A Proposal for Using Process-Based Soil Models for Land Use Life Cycle Impact Assessment

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Abstract

Life cycle impact assessment (LCIA) models regarding land use impacts are usually proxy-based models that lack regionalization or sufficient land use classes. In this dissertation, we introduce a paradigm shift from proxy-based to process-based models, by calculating biogeographically differentiated characterization factors (CF). The goal of the dissertation was to test the potential viability and accuracy of two spatially explicit process-based models to simulate soil dynamics, namely RothC and Denitrification Decomposition model (DNDC), which may enable an assessment based on scenarios to provide more accurate CFs for soil quality. Also, this dissertation tested the computational limitations of these process-based models when applied to LCIA. We proposed one LCIA midpoint method for land use impacts using Soil Organic Carbon (SOC) as an indicator on soil quality and used the region of Alentejo (Portugal) as a proof of concept. An additional advantage of using process-based models was that it enabled us to build scenarios that explicitly take into consideration expected future changes in temperature and precipitation under climate change.

In this dissertation, we present all the datasets necessary to run the models and their implementation. We also provide a sensitivity analysis of input parameters for the RothC model. A methodology that allows the calculation of CF’s obtained through results of RothC model is described. In the end the CFs are presented and compared with alternative models obtained in the literature.

Keywords: Life Cycle Impact Assessment, RothC model, DNDC model, Soil Organic Carbon, Characterization Factors

Resumo

Os modelos de avaliação de impacte em ciclo de vida (AICV) para determinação dos efeitos do uso do solo são, geralmente, modelos *proxy* que carecem de regionalizações e classes adicionais de uso do solo. Nesta dissertação, propomos uma mudança de paradigma na modelação do uso do solo em AICV calculando fatores de caracterização (FC) diferenciados biogeograficamente com recurso a modelos de solo baseados em processos. O objetivo desta dissertação é testar a potencial viabilidade e precisão de dois modelos baseados em processos espacialmente explícitos para simular a dinâmica de acumulação da matéria orgânico no solo, nomeadamente RothC e o modelo de Decomposição por Desnitrificação (DNDC), que poderão permitir uma avaliação baseada em cenários para fornecer FCs mais precisos para a qualidade do solo. Além disso, nesta dissertação foram testadas as limitações computacionais destes modelos baseados em processos quando aplicados ao LCIA. Propõe-se um método *midpoint* de LCIA para o impacto do uso do solo utilizando carbono orgânico do solo (COS) como indicador da qualidade do solo e usando a região do Alentejo (Portugal) como prova de conceito. Uma outra vantagem em utilizar modelos baseados em processos é que permite a construção de cenários que têm em conta, explicitamente, mudanças futuras esperadas de temperatura e precipitação sob mudanças climáticas.

Nesta dissertação, apresentamos todos os conjuntos de dados necessários para correr os modelos e a sua implementação. Além disso, é fornecida uma análise de sensibilidade dos parâmetros de entrada para o modelo RothC. O método que permite o cálculo de FCs obtidos através dos resultados do modelo RothC é descrito. Por fim, os FCs são apresentados e comparados com modelos alternativos obtidos na literatura.

Palavras-Chave: Avaliação de impacte em ciclo de vida, Modelo RothC, Modelo DNDC, Carbono Orgânico do Solo, Fatores de Caracterização

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List of Acronyms

B2C – Business to Consumers

CANDY – Carbon and Nitrogen DYnamics

CF – Characterization Factor

CLC – Corine Land Cover

DNDC – Denitrification Decomposition model

EC – European Commission

EC-JRC – Joint Research Centre of the European Commission

EDP - Environmental Product Declarations

EU – European Union

FOOD SCP RP - European Food Sustainable Consumption and Production Round Table

FU – Functional Unit

GHG – Greenhouse Gases

HWSD – Harmonized World Soil Database

ISO – International Standard Organization

LCA – Life Cycle Assessment

LCI – Life Cycle Inventory

LCIA – Life Cycle Impact Assessment

LCT – Life Cycle Thinking

LUCAS – Land Use/Land Cover Area Frame Survey

OEF – Organization Environmental Footprint

P – Phosphorous

PaSIM – Pasture simulation model

PDF – Potential Disappeared Fraction

PEF – Product Environmental Footprint

PNV – Potential Natural Vegetation

PRE – Monthly Precipitation

RothC – Rothamsted Carbon Model

OC – Organic Carbon

SETAC – Society of Environmental Chemistry and Toxicology

SOC – Soil Organic Carbon

SOM – Soil Organic Matter

treg – Regeneration Time

UAA - Utilized Agricultural Area

UN – United Nations

UNEP – United Nations Environment Programme

1. Introduction

1.1 Overview

Sustainable food and animal feed production are major challenges posed to our societies. The United Nations (UN) estimate that world population will increase to 9.7 billion people in 2050 and to 11.2 billion people in 2100 (UN, 2015). With the expansion of world population, the demand for natural resources, including soil support, provision and regulation services, is also going to increase. By 2050 agricultural production must increase by 60 percent to satisfy the expected demand for food and feed (FAO, 2014). Pressures such as soil degradation, groundwater depletion and extreme weather events create a problem that needs to be solved by enabling sustainable production of food and feed and the control of drivers of environmental damage, such as greenhouse gases (GHG) emissions, while achieving the Millennium Development Goal of ending hunger (Godfray et al., 2010).

Incorrect and intensive agricultural practices originated environmental issues such as water depletion, soil erosion and degradation, pollution, climate change, biodiversity loss, among others (Kutsch et al., 2009). Agriculture (including crop and livestock production), forestry and associated land use (LU) transitions (e.g. from agricultural to forest) are responsible for GHG emissions - about 20-24% of the total worldwide emissions (FAO, 2014). Land management practices such as tillage, fertilization, residue management and manure application may have a strong effect on carbon stocks. It is important to promote good management strategies in order to prevent soil degradation and assist with mitigation and adaptation of climate change (Godfray et al., 2010). To understand how agricultural practices affect production and environmental variables, it is essential to know how to achieve greater yields without compromising the environment (Tilman et al., 2011).

Another common concern is the increase of competition between the food sector and the bioenergy sector (biofuels) due to the necessity of accommodating bioenergy crops on land that was or could potentially be used for food and feed production. This demand for bioenergy crops may lead to an increase of food prices (Popp et al., 2014). In addition, climate changes are likely to increase land degradation (WMO, 2005). It is then probable that the demand for food and feed, though increasing, will have to be met in an equal amount (or lower) of the land available nowadays (Godfray et al., 2010).

While these problems are becoming more widely recognized, experts, governments and the population in general are becoming more concerned. There is a change in habits and perceptions that influences consumer choices and is increasingly conducive to environmental protection (Sengstschmid et al., 2011). Agri-food products are no exception. With this increased interest for environmental protection, there is an effort to lead the world into a greener economy, defined by the United Nations Environment Programme (UNEP) as "one that results in improved human well-being and social equity, while significantly reducing environmental risks and ecological scarcities" (UNEP, 2010). Such effort established an opportunity of effective marketing, strategic planning, environmental performance and development improvement for products. Companies started to present their products as “environmentally friendly”. To regulate such initiatives and further take advantage of this opportunity, environmental labels and declarations were created. These labels aim to help consumers differentiate between green or non-green products in order to capture consumer interest, to improve the products and services and to boost profits and competitiveness (EC-JRC, 2011), while preventing abuses and establishing confidence in claims of environmental quality.

There are three major voluntary environmental labelling types according to International Standard Organization (ISO) 14020 (ISO 14020, 2000): Type I – is assessed by a third-party and based on different attributes; Type II – self-declaration based on one attribute; Type III – based on the life cycle of a product and verified by a third party. The latter are also known as Environmental Product Declarations (EDP’s) (ISO 14020, 2000). All of these labels involve the application of life cycle thinking (LCT) to products or services.

1.2 Life cycle thinking

LCT is a way to get better and more informed decisions for the incorporation of sustainability accounting of the environmental, social and economic impacts of a product or service over its entire life cycle. It is a step forward from approaches that are only concerned with resolving problems on one specific source of pollution within the product’s life cycle (i.e. discharge of a pollutant to a river) (UNEP, 2012) and is one of the main concepts supporting Life Cycle Assessment (LCA).

Governments, businesses and the population, by taking a life cycle perspective of a product or service, can lead the society towards a greener economy. LCT helps to understand the environmental performance of products throughout their life cycle (Mont et al., 2007). By doing so, decision-makers have a holistic picture of an entire product or service system. Consequently, the main objective of LCT and one of its main advantages is to avoid burden shifting (Hellweg and Milà i Canals, 2014). This means that there is a concern for minimising impacts in a specific place and impact category (e.g. climate change) without increasing those impacts elsewhere, or in another category (e.g. biodiversity) (EC, 2010). In environmental declarations, using LCT is crucial as a mechanism that prevents “green washing” or resource waste, as companies who focus on single stage evaluations may be misdirected by their own preconceptions about where the environmental hotspots lie within their value chain.

LCT has been used as an important element in different policy instruments such as for the Thematic Strategy on the Sustainable Use of Natural Resources, Waste Framework Directive, the EU Ecolabel Regulation, Environmental Technology Verification Scheme (ETV), ECOdesign Directive, EMAS III Regulation and on the ISO 14000 family. It has been used to assess policy options, but also to assess sustainable production and consumption (EC-JRC, 2011). More recently, ISO 14001 revised in 2015 that addresses Environmental Management Systems, added life cycle perspective to the current requirements, so that organizations extend their scope to each step of the life cycle design of products and their development (ISO 14001, 2015). Currently, the only officially standardized method that assesses a range of potential environmental performance and associated impacts of services and products is the ISO 14044 (Lehmann et al., 2015a), a standard that introduced LCT by using LCA as its basis.

1.3 Life Cycle Assessment

LCA is an environmental management technique widely used in many sectors to support decision-making (Roy et al., 2009; Ferrão, 2009). It is used to study a product system or service's environmental aspects and potential impacts starting from raw material acquisition then production, use and disposal. Later developments are allowing also the assessment of social and economic aspects (Hellweg and Milà i Canals, 2014; Guinée et al., 2011). It is a tool that has been proven effective for the identification and comparison of impacts generated by different product systems (Peano et al., 2012; Mungkung et al., 2006) and may be used for different ends such as product development and improvement, strategic planning, public policy-making, marketing and improvement of environmental performance (ISO 14040, 2006). The European Commission (EC) recognizes LCA as the best framework currently available to assess the environmental impacts of products (Commission of the European Communities, 2003). According with ISO 14040 (2006) the process of LCA has four major phases: goal and scope definition, life cycle inventory (LCI) analysis, life cycle impact assessment (LCIA) and interpretation as described in figure 1.

The **goal and scope definition** phase determines aspects such as the decision context, intended applications and approaches (e.g. LCIA methods to be applied), the product system boundaries, the environmental impacts to be assessed and the functional unit (FU) that provides a reference unit for comparison of alternative products or services.

In the **LCI** phase data is compiled and is usually the phase that requires more time to be completed. It is an iterative phase that allows the quantification of the system flows.

The **LCIA** phase results in the evaluation of the products LCI regarding different impact categories. As justified later, the present dissertation focuses in particular in this stage.

The **interpretation** phase integrates insights from all of the other stages, in order to report the results in the most informative way possible and assist decision-making. This phase addresses the uncertainty and accuracy of the results.

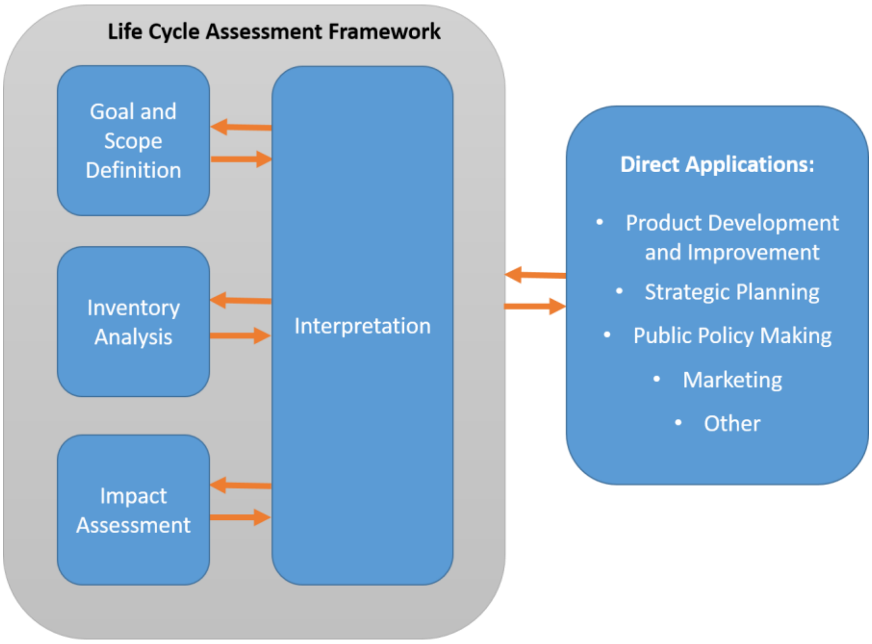


Figure 1- Stages of an LCA study (adapted from ISO 14040:2006).

1.3.1 LCIA phase

The ISO 14044:2006 divides the LCIA stage in four major phases:

- **Selection of impact categories, categories indicators and characterization models** - the impact categories are classes that represent environmental issues and are defined by their impact pathway and impact indicator. An example of an impact category is, according to IPCC (IPPC, 2007), global warming potential, where the indicator is kg CO_2eq. The LCI flows are assigned to the impact categories. The indicator results aggregated by impact category later enable the analysis of the environmental issues associated with the product system (ISO 14042:2006).
- **Characterisation** - where LCI results are converted to common units by applying characterization factors (CF) and are aggregated within the same impact category. These CFs express a change (positive or negative) of a property and are used to convert the life cycle results into a common unit. They reflect the contribution of each LCI flow in the impact category. The CFs are derived from characterization models used to assess environmental damages (e.g. the contribution of each GHG to climate change is determined using a characterization model).
- **Normalisation** – it is where the magnitude of impact indicator results in each impact category is calculated by dividing the indicator result by a reference value. This phase is usually optional.
- **Weighting** – it is the phase where the normalised results of each impact category are converted by applying a weighting factor based on value-choices. Like normalisation, this phase is usually optional.

Impact categories can report LCA results as endpoint or midpoint indicators. The impact categories addressed depend on the LCIA method chosen. There are several LCIA methods available, such as ReCiPe (Goedkoop et al., 2013), Eco Indicator 99 (Goedkoop et al., 2000), and ILCD (EC-JRC, 2011). Each method can differ widely, recommending different models for the assessment of similar impact categories (Roy et al., 2009).

Midpoint impact categories (problem-oriented approach) consider a point prior to the endpoint in the cause-effect chains correspondent to a particular impact category (Bare et al., 2000). Endpoint categories (damage-oriented approach) reflect causes of concern such as natural environment, human health or natural resources (ISO 14044, 2006). Endpoint indicators are calculated using midpoint indicator results (e.g. by characterizing the role of emissions with global warming potential, a midpoint impact category, on ecosystem quality, an endpoint). If the midpoint level is chosen, then the results of the calculations of the intermediary indicators will be more accurate, although their transition to endpoint indicators is more difficult since they involve more assumptions and value judgments. On the other hand, if the endpoint level is chosen, then the endpoint indicators will be easier to interpret, although they are harder to calculate and thereby are less accurate than the intermediary (midpoint) indicators (Ferrão, 2009).

