2 emissions by multiplying the C stock change by 44/12. This is based on the ratio of molecular weights.

$$\Delta C_{LU_i} = \Delta C_{AB} + \Delta C_{BB} + \Delta C_{DOM} + \Delta C_{SOC}$$
(B.2)

where ΔC_{LU_i} is the change in carbon stock for land use type *i* (i= cropland, pasture, forest, etc.), *AB* refers to above ground biomass, *BB* below ground biomass, *DOM* to dead organic matter and *SOC* to soil organic carbon. For the entire agriculture and land use sector, the sum of all carbon stock changes per land-use category is calculated as follows:

$$\Delta C_{tot} = \sum_{i} \Delta C_{LU_i} \tag{B.3}$$

where ΔC_{tot} is the total carbon stock change and ΔC_i is the difference in carbon stock for *i* land type. As noted in the IPCC methodology, carbon flows are different depending on the original and final land use. For example, soil organic carbon (SOC) from reforestation in formerly crop land usually increases carbon stocks; however, reforestation from previously pasture land usually reduces SOC pools. Some of these values, used as input parameters in the model, are considered from Guo and Gifford (2002) (Table B.1).

Land use Origin	Land use Destination	Δ SOC
Forest	Pasture	8%
Pasture	Secondary Forest	-20%
Pasture	Silviculture	-10%
Forest	Silviculture	-13%
Crop	Silviculture	18%
Forest	Crop	-42%
Crop	Secondary Forest	53%
Pasture	Crop	-59%
Crop	Pasture	19%

 Table B.1 Soil carbon stock mean value response to different land use changes. Source: Guo and Gifford (2002)

Appendix C. Brazil's agricultural technologies representation

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Service	Mechanisation	Installed Capacity GW	Capital Cost (MUSS/PJ)	Operational cost (MUS\$/PJ)	Biomass (PJ/PJ)	Biogas (PJ/PJ)	Biodicsel (PJ/PJ)	Diesel (PJ/PJ)	Electricity (PJ/PJ)	Gas (PJ/PJ)	Heavy fuel oil (PJ/PJ)	N2O (kt/PJ)	CH4 (kt/PJ)	Yield (Mha/PJ)
	Traditional	3.49	1.55	1.33	060.0	0.000	0.000	0.000	0.000	0.000	0.030	16.8	96.0	0.173
	Transitional	10.90	2.19	1.11	0.129	0.000	0.000	0.040	0.010	0.000	0.000	25.2	134.3	0.105
	Modern	8.72	2.78	0.96	0.000	0.000	0.000	0.200	0.102	0.010	0.000	42.0	172.7	0.053
Crops	(F 0SSU-Dasea) Modern (Renewable-based)	0.00	2.89	0.77	0.000	0.010	0.500	0.000	0.082	0.000	0.000	6.7	115.2	0.053
	Traditional	0.69	2.81	1.2	0.245	0.000	0.000	0.000	0.000	0.000	0.016	951.1	262.2	3.599
	Transitional	3.09	6.28	1.99	0.258	0.000	0.000	0.160	0.023	0.000	0.000	1426.7	367.1	1.100
	Modern	3.46	6.6	2.09	0.000	0.000	0.000	1.198	0.205	0.001	0.000	2377.9	472.0	0.094
Meat- based	(r ossu-basea) Modern (Renewable-based)	0.00	6.93	1.77	0.000	0.048	3.000	1.198	0.205	0.000	0.000	380.5	314.6	0.094
	Traditional	1.29	3.60	0.90	0.006	0.000	0.000	0.000	0.000	0.000	0.001	24.4	33.6	0.004
	Transitional	6.46	14.40	1.80	0.006	0.000	0.000	0.004	0.001	0.000	0.000	36.6	47.1	0.002
	Modern	3.23	13.50	2.25	0.000	0.000	0.000	0.012	0.004	0.001	0.000	60.9	60.5	0.001
Forestry products	(r ossu-vasea) Modern (Renewable-based)	0.00	18.00	3.00	0.000	0.003	0.030	0.000	0.004	0.000	0.000	9.7	40.3	0.001
1	Traditional	0.38	3.78	2.13	0.006	0.000	0.000	0.000	0.000	0.000	0.001	16.8	96.0	0.015
	Transitional	1.89	5.3	2.06	0.006	0.000	0.000	0.004	0.001	0.000	0.000	25.2	134.3	0.009
	Modern	0.95	6.31	2.02	0.000	0.000	0.000	0.012	0.004	0.001	0.000	41.9	172.7	0.004
Bioenergy	(r ossu-vasea) Modern (Renewable-based)	0.00	8.00	1.71	0.000	0.003	0.030	0.000	0.004	0.000	0.000	6.7	115.1	0.004
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Appendix D. Agricultural mechanisation by type of commodity



Figure D.1 Share of different agricultural mechanisation levels per agricultural service for each scenario





Figure E.1 Energy sector emissions in 2015, 2030, and 2050 for each scenario



Figure E.2 Power sector installed capacity by source for each scenario

Highlights

View nublication stats

- A novel energy-oriented agriculture and land use systems model has been developed
- Mechanisation levels are characterised using cluster analysis and linear optimisation
- Role of reforestation alongside measures in the energy sector in Brazil are studied
- By 2050, modern mechanisation could represent 54-63% of agricultural production
- Brazil has the potential to sequester around 5.6 GtCO₂ through reforestation

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