Many different LCIA models have been proposed for the calculations of the same impact categories. Each methodology has different outputs and assesses different environmental indicators (Hellweg and Milà i Canals, 2014). The amount of methodologies available for seemingly the same environmental issue, and the divergence of their results, creates confusion among decision-makers who are hindered in their ability to make informed decisions due to the lack of comparability between products of the same category. The lack of consensus on guidance and methods leads to a divergence on results and recommendations (EC-JRC, 2011). Even within the same characterization model, it is often impossible to compare similar products due to the range of flexibility allowed in each methodology and thereby the results may vary (Lehmann et al., 2015a; Manfredi et al., 2012; Zamagni et al., 2008).

It is important to reach a consensus on how LCA can lend credibility to results and their communication, by producing accurate and comparable information and preventing the lack of transparency between real claims and marketing plots ("green washing") of those who try to adjust the system to their own benefit, making claims that are inaccurate or insignificant (UNOPS, 2009).

In the past two decades, policies and strategies have been made by governments to improve and to take into account sustainable development and the environmental performance of services and products. Not only for business to consumer communications, LCA is also used for private companies to gain competitive advantages, such as costs savings, product differentiation, increase efficiency of production and to improve organizational performance (Hoffman et al., 2014; Hellweg and Milà i Canals, 2014).

The European Union (EU) created the Product Environmental Footprint (PEF) and the Organization Environmental Footprint (OEF) in order to harmonize and establish a common methodology applicable worldwide. The PEF and OEF are LCA-based guidelines used to evaluate the environmental performance of products and organisations, respectively. Together, they provide LCA practitioners with a tool that also helps on communicate the results to consumers and to business partners. They were created with the objective of improving how LCA declarations can be verified in the most efficient and effective way, to provide users a cheaper and easier tool to measure environmental performance and to produce and disseminate data for making environmental footprints available for free. They have as long term goals the possibility of comparing similar products based on their environmental performance throughout their value chain, to improve their access to green markets and to enable benchmarking for companies (Manfredi et al., 2012). PEF and OEF methods cover 14 impact categories, one of which is LU. PEF is now the reference method for LCA studies that applies to EU Eco-Labels within the EU (EC, 2013).

There are many improvements still necessary on PEF and OEF. For instance, methods regarding water consumption, LU, and abiotic resource are not considered adequate neither satisfactory (Lehmann et al., 2015a; EC-JRC, 2011). The EC encourages the test of alternative methods for these aspects in order to have more accurate assessments. These methods have a great importance in order to provide a successful application of LCA in food and feed production. Also, due to the great importance on the improvement of knowledge in this matter, the second pilot of PEF and OEF focuses on several sub-sectors of food and feed production (Lehmann et al., 2015b).

1.3.2 Life Cycle Stages of Food and Feed

Food and feed products life cycle chain may be divided in 5 major stages as described in the figure 2 (Sengstschmid et al., 2011):

Figure 2- Life cycle stages of food and feed products.

When assessing life cycle of food products, the agricultural stage usually has higher impacts than transportation and processing unless large transportation distances are involved and/or in the case of highly processed products (e.g. cheese) (Mogensen et al., 2009).

Even though food packaging is perceived as a significant stage of the life cycle of food products, and indeed it should be addressed, it often does not have significant environmental impacts (Sengstschmid et al., 2011). Also conservation methods and consumption patterns do not have a significant weight when compared with the overall of the environmental impacts (Jungbluth et al., 2000) except in the case of highly processed foods.

Agriculture is responsible for over 90% of eutrophication impacts and for 50% of GHG emissions of most food products (Sengstschmid et al., 2011). For products such as meat and dairy, the agricultural stage is responsible for significantly larger impacts the other stages of the food and feed value chain. Thereby, all other life cycle stages assessment are less significant

(Sengstschmid et al., 2011). This is due to the ratio of feed and meat production, i.e. 75-90% of the energy consumed by animals goes to body maintenance, manure and other products (e.g. skin and bones) whereas only the remaining energy is converted from feed to meat.

Land is a finite resource and the importance of LU is justified by the role of the agricultural stage of agri-food products being the main life cycle environmental hotspot (UNEP, 2012; Hörtenhuber et al., 2014). The higher need for feed/livestock brings pressure to LU that could be also used for food production (Röös et al., 2013). The availability of arable land per capita is declining (Bruinsma, 2009). While farmers need land for agriculture, they also need to maximize their profits and so they need to have the highest productivity possible. The quality of land is then a key factor for farm productivity. We can then conclude that LU impacts play a major role on assessing agriculture impacts. (Paloviita et al., 2015).

1.4 Land use and land cover

LU is defined as the way that a particular land is utilized, i.e. the arrangements, activities and inputs that humans undertake (e.g. forestry, agriculture, pasture, urban). A similar and often mistakenly considered as equal concept is land cover. Land cover refers to the biophysical characteristics of the earth's land (e.g. forest, cropland, grassland, mine). Nevertheless, the two concepts are related. LU is a function of land cover, and land use changes (LUC) may also affect land cover (FAO/UNEP, 1999). Changes in management and tillage practices and manure inputs are not considered LU or cover changes (Food SCP RT, 2013). In practice, there is an ambiguity between these definitions and it is common to encounter different perceptions of LU and land cover. Due to this inconsistency, in this dissertation we are will use either term "land use" or "land cover" as meaning both land utilization and its respective biophysical characteristics (i.e. a combination of both designations).

The Millennium Ecosystem Assessment (MEA, 2005) identified LU and LUC as one of the main direct drivers of biodiversity loss. LU influences biodiversity as well as the structure and functions of ecosystems (e.g. biomass production or water filtration) (Koellner et al., 2013b) and can cause damages to the areas of protection, i.e. areas that present value to human society (humans, biotic, abiotic and built environment) (Jolliet et al., 2004). LU changes also cause variations on carbon stocks, e.g., in a LU change from forest to agriculture, carbon stocks will vary due to microbial decomposition or aboveground biomass removal (IPCC, 2000). Soil carbon sequestration that is highly dependent of land management changes and LU changes is considered an important climate change mitigation option (Goglio et al., 2015).

In the past 40 to 50 years, agricultural land has expanded to regions that were previously forested and urbanized. Infrastructure expanded to areas previously occupied by agriculture (Holmgren, 2006). The higher demand for land for agricultural purposes or its allocation for the production of bio-fuels brings consequences such as deforestation and biodiversity loss (UNEP, 2012) While the use of mineral fertilizers and pesticides in conventional agriculture has deep effects on the environment, in comparison with organic agriculture, conventional agriculture needs less arable land (Roy et al., 2009). Land occupation is thusly one of the main variables required to understand the consequences of agricultural systems and practices.

LU and LUC are considered main contributors to GHG emissions and, as mentioned previously, there is an increasing pressure and competition on land due to the increase of the needs for food, feed and biofuels (Popp et al., 2014). When assessing LU impacts, soil represents an essential role by providing a range of ecosystem services (Antón et al., 2014).

1.5 Land use influence on soil properties

While assessing LU impacts, it is common to consider soil quality and respective properties (Garrigues et al., 2012). Soil physical and chemical properties such as texture, soil organic carbon (SOC), N content, clay fraction will influence soil quality. Soil quality is often defined as the capacity of soil to function, i.e. to provide soil ecological services but is also defined as the capacity to provide and sustain uses such as agriculture and habitation (Garrigues et al., 2012).

Soil is an essential non-renewable resource and its degradation is a global problem. Soil provides functions of recycling and storage of nutrients and organic waste, water flow control, protective action of groundwater quality and habitat for soil fauna amongst others (Andrews et al., 2004). Soil also has a major importance on the mitigation of climate change through the sequestration of carbon in soils from the atmosphere and thereby influencing overall GHG emissions (Goglio et al., 2015).

While agricultural activities have intensified, soil degradation, nutrient pollution, biodiversity loss and GHG emissions associated with LUC have also increased (UNEP, 2012). To assess soil quality on agricultural systems, specific land use and climate characteristics (e.g. temperature, precipitation) are necessary as well as management practices and goals (Andrews et al., 2004). An accurate characterization model assessing the role of LU must consider these factors.

1.6. Soil organic carbon and the soil carbon cycle

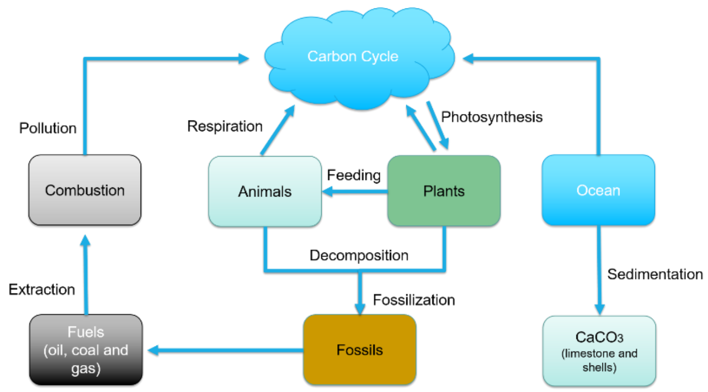


Figure 3- Carbon cycle simplified diagram.

Soil is not only a finite resource but also a shrinking one. Soil-stabilized carbon is an essential element to improve soil quality (Manna et al., 2016). A quarter of Earth's land suffered degradation due to soil carbon loss (Milne et al., 2014). Soil contains approximately 2 344 Gt of organic carbon globally (Stockmann et al., 2013), and are the largest global carbon terrestrial reservoir on Earth, second only to the oceans as the largest overall carbon pool (Ogle and Paustian, 2005). For this reasons, soil carbon sequestration has a major role to play within the carbon cycle, particularly in its uptake and release to the atmosphere. SOC is the carbon content of soil organic matter (SOM) (about 50 to 60% of SOM) (Kutsh et al., 2009). SOC has different benefits such as helping to create greater soil permeability, aeration, drainage and protection against erosion, providing substrate and energy to support microbial activity and providing a reservoir of organic N, P and other nutrients (Kutsh et al., 2009).

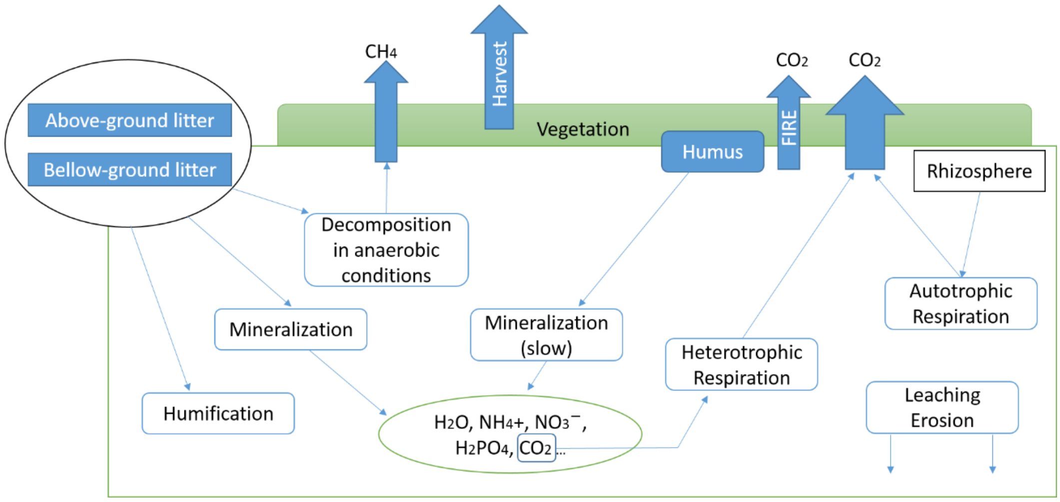


Figure 4- Soil carbon cycle simplified diagram, adapted from Kutsch et al. (2009).

Decomposition and mineralization processes of SOM play an important role on the losses of carbon from soil. Soil microorganisms, bacteria and fungus are responsible for carbon decay and therefore activity of soil organisms is crucial for soil dynamics. SOC is dependent on the microbial population of soil and on the properties of plants and vegetation and on the nutrients soil composition. Leaching processes are also important for the soil carbon balance, due to the loss of carbon via dissolved inorganic carbon (DIC) and dissolved organic carbon (DOC) (Chapin et al., 2006). Figure 3 and Figure 4 shows the mainly trades and processes of carbon between the atmosphere and soil.

SOC may be divided into different pools, based on SOC properties (composition, physico-chemical properties, rate of decomposition). Three pools are frequently considered based on decomposition rate: labile pool, slow pool and inert pool. The labile pool is composed by fresh plants residues, animal residues and micro-organisms. Mostly humus and resistant plant materials compose the slow pool. The inert pool is composed by the resistant components i.e. products at their last stage of decomposition, e.g. charcoal (Chan, 2008).

LU management has a large impact on SOC stocks and can cause CO_2 emissions or sequestration (Milne et al., 2014). Guo et al. (2002) estimated variations of soil carbon according to specific LU changes where the highest variations were from native forest to crop (loss of 42% soil carbon), from pasture to crop (loss of 59% soil carbon) and from crop to secondary forest (an increase of 53% of soil carbon). SOC is considered a proxy for soil quality due to its influence in many soil parameters and dynamics making it an important indicator for LCA of LU (Ogle et al., 2012). This indicator can be extended to other endpoint categories according to the impact pathways linked to LU proposed by Koellner et al. (2013a). Due to the goals of this dissertation on the study of different LU, management practices, and human occupation that can result in variations of soil quality and carbon stocks and due to magnitude of influence of SOC on soils, we chose it as a midpoint indicator for the assessment of LU impacts.

1.7 Land use and soil carbon in LCA

In the past years, there has been an effort to study LU impacts and soil dynamics and integrate them in LCA making credible frameworks for LU aspects, but most fail to provide a global consensus (Vidal-Legaz et al., 2016). The frameworks for accounting LU impacts on LCA are still attached to too many uncertainties due to the simplifications and assumptions made (Hörtenhuber et al., 2014).

1.7.1 Proxy Based Method – Land use model

Under the UNEP-SETAC Life Cycle Initiative, Milà i Canals et al. (2007) proposed a framework to account for LU interventions (occupation and transformation) and made an attempt to select environmental midpoint indicators and damage categories. It is the framework that carries more consensus of experts and is also the framework recommended by the Joint Research Centre of the EC (EC-JRC, 2011). Although it is the framework recommended, it is considered a framework with a limited scope and was only recommended to be used carefully. Further work within UNEP-SETAC, was developed by Koellner et al. (2013a) that provided an improved approach and addressed some limitations of the framework proposed by Milà i Canals et al. (2007), giving a larger importance to the bio-geographical differentiation of land-use impacts and proposing a cause-effect chain pathway linking LU with impact categories.

This framework considers two LU interventions (i.e. two types of LU flows): land transformation and land occupation. Land transformation is a process of changing land characteristics (cover and/or use) for a new intended LU and land occupation refers to a specific use of land maintaining its characteristics constant along the time (Milà i Canals et al., 2007). Transformation is measured in surface units (ha of land into new land) and occupation is measured in surface-time units (e.g. ha yr). For occupation, time and area are interchangeable (e.g. occupying 1 ha of land for 2 years is the same as occupying 2 ha for 1 year). These interventions will have an impact on land quality that can be measured using different indicators. After a land transformation, if there is no occupation process, the ecosystem will change gradually to its initial quality, even though the original ecosystem quality might not be reached (Koellner et al., 2013a). The LU impact is then the sum of land transformation impacts, land occupation impact and permanent impacts.

Brandão and Milà i Canals (2013) proposed a methodology for the calculation of transformation and occupation characterization factors, depicted in Figure 4, in order to reflect the impacts of these transformations in different LUs. The CFs calculated according to this model express SOC depletion. SOC loss is depicted by a positive CF and SOC gain is translated by a negative CF. This means that the indicator calculated by the indicator is “SOC depletion” (Brandão and Milà i Canals, 2013).

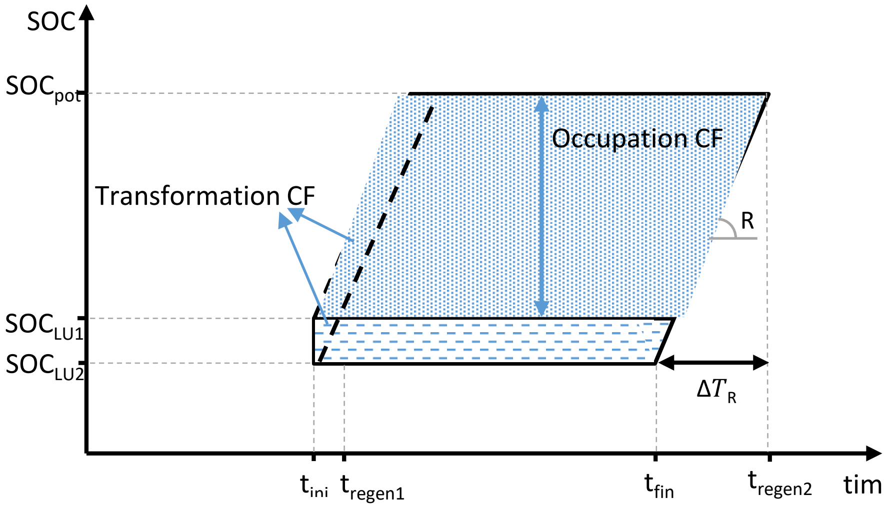


Figure 5- Depiction of the calculation of transformation and occupation characterization factors, based on Brandão and Milà i Canals (2013) - image adapted from Morais (2015).

CF – characterization factor; SOC_{LU1} - SOC content before transformation; SOC_{LU2} - SOC content in subsequent land use; R - regeneration rate; T_R- regeneration time; SOC_{pot} – potential SOC content in potential natural vegetation; SOC_{LU2} – SOC value after transformation or occupation; t_{ini} – instant when transformation and occupation occur; t_{regen1} – instant when SOC reverted to the previous land use; t_{regen2}- instant when SOC reverted to potential land use; t_{fin} – instant when occupation ends

The equation used to calculate transformation CFs (*CFtransf*) is described by equation (1)

$$CFtransf\ [kgC.year.m^{-2}] = (SOC_{pot} - SOC_{LU1}) \times (t_{regen1} - t_{ini}) + \frac{1}{2}(SOC_{LU1} - SOC_{LU2}) \times (t_{regen1} - t_{ini)} \quad (1)$$

where SOC_{pot} is the potential value of SOC that a land can have if undisturbed, SOC_{LU1} is the SOC value of a land before a transformation/occupation, SOC_{LU2} is the SOC value of a land after transformation/occupation, t_{ini} is the instant when transformation (which is assumed to have instant effects) and occupation happen, t_{regen1} is the instant where SOC reaches the value prior to transformation.

The occupation CF (*CFoccup*) is given by

$$CFoccup[kgC.year.m^{-2}year^{-1}] = SOC_{pot} - SOC_{LU2} \quad (2)$$

where t_{fin} is the instant when occupation intervention ends.

This framework raises many issues such as assuming that land transformation is instantaneous and land occupation is constant over time. Additionally, LU changes are calculated in relation to a baseline – reference situation. Different reference situations have been studied: the historic natural land state was used by Bentrup et al. (2002), Potential Natural Vegetation (PNV) by Saad et al. (2011), Koellner et al. (2013a), Alvarenga et al. (2015) and Morais (2015). Addressing the reference situation using a static PNV is a common approach but is also a problem because this approach does not reflect the ecosystems dynamics and natural evolution (Soimakallio et al., 2015).

Temporality aspects are another challenge on the evaluation of land changes. As reported by Othoniel et al. (2016), scenario-based modelling should be used to address this issue. Assuming a constant provision of LU over time is not accurate. For agriculture for example, due to the seasons of cultivation for each type of food, it is important to consider time aspects regarding cultivation, management practices and climate conditions that are not addressed in the current frameworks. Also, assuming a specific relaxation time, that is determined by expert knowledge, and that depends on the former type of occupation, the type of expected natural land cover and the biogeographical conditions (Milà i Canals et al., 2007) introduces high uncertainty. Wiedema and Liendeijer (2001) have already proposed a list of estimates of relaxation times for LU, but without considering regionalization. Constant relaxation times for each type of land cover or biome misses the dynamics of the ecosystems that are influenced by site-specific conditions, such as climate and soil properties - for example, a grassland in Portugal will have different impacts and relaxation times that the same grassland in Paraguay or Denmark.

Othoniel et al. (2016) highlights that the systems crawl back to a natural state under the influence of different pressures when the occupation states are abandoned. If we consider constant quality when calculating land occupation impacts, we are neglecting impacts such as climate change (independent from the system) or even the loss of a supporting function that was provided by the system and that was lost during the evaluation of the life cycle.

Transformation of land cover has another problem due to the double-counting of impacts. This happens due to the division of inventory flows into transformation “from” and transformation “to”. As discussed by Brander (2015), using natural regeneration as baseline (as suggested by Milà i Canals et al., 2007), if the land is maintained in agricultural use, the impact of foregone sequestration of carbon for example, is going to be present for each successive product-system utilising the land. So every time a new product-system is accounted, the foregone sequestration will be allocated. Unless this impact is distributed across all future production from the land, this problem will occur.

A final and important issue with this approach is that it is typically operationalized using data-intensive calculations. SOC maps are used to assign steady-state SOC levels to each land use/cover class in each region (e.g. climate or eco-regions). As a consequence, most LU LCIA models provide CFs for a very small number of land classes. For example, Morais et al. (2016b) provide CFs for LU in Europe using the LUCAS Topsoil database (Brogniez et al., 2015), which has approximately 20 000 observations. Nevertheless, they determined that if more than four land classes were used, the distinction between CFs for each class would not be statistically significant. In data-driven, proxy-based models the number of land classes seems to be limited. The most likely way of overcoming this limitation is by decreasing the need or direct observational data, using process-based models as a replacement.

1.7.2 Process-Based Modelling

Process-based models are used to assess a system, integrating many complex biogeochemical processes formulated on mathematical-ecological theory and taking into consideration climatic variations, agricultural management practices and soil conditions (Cuddington et al., 2013). They address different temporal and spatial scales.

In the “current modelling procedure”, such the one used by Brandão and Milà i Canals (2013), static natural reference situations are used for comparison. Transformation impacts are instantaneous and there is no variation on the degree of land occupation (Othoniel et al., 2016). The procedure is described on the left side of Figure 5, based on Othoniel et al. (2016).

The illustration on the right side of Figure 5 describes a “process-based method”, where there is no reference situation but an assessment based on real scenarios that characterize intra and inter-annual dynamics. These scenarios integrate site-dependent climatic and soil characteristics with seasons of cultivation and management practices for each type of product. This method requires more data than the proxy-based model (such as Milà i Canals et al., 2007; Koellner et al., 2013a) but carries higher level of detail and lower uncertainty allowing a more precise assessment (Othoniel et al., 2016). Also, process-based models are much more detailed when compared with proxy-based models (Filimonau et al., 2016). Models such as the ones described in the next section are very useful due to their capacity to simulate SOC turnover, according to specific site conditions and relate it to specific management practices (Monforti et al., 2015).

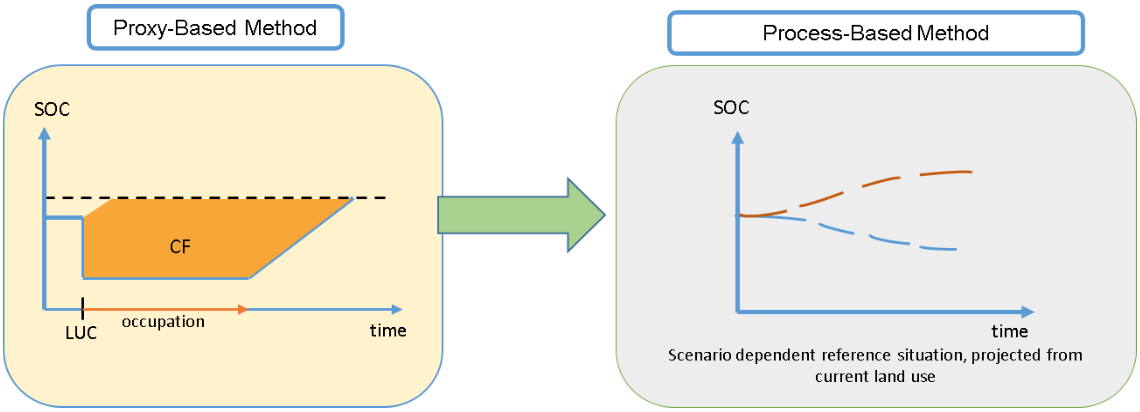


Figure 6- Illustration of the difference between proxy-based methods and process-based methods (adapted from Othoniel et al., 2016).

CF – characterization factor; LUC – land use change; SOC – soil organic carbon

1.7.3 Selection of impact pathway and indicator

The latest and more complete impact pathway for land-use impacts published is the one from Vidal-Legaz et al. (2016), depicted in Figure 6. It correlates soil properties and interventions with midpoint and endpoint indicators and categories, and also with areas of protection.

As explained previously, SOM is assumed to be the best single midpoint indicator to assess LU impacts by the ILCD Handbook (EC-JRC, 2011) and by the ENVIFOOD Protocol (Food SCP-RT 2013). Also, Brandão and Milà i Canals (2013) considered SOC as a stand-alone soil quality indicator. It is associated to the endpoint category of ecosystem services that was also proposed by Koellner et al. (2013a) as an endpoint category. SOC was thusly chosen as a midpoint indicator this dissertation. We measure the impact on land quality depending on the variation of SOC on soils across the simulations as a deficit of carbon where the FU is SOC depletion in tC/ha.

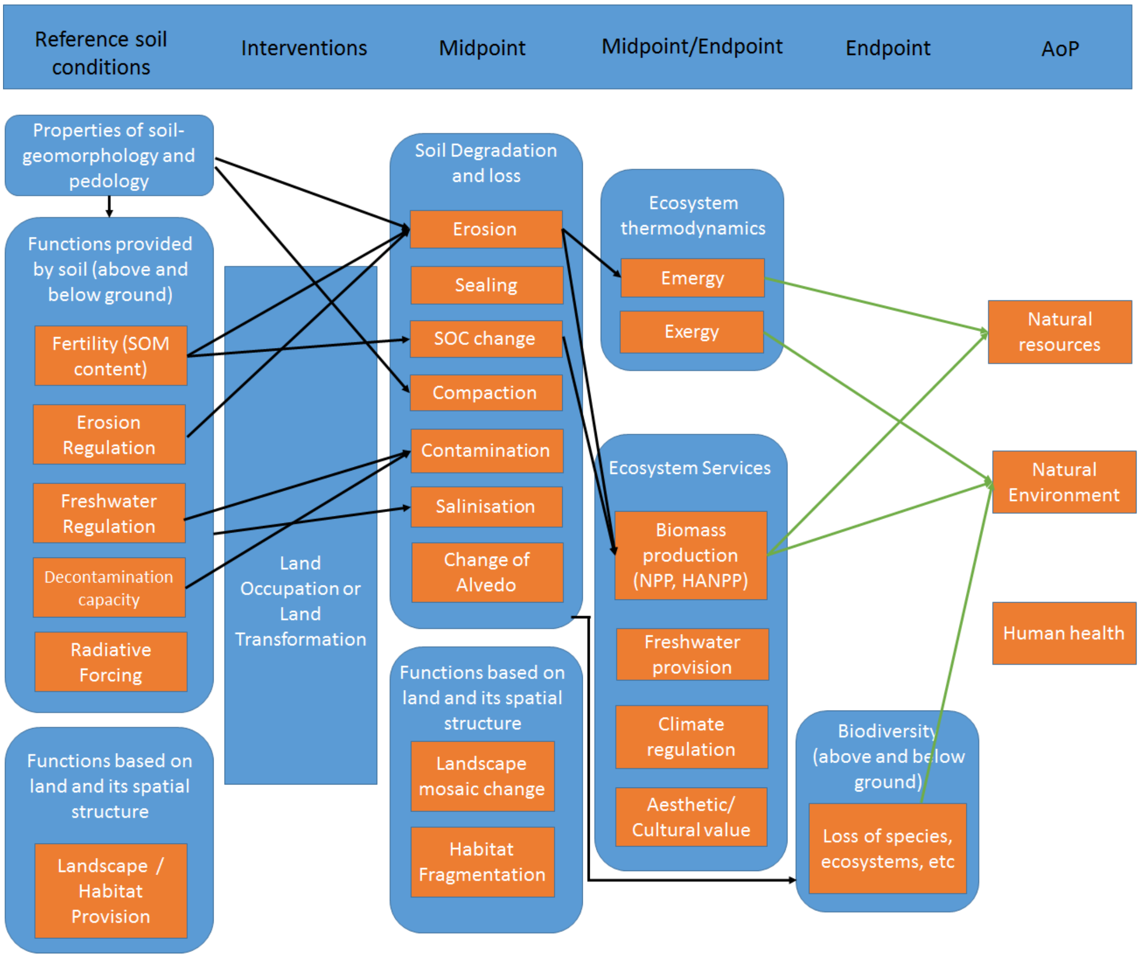


Figure 7- Impact pathway for land use, as presented by Vidal-Legaz et al. (2016).The arrows in black represent links to midpoint indicators while the green arrows represent links to endpoint indicators.

AoP – Areas of protection; NPP – net primary production; HANPP – human appropriation of NPP

2. Objectives of this dissertation

The main objective of this dissertation is to take a step forward from the frameworks that are currently being used, known as proxy-based modelling methods (Milà i Canals et al., 2007; Koellner et al., 2013a; Brandão and Milà i Canals, 2013) for the LCIA of LU. The goal is to test the potential LCIA applications of two process-based models, namely RothC and DNDC, which may enable an assessment based on scenarios to calculate more accurate CFs for soil quality. We apply this modelling process to obtain CFs for the LCIA midpoint LU category using SOC as an indicator, and obtaining regionalized CFs using a spatially explicit process-based model to simulate soil dynamics. A description of the main LCIA aspects covered by this dissertation is represented in Figure 8. One of the main limitations of typical LCIA models is the lack of regionalization, i.e. considering that the same type of LU may cause the same impacts at different locations of the globe (Jolliet et al., 2004). In this work, we calculate biogeographically differentiated CFs, as recommended by Koellner et al. (2013a).

The role of RothC and DNDC in this dissertation is to simulate the dynamics of SOC in soils using the region of Alentejo, Portugal, as a proof of concept. This application study aimed to determining the potential for global application of a similar procedure, identifying the main limitations of the approach and suggesting ways to move forward in that direction.

CFs are typically obtained using simpler mathematical procedures. The goals of this thesis are therefore exploratory. There is no prior experience with using scenario-based models that resulted in CF calculations (Vidal-Legaz et al., 2016). The approach in this thesis is a paradigm shift, where CFs are calculated based on scenarios. These scenarios will take into consideration expected future changes in temperature and precipitation under climate change. While proxy-based models are statistical and data-intensive, which limits the number of land classes evaluated, in our approach there is no such limitation, because each crop is analysed individually and are already calibrated in the case of DNDC model and can be calibrated indirectly using RothC.

We incorporate the site-dependency of the environmental impacts, accounting not only with the parameters of soil (for example pH, texture and bulk density for DNDC model) but also with the climatic parameters that have a major influence on all the dynamics of the soil. Instead of just modelling within a LU typology, we follow the example of Lugato et al. (2013) addressing the spatial location and its components by identifying unique homogenous territorial units overlaying climate data, with soil data and LU data.

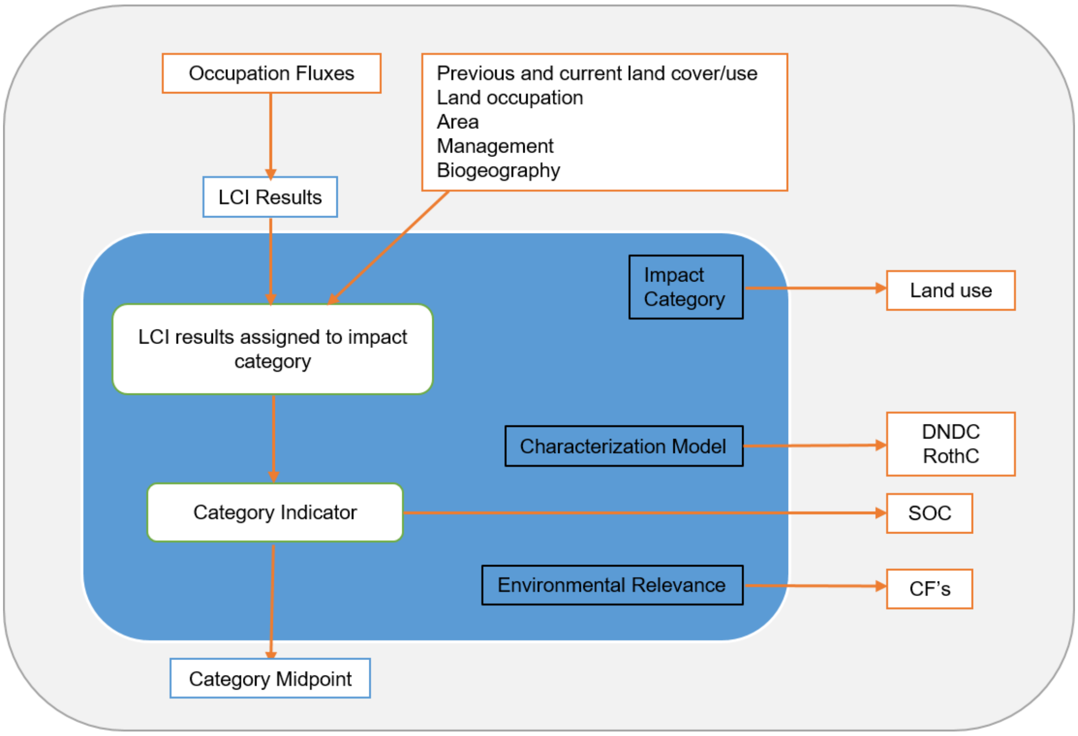


Figure 8- Main LCA Aspects covered in this dissertation (adapted from ISO 14042:2006). CF – characterization factor; SOC – soil organic carbon; LCI – life cycle inventory

The specific objectives of this dissertation are:

- To identify and select the most promising process-based models in order to estimate SOC depletion in LCIA;
- To model SOC dynamics as response to LU using the DNDC model and estimate SOC depletion;
- To model SOC dynamics using the RothC model and estimate SOC depletion;
- To determine the sensitivity of the RothC model to input parameters;
- To determine simple regression models that fit the results of RothC in order to simplify the calculation of CFs;
- To calculate CFs for the region of Alentejo and compare them to CFs obtained using proxy-based models.

This dissertation is divided in 5 main sections. Section 3 analyses different process-based models (their benefits and limitations) and selects the ones more appropriate to our objectives. Section 4 presents all datasets necessary to run the models. Sections 5 and 6 present the implementation of each model chosen. Section 7 analyses the sensibility of the models to their input parameters. This is followed by a complexity-reduction analysis in section 8 where results are approximated by simple equations. In the last section 9 CFs are calculated and compared with alternatives obtained from the literature. Since the results obtained for the CFs are in large tables, they are presented as supplementary material (duly cited in the text where relevant). This supplementary material is available at: https://fenix.tecnico.ulisboa.pt/homepage/ist172997/supplementary-materials.

3. Selection of models

3.1 Models available for the estimation of SOC dynamics

There are many different process-based models available for end-users. In order to choose which models to evaluate, we made a research and three main literature references (Ponce-Hernandez et al., 2004, Smith et al., 1997, Byrne et al., 2005) that evaluated different models. Byrne et al. (2005) evaluated DNDC (Denitrification Decomposition model), PaSim (Pasture simulation model), RothC and Century; Ponce-Hernandez et al. (2004) assessed Century and RothC; and Smith et al. (1997) evaluated RothC, Candy (Carbon and Nitrogen Dynamics), DNDC, Century, Daisy, NCSoil, SOMN, ITE and Verbene. After this analysis, we choose CENTURY, RothC, DNDC, Candy and PaSim that had a better overall evaluation on the articles, to research deeper.

RothC is a model of carbon turnover in non-waterlogged soils. It was developed to model the carbon turnover in arable soils, grassland and forest. It as in count the effects of temperature, moisture content and soil type. Nitrogen and carbon dynamics are not attached (Smith et al., 1997). The model uses a monthly step and is divided in five compartment systems: inert organic matter (IOM), easily decomposable plant material (DPM), resistant plant material (RPM), microbial biomass (BIO) and humified organic matter (HUM). IOM pool is resistant to decomposition and does not receive carbon inputs (Kutsch et al., 2009).

Each compartment, except IOM, decomposes according to a first-order process with specific parameters and a specific decomposition rate constant.

When an active compartment contains an amount of carbon (Y tC/ha), this amount will decompose in a particular month, where $Y\,(1-\ e^{-abckt})\ (tC/ha)$ is the loss of carbon in a monthly step, and where the parameters are defined as:

- a – rate modifying factor for temperature
- b – rate modifying factor for moisture
- c – soil cover rate modifying factor
- k – is the decomposition rate constant for the specific compartment
- t – is 1/12 due to k being an yearly decomposition rate

DNDC models the dynamics of carbon and nitrogen biogeochemistry in agricultural ecosystems and that operates at a daily step. It is composed by 6 sub-models: soil climate, crop growth, decomposition, nitrification, denitrification and fermentation. The first three sub-models are used to predict soil temperature, moisture, pH, redox potential and substrate concentration. With the outputs of the first three sub-models, the model runs the last three sub-models to predict carbon dioxide, methane, ammonia, nitric oxide, nitrous oxide and dinitrogen emissions. Crop residues (namely litter) are considered an essential input for SOM. There are three different soil litter pools in which the crop residues go depending on their C/N ratio: very labile litter pool, labile litter pool and resistant litter pool. SOM is divided in 4 different pools: plant residue, microbial biomass, active humus and passive humus. Soil decomposition rate is influenced by pool size, specific decomposition rate, soil clay content, N availability, soil temperature and soil moisture parameters. When SOC residing in a pool decomposes, a portion is lost as CO_2 while the rest is integrated into other SOC pools. Does not considers layers on the vertical horizon of soil. Water availability depends on parameter of precipitation, snowfall, drainage and actual pan evaporation. Nitrification and denitrification are influenced by the dynamics of soil Eh and substrates of DOC, NH_4^+, NO_3^-, NO, N_2O. DNDC can be run in two different modes: site or regional.

CENTURY 5 Agroecosystem is a model that is used to simulate carbon and nutrients (Nitrogen (N), Phosphorous (P) and Sulphur(S)) dynamics for different types of ecosystems (grassland, agricultural crop, forest and savanna). The model runs using a monthly time step and can simulate the dynamics of SOM for one year, centuries or even for thousands of years. The model is divided in 6 sub-models: SOM, nitrogen, phosphorus, sulphur, plant production and water budget, leaching and soil temperature sub-model.

The SOM sub-model includes three SOM pools (active, slow and passive). The active pool represents soil microbes and microbial products, the slow pool includes resistant plant material derived from the structural pool and soil-stabilized microbial products and the passive pool includes physically and chemically stabilized products. For plant residues and organic animal excreta there is a structural pool and a metabolic pool, where both are function of the lignin to N ratio in the residue. Each one of this pools have different turnover rates. SOM dynamics are only simulated in the first 20 cm of soil. The model also considers leaching of organic matter, aerobic and anaerobic conditions, soil texture and content. The flows of N, P, and S are calculated by multiplying the carbon flow rates by C:N, C:P, and C:S ratios of the state variables (Parton et al., 1988). For the organic matter decomposition, the model assumes factors of soil moisture, soil temperatures, clay content and N content. Management options such fertilizer addition, different types of harvest, effects of fire and grazing, senescence for crops, addition of organic matter, irrigation and erosion are available in the event commands of the model.

PaSim is a model based on the Hurley Pasture Model (Thornley, 1997) that simulates water, carbon and nitrogen cycles. The time step used is 1/50 of a day and several years may be simulate. Soil horizon is assumed homogeneous. It is divided in sub-models for plants, animals, microclimate, soil biology, soil physics and management. Photosynthetic carbon is divided into two departments (root and shoot) and can be lost due to ecosystem respiration, animal milking and enteric CH4 emissions. Aboveground biomass has three destinations: cutting, grazin or litter pool. N deposition, N fertilizer and symbiotic N2 fixation are the inputs considered by N cycle. At the animal module, it is possible to simulate classes of suckler cows, dairy cows and heifers, where temperature will affect forage digestibility and ingestibility. Agricultural management has options of tillage, irrigation and N fertilization. In recent improvements, this models enables the simulation of diet of animals and associated methane emissions. It enables the determination of optimal forage yield to feed animals at barn. The soil biology sub-model is derived from the CENTURY model (Lardy et al., 2012).

CANDY model simulates carbon and nitrogen dynamics in mineral soils, up to a depth of 2m. Its purpose is to model carbon stocks, organic matter turnover, nitrogen, leaching and water quality. It is divided in different modules: soil and temperature dynamics, soil water dynamics, soil structure dynamics, pedotransfer functions, biologic active time, SOM turnover, N dynamics and crop. Each simulation starts with a set of parameters of soil, agricultural management and weather. Soil and temperature dynamics module is responsible for the simulation of the variation of soil temperature, that will influence chemical and biological processes. Soil water dynamics module will simulate the amount of water available that will the influence plant growth, soil temperature, chemical transport and ground water recharge. Water percolation and interception, snow accumulation and melting, evaporation are all modelled. Soil dynamics module is responsible for the simulation of SOC content, where bulk density, soil loosening, re-compaction, cryoturbation and bioturbation are all modelled. Pedotransfer functions module is responsible for the estimation of properties of soil texture, bulk and particle density, pore volume, water parameters and retention. Biologic active time and SOM turnover modules will allow the simulation of SOM turnover due to biologic activities. N dynamics module allows the simulation of mineral nitrogen (nitrate or ammonium), where the organic pools are dependent on the carbon amount and C/N ratio. Crop module will enable the simulation of plant growth and crop development. CANDY also has a weather generator and an auto fertilizer scheme (Franko et al., 2015).

All of these models have been used in previous scientific works. Century, Daycent (daily-step version of CENTURY) and DNDC were used by Smith et al. (2012), to investigate SOC stock changes due to crop residues removal, concluding that the predictions resulting from the use of this models were within the range of uncertainty as estimates derived from field experiments. Lugato et al. (2010) successfully estimate C and N cycles at Beano site (Italy) with DNDC for different site specific parameters and management practices. Leip et al. (2008) used DNDC to estimate GHG fluxes and carbon stock changes for agricultural soils in Europe, for different management practices, linking it with CAPRI (Common Agricultural Policy Regional Impact Assessment) economic model for agriculture. Wattenbach et al. (2010) modelled winter wheat and maize on European croplands with 4 different models, recognizing DNDC being the one with more options of crops and management practices even though it lacks accuracy on simulating carbon fluxes. Smith et al. (1997) compared nine different models against twelve datasets with different LUs and management practices. The results showed that both RothC and DNDC had a low root mean square error. Francaviglia et al. (2012) used RothC successfully to estimate SOC stocks in Mediterranean systems for different management processes. Also for Mediterranean systems, Nieto et al. (2010) used RothC to predict SOC changes in the LU change from native vegetation to olive groves. Álvaro-Fuentes et al. (2012) simulate the dynamics of Spanish soils with CENTURY and RothC, for different tillage practices and different fertilization applications.

3.2 Selecting the model

The criteria for selecting the model in use were adapted from Ponce-Hernandez et al. (2004):

a) The required inputs needed to match with available data in databases;
b) The model should integrate site-specific parameters of soil, climate and land management;
c) The model should generate output variables needed and appropriated for the study.
d) The model should be able to simulate not only agricultural crops but also forest.
e) The model should be computationally doable, i.e. the simulations should require fewer time and the computer required should not be a supercomputer.

The objective of the application in this thesis is LCIA modelling. There are limitations and particular features required by LCA, namely the types of inventory flows commonly available to use as source data and the need for simplicity and global coverage. Inventories typically provide only area occupied and/or transformed by major land classes (e.g. agriculture, forest) with no additional qualification. Additionally, the fact that LCA focuses on products that very often are the result of global production chains means that models must be run effectively to obtain approximated results for the entire planet rather than site-specific, detailed results. This means that we added two additional criteria:

f) The model should require only information available in LCIs;
g) The model should be applicable, in simplified/approximated form, to entire regions and not particular case studies.

Table 1 - Summary of the characteristics of the different models (RothC, DNDC, Century, PaSim and Candy).

	RothC	DNDC	Century 5	PaSim	Candy
Inputs availability	Available.	Yes, although difficult to find regionalized data.	Yes, although difficult to find regionalized data.	No, difficult to find available data.	No, difficult to find available data.
Soil, climate and land management parameters	Yes.	Yes.	Yes.	Yes	Yes.
Appropriated outputs.	Simulates SOC dynamics.	Simulates SOC dynamics.	Simulates SOC dynamics.	Simulates SOC dynamics.	Simulates SOM dynamics.
Simulation crops (agricultural and forest)	Yes.	Yes.	Yes.	Yes.	Yes.
Computational efficiency (simulation running time)	Efficient with the modified version in Matlab.	Not efficient.	Not efficient.	Not efficient.	Not efficient.
Allows simulations for multiple regions	No, only with a modified version.	Yes	Yes	Yes	Yes
Support and guidance	Yes.	Yes.	Incomplete guide to use the model.	Yes.	Yes.

According with these criteria and our research, RothC and DNDC were the models recognized to perform better. They were chosen due to the few requirements of inputs and easiness of application against models such CENTURY that are an ecosystem model and more complex and difficult to execute. Also the successful applications in similar studies and their ability to perform simulations for different locations (each location with different characteristics) simultaneously were an important factor. Another critical factor for not choosing CENTURY, despite its successful application in other studies, was the lack of support and guidance to use it. Guidelines for the model are available on the website, but instructions, for example on how to construct the input files, are unavailable yet. Even though RothC has not been parameterized for forests, this model has been successfully used to simulate these systems (Palosuo et al., 2012).

In our analysis we recognized then that these models had different degrees of complexity and number of inputs required. We choose RothC and DNDC also to establish a frontier, represented at Figure 9, of what is viable or not in LCA. Models such as CENTURY or PaSim are too complex for LCIA at the moment, so the question is whether a manageably complex model such as DNDC would perform better than a less complex model such as RothC, or if for LCA purposes RothC is the right balance between complexity and information required for the simulations.

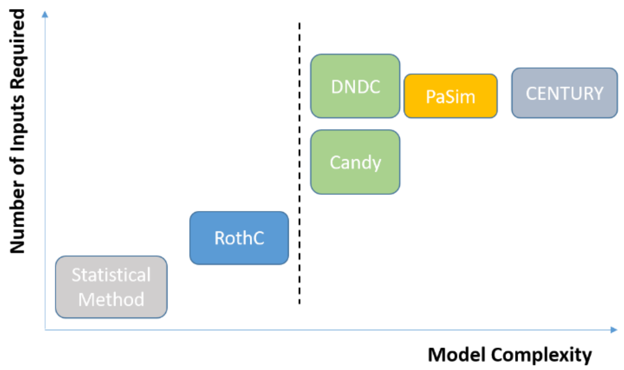


Figure 9- Illustrative graph of number of inputs required and model complexity of the models in study: statistical method (proxy-based method), RothC, DNDC, Candy, PaSim and Century. The dotted line shows a tentative frontier of complexity for application to LCA.

4. Datasets

4.1 Study Region – Alentejo

The region in study is the NUTS II region of Alentejo located at the center-south of Portugal. It comprises the districts of Portalegre, Évora, Beja, half of the south part of Setúbal and part of Santarém. It has approximately 760 thousand inhabitants (2011 Census) and an area of approximately 31 600 km^2.

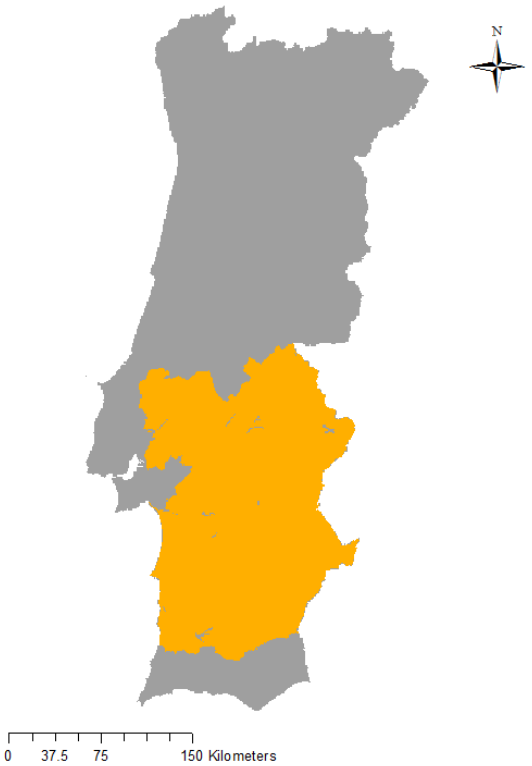


Figure 10- Portugal map with Alentejo's region depicted in yellow.

Alentejo has a Mediterranean climate, with a dry and hot summer and precipitation scarcity, and a cold winter, with some excess precipitation. It is the region in Portugal with the lowest ratio between precipitation and potential evaporation (0.7 ratio) (CEDRU, 1996). The Alentejo landscape is characterized by "montado" that may be defined as areas covered by multifunctional holm and cork forests where crop and livestock production may be present (Pimenta et al., 2014). Alentejo's utilized agricultural area (UAA) represents 53% of the total UAA in Portugal even though the largest number of agricultural farms is in the North and Center regions of Portugal (INE, 2013).

Table 2- Identification of the major agricultural crops in the Alentejo region and total production (ton) and farm area (ha) in Portugal and Alentejo.

Crops (2015)	Production Portugal (ton)	Total Area per crop Portugal (ha)	Production Alentejo (ton)	Total Area per crop Alentejo (ha)	Weight of Alentejo Crops in Portugal (%)
Grapes	934,633	178,957	242,265	32,764	18
Maize (grain)	808,995	88,547	435,305	32,234	36
Forage Maize	3 152,230	80,781	234,008	4,287	5
Tomato	1 832,467	19,360	1 511,871	15,931	82
Potato	444,166	20,267	69,199	2,450	12
Rice	184,918	29,142	118,599	17,667	61
Barley	44,402	21,170	41,477	19,477	92
Wheat	80,393	39,736	67,841	30,807	78
Oats	48,402	40,415	53,515	32,169	80
Forage Oat	1 976,056	130,559	1 364,619	81,991	63
Olive	722,893	351,340	51,810	179,387	51

According to the data provided by Instituto Nacional de Estatística (INE) (available at https://www.ine.pt/xportal/xmain?xpid=INE&xpgid=ine_base_dados), barley is the most produced crop in Alentejo (92% of all Portuguese production), as well as tomato (82%), oats (80%) and wheat (78%), as shown in Table 2. Table 3 compares the area of forest in Portugal and Alentejo. These values confirm the importance and weight of Alentejo's agriculture and forest in Portugal and were also obtained at INE portal.

Table 3- Identification of forest area in Portugal and Alentejo and respective weight percentage of Alentejo forest area comparing with total Portuguese forest area.

	Portugal Continental (kha)	Alentejo (kha)	Proportion of Portuguese forest in Alentejo (%)
Stone Pine	170	114	67
Pine	621	48	7
Cork	717	622	86
Eucalyptus	749	194	26
Oaks	64	4	6
Holmoak	325	299	91

Land degradation is recognized as one of the major issue in Mediterranean soils. Misuse of water resources and pollution, climatic variations and human exploitation and impact are one of the main causes for this degradation in this area (Geeson et al., 2002). Mediterranean countries are characterized by having the lowest SOC values in Europe (Brogniez et al., 2015). In the specific case of Alentejo, according to the LUCAS Topsoil Database (Brogniez et al., 2015) the values of SOC in the first 20 cm soil layer vary from 23 tC/ha to 224 tC/ha.

4.2 Crop Parameters – GPP

Information about management practices of each crop system simulated with data taken from GPP (2001). These data are described at Table 4 and involves practices of irrigation, flooding, tillage, pruning and planting and harvest dates. GPP (2001) crop fact sheets are the most complete data sets available, including more details about each crop system for the region of Alentejo. However, due to their key importance, application of manure and fertilizers were updated using Morais et al. (2016a).

Table 4 - Crop parameters - adapted from GPP (2001).

Crop	Irrigation System	Planting Date	Harvest Date	Tillage Date	Pruning	Irrigation Date	Flooding Date	Irrigation (mm/m^2 year)
Oats	Rainfed	October	July	October				
Olive	Rainfed		December	March	March			
Olive	Irrigated		January	March	March		July to September	18
Grape	Rainfed		September	February & June	November			
Orange	Irrigated		May		June	May to September		35
Peach	Irrigated		July	April	January	May to August		40
Maize	Irrigated	May	October				July	24
Forage Maize	Irrigated	May	November				July	24
Tomato	Irrigated	April	September	March		June to September		48
Potato	Irrigated	May	September			June to September		30
Rice	Irrigated	April	September	March & April				150
Barley	Rainfed	October	July	April & October				
Wheat	Rainfed	November	July	April				

4.3 Input Data Comparison – RothC and DNDC

Table 5 presents a comparison and summary of RothC and DNDC inputs required for the simulations. The inputs needed for these models are divided in different categories: soil, fertilization and manure, management, crop, climate and others. As we can see, DNDC models needs a total of 41 different inputs, against RothC that only needs 12 different inputs.

Table 5- Input comparison between DNDC and RothC.

DNDC		**RothC**	
Soil Parameters	Units	**Soil Parameters**	Units
N concentration in precipitation	ppm	-	
Maximum and minimum SOC content	kgC/kg	SOC initial content	tC/ha
Maximum and minimum soil clay fraction	%	Clay content of the soil	%
Maximum and minimum soil pH			
Maximum and minimum soil bulk density	g/cm3		
Slope			
Soil Salinity index	0 - 100		
Fertilization		**Fertilization**	
Fertilizer Application Rate	kgN/ha		
Flooding		**Flooding**	
Start and end date			
Flooding method for each event			
Irrigation		**Irrigation**	
Irrigated percent for each upland crop			-
Manure		Manure	
Manure Application rate	kgN/ha	Monthly input of farmyard manure	tC/ha
Management		**Management**	
Planting and Harvest Dates			
Percent of Above-Ground crop residue		Monthly input of plant residues	tC/ha
Tilling date and method			
Crop Parameters		**Crop Parameters**	
Maximum yield	kgC/ha		
Accumulative temperature	ºC		
Water requirement	kg water/kg		
Climate		**Climate**	
Daily Maximum and minimum air temperature	ºC	Average monthly mean air temperature	ºC
Daily Precipitation	cm	Monthly rainfall	mm
		Monthly open pan evaporation	

DNDC		RothC	
Other Soil Texture Parameters		**Other Soil Texture Parameters**	
Porosity			
Soil saturation conductivity	m/hr		
Field Capacity			
Wilting Point			
Other Crop Parameters		**Other Crop Parameters**	
		Depth of soil layer sampled	cm
		Soil cover (0 or 1)	
Maximum total crop biomass at maturity	kgC/ha		
Grain fraction of total biomass			
Leaves+stems fraction of total biomass			
Root fraction of total biomass			
C/N ratio for total plant			
C/N ratio for grain			
C/N ratio for roots			
C/N ratio for leaves+stems			
Water requirement			
Maximum leaf area index			
Maximum plant height	m/hr		
Accumulative air temperature			
N fixation index			
Optimum Temperature	ºC		

4.4 Common Input Data for DNDC and RothC models

4.4.1 Soil Data - LUCAS Database

Soil datasets were obtained from the LUCAS Topsoil (20 cm) Database (Toth et al., 2013). A topsoil survey was conducted at the intersections of 2 x 2 km^2grid, except areas above 1000 m altitude, covering the EU (except Romania and Bulgaria) with 20 000 sampling sites. Soil coarse fragments layer and texture layers (clay, silt and sand) were mapped with a 500m grid cell resolution applying the Multivariate Adaptive Regression Spline model and texture is expressed as the relative percentage of sand (> 5×10^{-2} mm), silt ($2 \times 10^{-3} - 5 \times 10^{-2}$ mm) and clay (< 2×10^{-3} mm). Bulk density values were derived from packing density and clay content, following the equation of Jones et al. (2003) (EC-JRC, 2013).
SOC values for topsoil (0-20 cm) were obtained through a map created according to LUCAS-topsoil carbon data (Brogniez et al., 2015).

4.4.2 Soil Data – HWSD

Soil datasets obtained from LUCAS topsoil database were lacking pH values. These values were obtained with the Harmonized World Soil Database (HWSD) (FAO et al., 2012). The data layers have a 30 arc-second resolution, with 15773 different soil mapping units. This database is a combination of existing regional and national updates of information worldwide. For the purpose of this thesis, we only used the parameters related to Alentejo pH and texture.

Reliability of the information presented in this database is variable: the parts of the database that still make use of the Soil Map of the World such as North America, Australia, West Africa (excluding Senegal and Gambia) and South Asia are considered less reliable, while most of the areas covered by SOTER databases are considered to have the highest reliability (Southern and Eastern Africa, Latin America and the Caribbean, Central and Eastern Europe) (FAO et al., 2012). The properties considered are for the top-soil layer (0–30 cm).

4.4.3 Land Cover Data – Corine Land Cover

Datasets regarding land cover were taken from the CORINE land cover – 2006 (CLC, 2006) obtained at European Environmental Agency (available at http://www.eea.europa.eu/data-and-maps/data/corine-land-cover-2006-raster). This dataset provides the physical characteristics of Europe's surface (Büttner et al., 2011) and is one of the most complete datasets available (Lugato et al., 2014). The dataset used has 100 m resolution. CLC was used instead of Use and Land Occupation Charter of Portugal (COS) due to the availability of level 3 data map. COS is publicly available until level 2 only.

CLC divides the characterization of land cover in 3 different levels of detail, all with different classes. Level 3 of CLC is the most detailed available. For the objectives of this dissertation we aggregated some of the different classes, finishing with a total of 13 classes described at Table 6, allowing a simpler analysis of the results. Note that it would be possible to include all CLC level 3 classes. That is precisely the advantage of this approach – all classes may be simulated as long as input parameters are available. There is no statistical limitation due to reliance on large SOC databases, as in proxy-based models. Since, however, the goal of the thesis is to demonstrate the potential of the approach, we opted to aggregate some classes.

Table 6- Corine land cover classes and aggregation of classes obtained for this dissertation.

CLC level 3	**Agreggated classes (this dissertation)**
Continuous urban fabric	Artificial Surfaces
Discontinuous urban fabric	
Industrial or commercial units	
Road and rail networks and associated land	
Port areas	
Airports	
Mineral extraction sites	
Dump sites	
Construction sites	
Green urban areas	
Sport and leisure facilities	

CLC level 3	Agreggated classes (this dissertation)
Permanently irrigated land	Permanently irrigated land
Rice fields	Rice fields
Vineyards	Vineyards
Fruit trees and berry plantations	Fruit trees and berry plantations
Olive groves	Olive groves
Annual crops associated with permanent	Non-Irrigated Arable Land
Complex cultivation patterns	
Land principally occupied by agriculture, with	
Non-irrigated arable land	
Agro-forestry areas	Agro-forestry areas
Broad-leaved forest	Broad-leaved forest
Coniferous forest	Coniferous forest
Mixed forest	Mixed forest
Natural grasslands	Pasture
Moors and heathland	
Sclerophyllous vegetation	
Pasture	
Transitional woodland-shrub	Forest
Beaches, dunes, sands	Not Used
Bare rocks	
Sparsely vegetated areas	
Burnt areas	
Glaciers and perpetual snow	
Water courses	
Water bodies	
Coastal lagoons	
Estuaries	
Sea and ocean	
Inland marshes	Wetland
Peat bogs	
Salt marshes	
Salines	
Intertidal flats	

4.4.4 Climate Datasets

Climatic datasets were retrieved from 12 different meteorological stations within the Alentejo Region, available on Sistema Nacional de Informação de Recursos Hídricos (SNIRH) (available at http://snirh.pt/index.php?idMain=2&idItem=1) for the years since 2003 to 2008. The datasets retrieved were: hourly temperature, daily precipitation and daily pan evaporation and are the more complete available for Portugal's Alentejo region.

4.4.5 Climate Change Scenarios

Our analysis uses a fixed time horizon of 100 years. This assumption, used for simplicity purposes, is analysed in the Discussion. To make 100 year simulations, climatic data from the past cannot simply be extended further in time. In light of climate change, climate scenarios must be included in the variables of the model. We analysed different scenarios for the climate data needed (temperature, pan evaporation and precipitation). Compared to other countries, starting from 1990 and until 2100, the temperature increase in Portugal will be higher than the other regions in Europe (Santos et al., 2002). Thereby, it is important to take into account these changes for Alentejo region in order to have more accurate assessments.

These scenarios were retrieved from the Portuguese Project "Climate Change in Portugal. Scenarios, Impacts and Adaptation Measures" (SIAM) (Santos et al., 2002). This project started in 1999 and describes different climatic future scenarios based on models of atmosphere general circulation (Santos et al., 2002).

For the temperature change values, we calculated the mean and deviation standard for all the scenarios evaluated by SIAM generated by the following general circulation models: CSIRO, ECHAM4, CGCM1, HadCM2-GGa2, HadCM2-GSa2, HadCM3-GG, HadCM3-GS, GFDL, NCAR and CCSR (Santos et al., 2002). These models are based on approximations to a large-scale of physical laws that represent the climate system. The models differ on, for example, numerics on atmospheric, ocean, cryospheric and terrestrial processes, horizontal and vertical resolution, parameterization (Randall et al., 2007).

The precipitation values have a higher uncertainty. This is due to the irregular variations within the runs of the models and the larger differences from model to model than the temperature predictions (Santos et al., 2002). For these values, we calculated the mean and standard deviation for the precipitation changes from 2000 to 2100, for the proposed scenarios of SIAM on the Centre and South of the Western Iberia: HadCM2 GGa2, HadCM3 GG, HadCM2 GSa2 and HadCM3 GS. In the end, we obtained the values for temperature and precipitation increase described at Table 7.

Table 7- Temperature and precipitation monthly increment and respective standard deviations obtained at Santos et al. (2002).

	Increment	**Standard Deviation**
Temperature	$0.004 \pm 0.001\ ^{\circ}\mathrm{C}\ month^{-1}$	$0.001 \pm 0.0001\ ^{\circ}\mathrm{C}\ month^{-1}$
Precipitation	$-0.07 \pm 0.11\ \mathrm{mm}\ month^{-1}$	$0.11 \pm 0.01\ \mathrm{mm}\ month^{-1}$

4.5 Unique Homogeneous Territorial Units

The Alentejo region is not homogenous in terms of soils, climate and LU. For the intended regionalization of the simulations, Unique Homogeneous Territorial Units (UHTU) in Alentejo were obtained by the overlay of soil and climatic datasets described in Figure 11. Each UHTU was characterized by a distinct set of parameters corresponding to the intersection of the four variables indicated in Figure 11. The data sources for each of these variables are indicated in detail in sections 4.4-4.10 below.

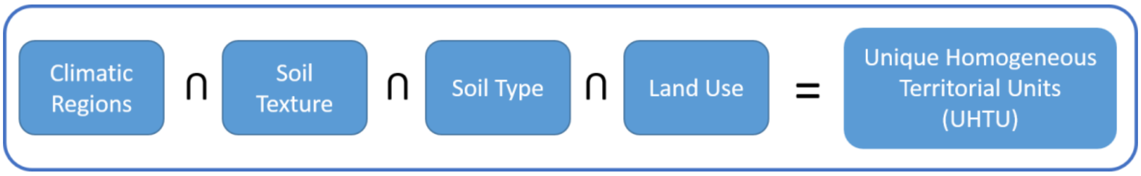


Figure 11 - Unique homogeneous territorial units (UHTU) composition.

After the overlay of these datasets, we obtained 2041 UHTU's for the Alentejo region. These UHTU's were used for simulations using DNDC and RothC.

4.6 Specific DNDC datasets

As shown in Table 5, DNDC requires additional data when compared to RothC. These additional data and the sources used are presented in the next sections.

4.6.1 Climate Data and N concentration in precipitation

Climatic data were retrieved from SNIRH for the same years of RothC data (from 2003 to 2008). The values needed to run DNDC are daily precipitation, maximum temperature and minimum temperatures. Climatic change scenario previously described was also applied to the program, in the alternative climatic options menu. N concentration in precipitation data was retrieved from EMEP (2016) map of NH_4 wet deposition and NO_3 wet deposition (annual means). These data were measured directly from monitoring stations for the United States and Western Europe for the years from 1989 to 1994. The maps have a resolution of 0.5 x 0.5 degrees.

4.6.2 Soil parameters

Values for pH (maximum and minimum) were retrieved from HWSD (FAO et al., 2012). Soil bulk density, SOC and clay content (maximum and minimum) was retrieved from LUCAS topsoil database (Toth et al., 2013). HWSD values are for a 30 cm soil depth, while LUCAS topsoil database are for 20 cm. In order to exceed this mismatch, we assume that all the properties remain equal regardless of the depth. Salinity values for the region were retrieved from ESDAC (available at http://esdac.jrc.ec.europa.eu/content/potential-threats-soil-biodiversity-europe).

4.6.3 Crop parameters

DNDC provides datasets that can be used in the simulations. For this dissertation, we used the default cumulative temperature (ºC) data available on DNDC for each crop chosen. Also, we used for each 12 soil texture types in use, detailed data provided by DNDC: clay fraction, porosity, soil saturation conductivity (m/hr), soil moisture in water filled porosity at the field capacity point and at the plant wilting point.

Due to the lack of information about water requirements for Alentejo's crops, we estimate an upper bound value for each irrigated crop by summing precipitation and irrigation values.

Maximum grain yield (kgC/ha) for each crop was estimated according to the productivity values of INE, for the maximum value for 10 years data (available at https://www.ine.pt/xportal/xmain?xpid=INE&xpgid=ine_base_dados). To convert these values into carbon values, we assume that dry matter has 45 % of carbon content, according to Farina et al. (2013).

4.6.4 Crop management practices

DNDC requires data of irrigation area (%) for each UHTU. For irrigated crops we consider a value of 100% of area irrigated. Otherwise, for rainfed crops, irrigation area is zero. Crop management parameters such has planting and harvesting dates, flooding events and tillage practices were taken from GPP (2001) has described at Table *Table 4*. Fertilizer and manure application values (kgN/ ha) for each crop were retrieved from Morais et al. (2016a).

DNDC also requires the percentage of above-ground biomass that stays on the ground, i.e. that is a crop residue. To estimate these parameters, we assume that the biomass above-ground that is not harvest becomes a crop residue. According to specific harvest indexes the fraction that stays in the ground will be

$$Aboveground\ residue\ percentage = 1 - Harvest\ Index\ . \quad (3)$$

4.7 Specific RothC Datasets

Despite requiring less data, RothC also has specific data requirements that are different from DNDC's. For RothC simulations, the model needs specific input parameters described in Table 5, for each one of the UHTUs. The datasets were spatially referenced on ArcMap. A Visual Basic routine was created to put all the inputs from ArcMap in the program.

4.7.1 Climate Data

Climatic data were retrieved from SNIRH values for 12 different meteorological stations for the years from 2003 to 2008 (available at http://snirh.pt/index.php?idMain=2&idItem=1). The climate change scenarios described above were applied to the values of temperature and precipitation.

Base monthly open pan evaporation values and monthly precipitation (for present time) were obtained from daily open pan evaporation values and daily precipitation values respectively. We summed all the daily open pan evaporation and daily precipitation for each month and divided them by the number of years. Average monthly mean temperature values were calculated based on hourly mean temperature. In order to calculate monthly mean temperature, we grouped all the hourly values for each month and calculated the mean temperature of each month for each year. Then we aggregate all the values in 12 groups, where each group represents a month, i.e. all the mean values of January are aggregated, independently the year they were recorded, and calculated the mean of these values. This way we obtained average monthly values of pan evaporation, monthly precipitation and temperature, and respective standard deviations. We assume that all these three parameters have a normal distribution.

4.7.2 SOC and Clay Data

Inputs for SOC initial values and clay content for each UHTU were obtained from Brogniez et al. (2015) map based on LUCAS-topsoil carbon data. Clay content values were retrieved from the LUCAS Soil Database. The input for RothC of depth of soil layer simulated is 20 cm, the same as LUCAS Soil Database topsoil samples. Also for these two parameters, we recorded the standard deviation values obtained and assumed a normal distribution for each.

4.7.3 Soil Cover

Soil Cover inputs are required due the higher decomposability of carbon in the presence of fallow soils. For simulation aspects soil cover was considered zero for fruit, olives, wine crop. For forest, grasslands and shrublands we assume that soil cover is presented for the entire year. For irrigated and rainfed cereals crops we assumed:

- 1 for the months from seed to harvest;
- 0 for the other months.

4.7.4 Calculation for the carbon inputs from plant residues

To estimate the crop residues (tC/ha) and forest residues (tC/ha) we made an extensive search for crop residues values and for indirect parameters of harvest index, shoot-to-root ratios and residues/crop yield of each crop that enable the estimation of the residues. Crop residues are the wastes left on the ground resulting from the crops itself. These residues are a consequence of pruning and harvesting.

The yield for each crop, represented at Table 8, was retrieved from INE database (available at https://www.ine.pt/xportal/xmain?xpid=INE&xpgid=ine_base_dados), where we obtained the average values for the last 10 years of data available. We assume that dry matter from production values as 45 % of carbon content, according to Farina et al. (2013).

Harvest index was used to estimate the values of aboveground biomass produced by each crop, according to

$$HI = \frac{Yield\ (g)}{Aboveground\ Biomass\ (g)}. \tag{4}$$

Shoot-to-root ratios (S:R) were used to estimate the belowground biomass values for each crop according to

$$S{:}R = \frac{Aboveground\ Biomass\ (g)}{Belowground\ Biomass\ (g)}. \tag{5}$$

After equations (4) and (5), crop residues are obtained according to

$$\begin{aligned} &Crop\ Residues[tCha^{-1}] \\ &\quad = (Aboveground\ biomass - Yield) + Belowground\ Biomass. \end{aligned} \tag{6}$$

We took the yield from the aboveground biomass because the yield is the portion that is taken from the soil, while the rest of the aboveground biomass stays on the ground.

Crop residues were also obtained according to the ratio of residue-crop defined by

$$Crop\ Residues\ [tCha^{-1}] = \frac{Residues}{Yield}. \tag{7}$$

The values for residues that we found for each crop using different methods often differed. For example, in the case of tomato crops, we estimate residues of 0.76 tC/ha and 91 tC/ha using different parameters for the same crop (tomato) and with the same yield (obtained from INE). To overcome this limitation and to understand which values were the most appropriate and knowing that for some cases calculating a mean of the input values would be inaccurate, like the case of tomato, we simulate all the options available using a uniform probability distribution.

Table 27 in the Appendix shows the values found in the literature review, with respective conversion to values in $tCha^{-1}$ (input value necessary to RothC model), by applying the productivity values for Alentejo region (described at Table 7).

Table 8- Alentejo crops productivity, ten year average - retrieved from INE.

Crop	Productivity (kg/ha) – ten year average (2006-2015)
Oats Forage	17,198
Olive	1,473
Grape	5,439
Orange	8,743
Peach	13,748
Forage Maize	53,633
Irrigated Maize	10,824
Tomato	71,931
Potato	16,866
Rice	6,125
Barley	1,837
Wheat	1,827

4.7.5 DPM/RPM ratio

As discussed above, in the RothC model SOC is initially distributed through 2 different compartments: decomposable plant material (DPM) and resistant plant material (RPM). Their ratio of distribution (DPM/RPM ratio) is an input needed for the model. RothC advises the value of DPM/RPM ratio of 1.44 for agricultural crops and improved grassland. For tree fruits, olives and vineyards we assumed a DPM/RPM ratio of 1, due to the greater content of lignin, which has higher resistance to decomposition (Jebari, 2016). RothC was not calibrated specifically for forest even though it was already used to simulate it. To estimate SOC changes we assumed a DPM/RPM ratio of 0.25 for forest simulations (Jekinson et al., 1991). Farmyard manure inputs have a different distribution for each compartment. The ratio of distributions is: 49% to DPM, 48% to RPM and 2% to humus (Coleman et al., 2014).

4.7.6 Monthly Distribution of Carbon Inputs

Carbon crop residues values are valid for an entire year and had to be distributed monthly. Monthly distribution of carbon residue inputs is dependent on the primary production and life stages of plants. Based on the methodology of Jebary et al. (2016) we assumed for cereal crops a distribution of 50% for the months of harvesting and other 50% in the three months earlier. For permanent crops such as fruit trees, olives and vineyards we assumed a distribution of 70% of inputs in the pruning months and the 30% rest on the 4 months earlier. The months of harvesting and pruning are indicated in GPP (2001). For forest trees, assuming no pruning neither harvesting, we assumed as a simplification a constant provision of carbon residue inputs equally distributed during the year.

4.7.7 Monthy Farmyard Manure Carbon Inputs

Farmyard manure carbon inputs were retrieved from Morais et al. (2016a). Yearly values also had to be distributed among the months when farmyard manure is applied to the crops. These months are indicated by GPP (2001). Table 9 summarizes all the information for the crops where farmyard manure is applied.

Table 9- Farmyard manure annual values and respective standard deviation and application months.

	Manure (tC/ha)	Manure Standard Deviation (tC/ha)	Application Months
Tomato	9.9×10^{-3}	3.7×10^{-4}	May to July
Maize Forage	8.8×10^{-2}	3.3×10^{-3}	June
Maize Irrigated	1.7×10^{-2}	6.6×10^{-4}	July
Orange	1.3×10^{-2}	4.9×10^{-4}	April
Peache	1.1×10^{-3}	4×10^{-4}	June
Potato	2.2×10^{-1}	8×10^{-3}	May

4.7.8 Irrigated Crops – Irrigation Values

RothC does not provide irrigation options. Water input values are disregarded and are not modelled by the program. For irrigated crops, this is an information with major importance. With more availability of water in the soils, carbon decomposability will be higher (Kutchs et al., 2009). To overtake the lack of irrigation in RothC, we sum water from irrigation to the precipitation data. For each irrigated crop, we retrieved the irrigation water values from GPP (2001), divided them throughout the irrigation months for each crop and summed them to the precipitation for each month. These data are shown in Table 4.

4.7.9 Model Initialization

The version used of RothC is a modified version, already parameterized for the Mediterranean region by Farina et al. (2013). To initialize the program, we needed to distribute SOC initial values through the five compartments of SOC: RPM, DPM, Hum, BIO and IOM. According to Weihermüller et al. (2013) SOC is distributed through these departments according to

$$IOM = 0.049\, SOC^{1.139}, \tag{8}$$

$$RPM = (0.1847\, SOC + 0.1555) \times (Clay\ Fraction + 1.2750)^{-0.1158}, \tag{9}$$

$$HUM = (0.7148\, SOC + 0.5069) \times (Clay\ Fraction + 0.3421)^{0.0184}, \tag{10}$$

$$BIO = (0.0140\, SOC + 0.0075) \times (Clay\ Fraction + 8.8473)^{0.0567}, \tag{11}$$

where "Clay Fraction" is the clay content expressed in %, IOM is the inert organic matter expressed in tC ha^{-1} ,RPM is the resistant plant material expressed in tC ha^{-1}, BIO is the microbial biomass expressed in tC ha^{-1}, HUM is the humified organic matter expressed in tC ha^{-1}, SOC is soil organic carbon expressed in tC ha^{-1}.

These distributions are only dependent on the initial SOC values and clay fraction of the soil. DPM compartment distribution is calculated according to the results of these equations. If the SOC value is higher than the sum of the four compartments described above, then DPM compartment will have the rest of SOC fraction that was not distributed. A schematic distribution of SOC through these compartments is shown in Figure 12.

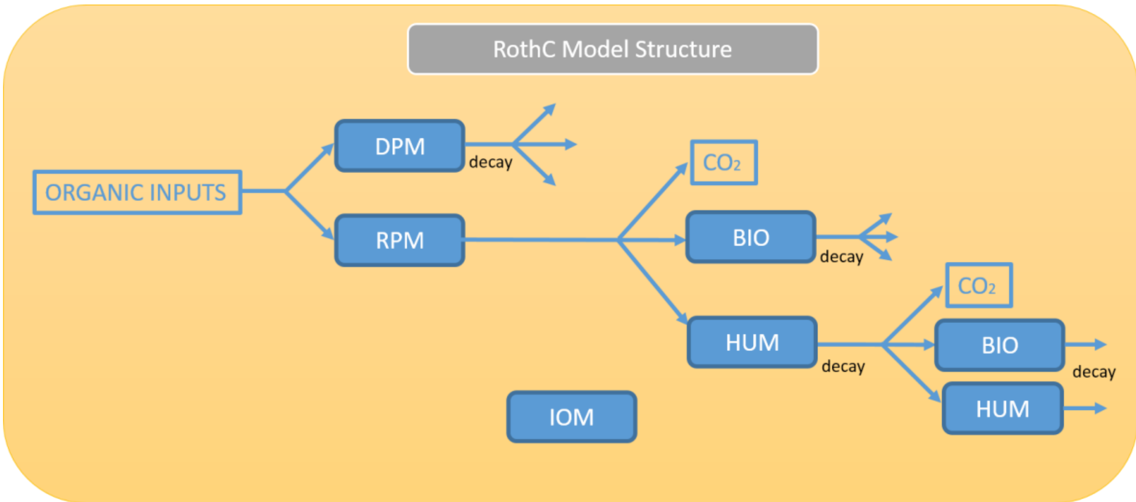


Figure 12 – Schematic of RothC model pools structure - adapted from the RothC manual.

DPM - decomposable plant material; RPM - resistant plant material; IOM - inert organic matter; BIO - microbial biomass; HUM - humified organic matter

5 Estimation of SOC depletion due to land use with DNDC

5.1 Summary

The goal with DNDC was to simulate soil dynamics for each UHTU in order to enable the calculation of CFs based on scenarios. Due to computational problems, i.e. the amount of time required to run a simulation with all the UHTU was 5 days and for just one UHTU was 4 minutes, we started to make an analysis for only one specific UHTU. In this section we describe the implementation of DNDC and the problems encountered. All the datasets used are described at the previous chapter.

5.2 Method

In this dissertation, DNDC was run in regional mode, to simulate the dynamics of C and N for different UHTU. Runing DNDC in regional mode requires information of location, climate, soil properties, cropping systems and farming management practices for each UHTU. DNDC provides default settings for 88 different crops and 12 soil types that can be modified by the users.

We started with the preparation of all the information for each UHTU and ran the program. In this thesis we chose one UHTU only to analyse results, which were similar regardless of the region chosen. This UHTU had a present LU of Artificial Surface, and the intended LUC was rainfed barley. We also performed a sensitivity analysis in order to understand which parameters would have a greater effect on the results. By this time, we had already successfully simulated this UHTU for transformation to rainfed barley, and knew that the results showed an increase of SOC stocks (as shown in Chapter 6).

In order to understand the sensitivity of the model to the inputs, we made different simulations, changing one input at a time and understanding its impact on the final results. In the end we made 14 different simulations. The results of these simulations are explained next.

5.3 Results

Table 10 and Table 11 present the initial input values for transformation to rainfed barley in UHTU 1.

Table 10- Soil parameter inputs given to DNDC for UHTU 1 region.

Soil	Value	Soil	Value
Lon	-7	pH max	6.8
Lat	39	pH min	6.7
N-dep	3×10^{-2} (ppm)	Max Bulk Density	1.38 (g/cm^3)
SOC max	1.3×10^{-2} kgC/kg soil	Min Bulk Density	1.34 (g/cm^3)
SOC min	1.2×10^{-2} kgC/kg soil	Slope	45
Clay max	2.8×10^{1} (fraction)	Salinity	0
Clay min	2.2×10^{1} (fraction)		

Lon – Longitude; Lat – Latitude; N – Nitrogen; dep – deposition; SOC – Soil Organic Carbon; max – Maximum; min – Minimum

Table 11- Crop and management parameter inputs given to DNDC for UHTU 1 region.

Crop	Value	Management	Value
Maximum Grain Yield	947 kg C/ha	Fertilization	40 kgN/ha
TDD	1,300 ºC	Flooding	0
Water demand	250 kg water/kg dry matter	Irrigation	0
Plantation	October	Fraction of aboveground residue	5.6×10^{-1}
Harvesting	July	Tillage	April, 10 cm
		Manure	

TDD – thermal degree days

According to the initial values described in Table 10 and Table 11, and running a 100-year simulation on DNDC for transformation from artificial surface (the current LU in UHTU 1) to rainfed barley, we obtained SOC changes depicted in Figure 13.

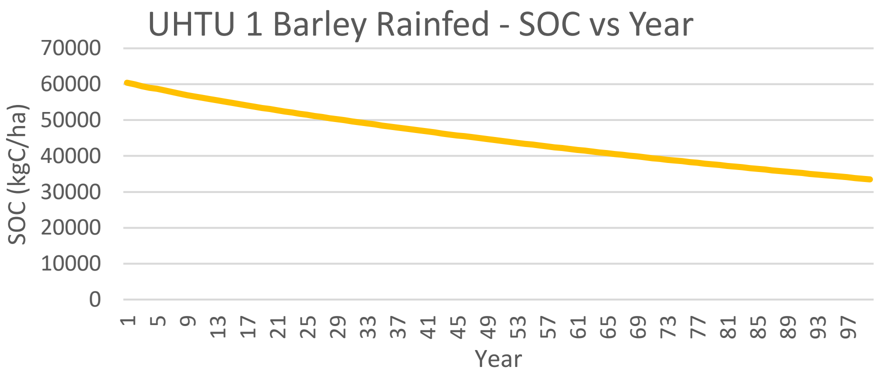


Figure 13- SOC dynamics using a 100-year simulation in DNDC for UHTU 1.

UHTU – Unique Homogeneous Territorial Unit; SOC – soil organic carbon

The curve has a downward slope which is unexpected considering that, in the original SOC data, rainfed barley plots typically have higher SOC than artificial plots. We thus proceeded with the sensitivity analysis of parameters to understand this behaviour. We made a total of 14 different simulations, where in each simulation one input changed. The left column of Table 12 indicates the input that was changed in each simulation, while the right column represents the total SOC change for the 100-year simulation. A negative SOC change value indicates a depletion on SOC stocks and a positive value on SOC change indicates a gain on SOC stocks. We can see that the main contributors to the results are SOC initial values, clay fraction and bulk density. However, there is SOC depletion in every case.

Table 12- Description of the different DNDC simulations, indicating input parameters changed and the consequent results for SOC differences between year 100 and year 0.

Simulation Type	SOC difference after 100-year simulation tC/ha
Original	-27.15
Maximum Grain Yield x5 = 4735 kgC/ha	-27.11
Water demand = 0	-27.10
Fertilization x10 = 400 kgN/ha	-27.17
Manure = 100 kgN/ha	-27.15
Intial SOC divided by 10	-2.68

Initial SOC divided by 100	-0.22
Clay min and max +20 %	-19.98
Clay min and max -20%	-20.1
pH = 9.8	-27.14
pH = 3.8	-27.13
Bulk max = 2.38 **Bulk min = 2.34**	-46.88
Bulk max = 0.38 **Bulk min = 0.34**	-7.20
Salinity = 1	-27.15

Bulk – bulk density; min – minimum; max – maximum; SOC – soil organic carbon

5.4 Discussion

The first results obtained using the base simulation (where the most likely estimates for each variable were used) showed a SOC decrease of almost 30 tC/ha as we can see at Figure 12. Also, for other UHTU's the same decrease dynamic was encountered while testing DNDC simulations. The sensitivity analysis showed that, even when assuming values with completely different magnitudes, e.g. dividing the SOC initial value by 100, we would still obtain a decrease of SOC stocks following LUC. A possible explanation for this problem is that the model is not calibrated for the Mediterranean region. Also, because the simulations had to be made in regional simulation mode, the program does not allow a calibration with other parameters.

Another aspect encountered using the DNDC model is that manure is not being included in the calculations. We can see at Table 12 that the results remain equal to the base case simulation when manure inputs are changed. We tried different ways to write this input at the DNDC input text files. DNDC has a user guide available, with the steps required to implement the model and how to present and write in text files the input values. DNDC also has an example for a region called Shangrila, showing example text files for the user to try to run the simulations and to learn how to implement the model. We observed that the instructions of the user guide available on how to create the text files were different from the text files for the Shangrila example. We also tried to run the example simulation given already on DNDC and changed the manure input and saw that results remained at the same levels. This means that this input is unaccounted for in the results.

5.5 Conclusion

DNDC is a much more complex model than RothC, with more specific inputs needed for the simulations. With all the limitations on the instructions of the user guide of DNDC, which are partially incomplete, the manure input value un accounted for in simulations, the computational limitation of running time and the lack of regional calibration of the model, we concluded that it would be impossible to obtain accurate regionalized CFs even for simply one UTHU in Alentejo.

6 Estimation of SOC depletion due to land use with RothC – Simulations

6.1 Summary

We simulated soil dynamics using RothC with the objective of obtaining SOC changes as a consequence of LUC, which is essential to calculate CFs. For each simulation with RothC we obtained a curve representing SOC changes for each UHTU and for each LUC intended. One key variable here was the amount of carbon in crop residues. We used the most likely estimates to run the simulations. The crop residues variable will be further analysed in the next section of this dissertation. All other datasets needed were previously described in section 4.9 of this dissertation. In this section we present the method used to prepare and run the simulations and the results obtained.

6.2 Method

6.2.1 Matlab Implementation

The original version of the RothC model runs one region or location (i.e. on UHTU) at a time. This characteristic would be a computational problem given the amount of UHTUs in our work. In order to overcome this issue, we obtained a modified version of RothC for Microsoft Excel. This RothC version was provided by Jorge Álvaro-Fuentes from Estación Experimental de Aula Dei. This modified version allowed us to run all UHTUs simultaneously, although it took 7 hours to complete one simulation for the 2041 UHTUs and obtain SOC dynamics for 100 years. Due to our necessity to run different simulations for each UHTU in order to simulate different LUC, this amount of time was a computational problem. To reduce the amount of time required for the simulations, we wrote a version of RothC in Matlab that requires only 30 seconds to complete a simulation for the 2041 UHTUs. With this new version, we eliminated time restrictions and were able to make deeper analyses of RothC and its parameters.

This analysis was made using two different procedures: (1) using the most likely estimate for each variable; and (2) assigning an uncertainty distribution to each variable and using a Monte Carlo simulation. This type of simulation is used to account the variability and uncertainty in the assessments (explained in Chapter 7), studying the contribution of each parameter to the range of results. A model that does not explicitly address uncertainty is a deterministic model. Because we assumed that the input values used in case (1) are the mean values (the most likely estimates), this deterministic model is considered a base case scenario. In the case of Monte Carlo simulation, each input parameter has a statistical distribution and, for each distribution, random samples are calculated. These random samples were then the input values for the simulations (Raychaudhuri, 2008).

To enable this analysis, in order to account for a wider range of values and associated error, we modified once again the Matlab version of the RothC model. Instead of giving only one input value for each parameter, the program is given a mean value and a standard deviation for each variable, namely pan evaporation, temperature, precipitation and farmyard manure for each UHTU. The program, by running several iterations (up to 100), generates random numbers for a normal distribution and runs the simulations for each iteration. In the case of crop carbon residues, due to a lack of data, we were unable to calculate the parameters of a normal distribution. In that case we assumed a uniform distribution where any number within the range determined by the lower and higher estimate was assigned equal probability. Thereby, each iteration has as inputs different random values within the ranges defined in the beginning of the model and the model ran with that distinct set of parameter in each iteration. We calculated the mean of each parameter, for 100 iterations for each UHTU and respective standard deviation. This later version of the RothC model in Matlab takes 10 minutes to complete a simulation for the 2041 UHTU's for 100 iterations.

6.2.2 RothC simulations

With the modified version for Matlab of RothC we were able to simulate soil dynamics for all UHTUs. To start this process, RothC was given values of SOC content and clay fraction that are the initial characteristics of each UHTU. The information of which LU is present at year 0 is given by the classification in CLC (2006). Although this information does not interfere with the simulations at this point (it only intervenes in the calculation of CFs), it was useful for our interpretation. From that starting point of SOC content and clay fraction, RothC simulates the soil dynamics, according with the climate data and the management options given. In this simulation we go from one specific initial land use (LU_1), to another land use (LU_2) defined by the management options. A schematic representation of this procedure is shown in Figure 14.

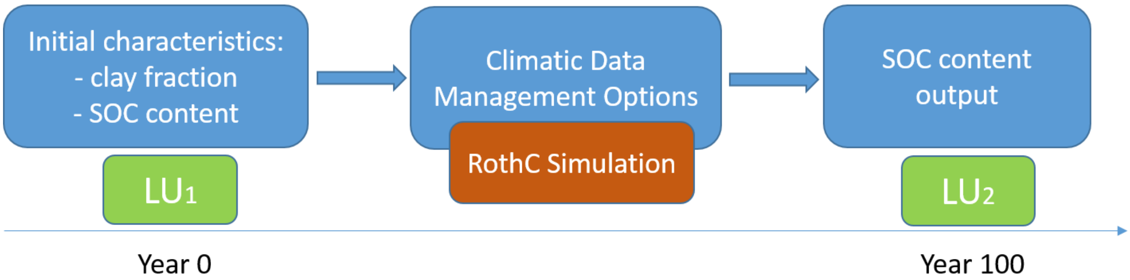


Figure 14- Schematic of a RothC simulation starting from a land use 1 (LU1) and changing it to a land use 2 (LU2).

LU1 – first or baseline land use; LU2 – second land use (after transformation)

We simulated each UHTU different times, with different management options, in order to obtain different LU_2. This way we obtained different outputs (LU_2) for each UHTU. The possible LU_2 are indicated in Table 13. This means that we calculated the resulting SOC dynamics in each UHTU for each LU_2 independently.

Table 13- Crops types intended for the results obtained through RothC model.

LU_2	Irrigation Option
Tomato	Irrigated
Oats	Rainfed
Wheat	Irrigated
Barley	Rainfed
Forage Maize	Irrigated
Maize	Irrigated
Rice	Irrigated
Peach Tree	Irrigated
Orange Tree	Irrigated
Vineyards	Rainfed
Olive	Irrigated
Olive	Rainfed
Pasture	Rainfed
Potato	Rainfed
Pine	Rainfed
Eucalyptus	Rainfed
Cork	Rainfed
Holmoak	Rainfed
Oak	Rainfed
Shrublands	Rainfed
Grasslands	Rainfed

LU2 – Land use after the transformation process

We thus ran a total of 20 different simulations for each UHTU with the objective to obtain all the intended LU_2. After these simulations, for the CFs calculation in Chapter 9, we needed to make additional simulations. Now, instead of starting from the initial SOC content of LU_1, we started with an initial SOC content obtained from the last SOC content value of LU_2, and simulated each UHTU in order to obtain a third LU. This third LU is the respective PNV of each UHTU. Figure 15 is a representation of the process. The justification to this extra simulation to PNV is explained in section 9.1.2 (page **Error! Bookmark not defined.**). For this last process, 20 additional simulations had to be run with RothC.

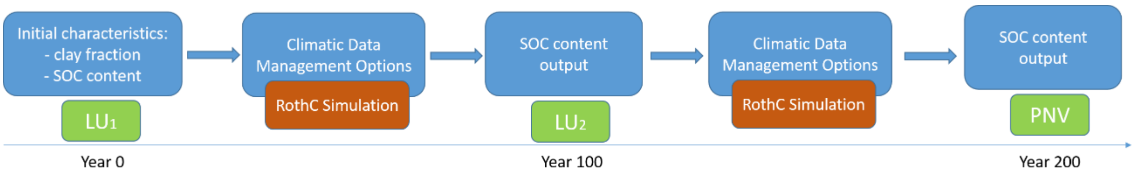


Figure 15- Schematic of a RothC simulation starting from a land use 1 (LU1), changing it to a land use 2 (LU2) and then changing it to a land use 3 that corresponds to the potential natural vegetation (PNV).

LU1 – first land use; LU2 – second land use (after first transformation); PNV – potential natural vegetation

After this procedure, we obtained the dynamic SOC curves needed in order to calculate the CFs. With the modified version of Matlab, we obtained results for the Monte Carlo simulations and for the best case scenario. The latter is obtained through a simulation using only the mean values of each parameter, without the deviation standards.

6. 3 Results

RothC simulates the dynamics of soils, starting from an initial value of SOC for each UHTU for year zero. From that point, RothC gives SOC stock values for each of the 100 years simulated. Table 13 shows the mean SOC initial values given to RothC for the year zero for each of the CLC reclassification proposed in Table 6. To obtain these values presented at Table 13, we aggregated each UHTU to its respective CLC class and calculated the mean SOC stocks using the LUCAS topsoil database. The classes that present lowest SOC stocks are permanently irrigated land, vineyards and olive groves. Artificial surfaces are the fifth class with lowest values. All the forest classes, pasture and wetlands have the highest values. Starting with these baseline SOC stocks, we simulated different LUC. The results of these simulations are presented in Table 15, Table 16, Table 17, Table 18 and Table 19 for barley, wheat, tomato, olive rainfed and pine, respectively. The values in the tables are the change in SOC stocks, i.e. $SOC_{year\ 100} - SOC_{year\ 1}$ and thereby positive values represent a gain in SOC stocks along 100 years, while negative values are losses of SOC stocks. These tables, in general, represent a SOC change for a LUC of "what is there at year 0" to something else. The present land use (LU_1) is shown in the first column, with 14 different land use classifications. The LU obtained after the transformation (LU_2) is represented by the next three columns, where the "best estimate" column represents the values of the simulation with mean (or "best estimate") values for all the inputs, without considering the associated error. The "100 iteration" column represents the average values obtained after 100 iterations. The "Standard Deviation" column represents the standard deviation results obtained after 100 iterations.

Table 14 - Initial SOC input values for the reclassified CLC. Each UHTU was aggregated into the correspondent CLC class.

Initial SOC input values mean	tC/ha
Artificial Surfaces	49.51
Non-Irrigated Arable Land	50.44
Pastures	65.68
Wetlands	65.39
Permanently Irrigated Land	42.87
Rice	44.33
Vineyards	42.04
Fruit trees and berry plantations	42.17
Olive Groves	45.48
Agro-forestry areas	55.24
Broad-leaved forest	66.21
Coniferous forest	71.91
Mixed Forest	73.13

Forest	68.37

SOC – soil organic carbon

When some LUC results, for instance, in a decrease of SOC, it means on average SOC decreases over 100 years in the study region, not for each UHTU individually. It means that the mean of the overall values of UHTU organized in their respective CLC classes are negative. All results presented are obtained using the most relevant crop carbon residue. A further analysis of this parameter is described at section 7. The values presented here are a mean of the SOC changes obtained for different UHTU, and not the results for one specific UHTU.

Table 15 depicts LUC to barley. Crop carbon residue used for this simulation was 0.991 tC/ha (APA, 2011). Regardless of the baseline LU, SOC always decreases after transformation to barley. The classes with a higher SOC decrease for transformation to barley are pasture, wetlands and the five forest classes. The best estimate simulations are within the range of the 100 iteration simulation values, considering the standard deviation.

Table 15- SOC change ($SOC_{year\ 100} - SOC_{year\ 1}$) mean values for best estimate and 100 iterations and respective standard deviation for the last case. Land use change to barley.

Final land use (tC/ha)	Barley - Best Estimate	Barley 100 iterations	Standard Deviation
Artificial Surfaces	-9.08	-12.87	8.24
Non-Irrigated Arable Land	-10.29	-14.40	9.30
Pastures	-16.55	-22.00	11.11
Wetlands	-18.78	-22.31	12.60
Permanently Irrigated Land	-6.47	-10.18	8.24
Rice	-6.90	-10.79	8.27
Vineyards	-4.23	-8.86	7.96
Fruit trees and berry plantations	-4.44	-9.02	7.65
Olive Groves	-7.20	-11.22	8.87
Agro-forestry areas	-13.06	-17.26	9.73
Broad-leaved forest	-19.20	-23.54	11.26
Coniferous forest	-22.19	-26.52	11.16
Mixed Forest	-23.28	-27.20	12.05
Forest	-20.20	-24.62	11.86

Next we present the values for LUC to rainfed wheat in Table 16. The crop carbon residue used was 1.499 tC/ha (Álvaro-Fuentes et al., 2014; Jebari, 2016). There is an increase in SOC stocks in the LU1 classes of permanently irrigated land, vineyards and fruit trees and berry plantations for the best estimate simulation. In the case of 100 iteration simulation, all the classes present a decrease on SOC stocks.

Table 16 - SOC change ($SOC_{year\ 100} - SOC_{year\ 1}$) mean values for best estimate and 100 iterations and respective standard deviation for the last case. Land use change to wheat.

Final land use (tC/ha)	Wheat - Best Estimate	Wheat 100 iterations	Standard Deviation
Artificial Surfaces	-1.39	-6.28	9.37
Non-Irrigated Arable Land	-3.60	-7.90	10.39
Pastures	-9.50	-15.28	12.34
Wetlands	-12.69	-16.39	14.07
Permanently Irrigated Land	0.21	-3.65	9.38
Rice	-0.85	-4.51	9.21
Vineyards	2.75	-2.25	9.19
Fruit trees and berry plantations	2.75	-2.13	8.97
Olive Groves	-0.06	-4.51	9.88
Agro-forestry areas	-6.67	-10.93	10.71
Broad-leaved forest	-13.00	-17.31	12.16
Coniferous forest	-16.40	-20.95	12.05
Mixed Forest	-17.31	-21.11	13.14
Forest	-13.90	-18.41	12.83

For the LUC to tomato, simulations for the best estimate case, presented in Table 17, show SOC stocks increase for the classes of permanently irrigated land, rice, vineyards, fruit trees and berry plantations and olive groves. All 100 iterations have a decrease in SOC stocks. The decrease is smaller for the same classes that presented an increase for the best estimate case. The crop carbon residue input used for these simulations was 1.5 tC/ha, a mean value obtained from the two lowest values found in the literature review (Dias and Azevedo, 2004; Alves, 1995).

Table 17- SOC change ($SOC_{year\ 100} - SOC_{year\ 1}$) mean values for best estimate and 100 iterations and respective standard deviation for the last case. Land use change to tomato.

Final land use (tC/ha)	Tomato Best Estimate	Tomato 100 iterations	Deviation Standard
Artificial Surfaces	-1.66	-6.55	9.34
Non-Irrigated Arable Land	-2.99	-7.51	10.47
Pastures	-9.09	-15.22	12.35
Wetlands	-11.94	-16.02	13.88
Permanently Irrigated Land	0.88	-3.20	9.48
Rice	0.43	-3.50	9.55
Vineyards	3.41	-1.80	9.06
Fruit trees and berry plantations	3.26	-2.10	9.03
Olive Groves	0.30	-4.27	10.08
Agro-forestry areas	-5.91	-10.61	10.80
Broad-leaved forest	-12.22	-16.89	12.36
Coniferous forest	-15.45	-20.17	12.17
Mixed Forest	-16.53	-20.43	13.22

Forest	-13.14	-17.85	12.90

For the case of LUC to rainfed olive, the only case where we obtained a gain (almost null) in SOC stocks is the change from vineyards for the case of best estimate, as shown in Table 18. For the 100 iterations, all the mean values obtained show SOC losses. The values used for crop carbon residues were a mean value of 1.7165 (Blasi et al., 1997 and Nieto et al., 2010).

Table 18- SOC change ($SOC_{year\ 100} - SOC_{year\ 1}$) mean values for best estimate and 100 iterations and respective standard deviation for the last case. Land use change to rainfed olive.

Final land use (tC/ha)	Olive Rainfed Best Estimate	Olive Rainfed 100 iterations	Standard Deviation
Artificial Surfaces	-5.77	-11.38	9.54
Non-Irrigated Arable Land	-7.40	-12.52	10.24
Pastures	-14.75	-21.42	11.91
Wetlands	-16.28	-20.55	13.91
Permanently Irrigated Land	-2.62	-7.34	9.30
Rice	-2.66	-7.91	9.20
Vineyards	0.02	-5.96	9.21
Fruit trees and berry plantations	-0.53	-6.41	9.17
Olive Groves	-3.88	-8.90	9.84
Agro-forestry areas	-10.46	-15.73	10.66
Broad-leaved forest	-17.91	-23.43	11.86
Coniferous forest	-21.16	-26.90	12.16
Mixed Forest	-22.53	-27.72	12.67
Forest	-18.98	-24.39	12.29

The last case presented in this section is a LUC to pine forest. The crop carbon residue used for this simulation is 2.96 tC/ha (APA, 2015). We can observe a significant gain in the SOC stocks for all the LU classes for both the best estimate and 100 iterations simulations.

Table 19-SOC change ($SOC_{year\ 100} - SOC_{year\ 1}$) mean values for best estimate and 100 iterations and respective standard deviation for the last case. Land use change to pine forest.

Final land use (tC/ha)	Pine Best Estimate	Pine 100 iterations	Standard Deviation
Artificial Surfaces	40.47	29.48	16.96
Non-Irrigated Arable Land	35.52	26.58	17.43
Pastures	31.51	20.28	19.18
Wetlands	26.88	20.20	21.73
Permanently Irrigated Land	39.49	31.02	16.63
Rice	38.31	30.36	16.23
Vineyards	43.87	33.04	16.89
Fruit trees and berry plantations	43.71	32.75	17.10
Olive Groves	39.79	30.23	17.29
Agro-forestry areas	32.43	23.56	17.70
Broad-leaved forest	25.40	17.08	18.86

Coniferous forest	21.86	13.97	18.74
Mixed Forest	20.80	13.37	19.94
Forest	25.04	16.33	19.43

The results obtained for the other simulations are represented in the Appendix from Table 28 to Table 42.

6.4 Discussion

The values obtained for the baseline SOC stocks, described at Table 14 were directly obtained using the CLC (2006) maps and LUCAS Topsoil database. In the specific case of artificial surfaces, we can see that SOC values obtained are higher than some agricultural crops (permanently irrigated land, rice, vineyards, fruit trees and berry plantations and olive groves). These values for artificial areas mean that while there are some UHTUs with a LU of artificial surface with a lower SOC content (e.g. 30 tC/ha) there are other UHTUs significantly higher values (e.g. 80 tC/ha). Such high SOC contents are unexpected for an artificial surface. This is nevertheless a direct observation of the data reported in the LUCAS database. It is possible that this is explained by the sampled locations – so-called “artificial areas” are probably vegetated areas in urban locations, which would explain the high SOC concentrations. All the other baseline SOC stocks are within the expected range. The classes of forests, pasture and wetlands present the highest mean SOC values against permanent and annual crops.

Analysing the simulations results obtained through RothC, in Table 15, the values obtained for all LUC to barley are lower than expected. We expected a decrease of SOC stocks for classes such as pasture, wetland and forests, considering the average SOC measurements in the LUCAS database for each LU class. The negative values of Table 15 can be explained by the low estimate of crop carbon residue given to RothC. In this case the value given was the highest possible obtained in the literature review: 0.991 tC/ha. Even though it was the highest found, it is still fairly low when compared to the estimates found for other similar crops. In the simulation of LUC to wheat, the values obtained for the best estimate case are more in line with expectations that the ones obtained for barley. This is true despite the fact that for non-irrigated arable land classes (i.e. the class where wheat is aggregated), it presents a loss of more than 3 tC/ha, while the expected value for this specific case would be a SOC change near to zero. The value of crop carbon residue used was 1.5 tC/ha, a value much higher than the one used for barley.

The correspondent class of CLC for tomato is permanently irrigated land. For LUC from permanently irrigated land to tomato, using the best estimates, we can see that the values for this class are nearly constant, as it would be expected from the original data. Permanently irrigated land is the CLC class for tomato and as such no large variation of SOC was, at first glance, likely. Regarding the crop carbon residue values obtained for tomato in our literature review, we found values with different magnitudes. If we used any value other than the ones by Dias and Azevedo (2004) and Alves (1995), the values would be higher that any value found for forest crops in our literature review. These values would then lead to completely different results, much higher that forest classes.

As we can see in Table 37, LUC from the CLC class of Pasture to Pasture (obtained using the best estimate simulation of RothC) will result, in the best estimate case, in a substantial decrease of SOC of 16.2 tC/ha. For this case the values were expected to remain approximately constant. We can then conclude that such results are a consequence of the lower value of crop carbon residue obtained at the literature review of 0.8 tC/ha as described in Table 27.

For pine forests, we obtain a SOC increase for the best estimate case of 33 tC/ha for all regions. These results should be interpreted as valid for young forests only, when more C is stored, corresponding to the C input we considered. Another reason for the higher results is that we assumed permanent soil cover in this simulation.

An example of the impact of soil cover is, for instance, the comparison of this last simulation (pine forest) with the results obtained for potato. For potato, whose results are described in the appendix in Table 29, we obtained gains of SOC almost as large as to the ones obtained in the forest simulations (oak, holmoak, cork). These high results are partially explained by the high values found in the literature review for potato carbon residues, but not entirely since potato residues are actually higher than pines.. The difference is that for pine forest we assumed the soil was covered for the entire year, and only between seeding and harvest months in the case of potato. Potato carbon residues generate high increases of SOC stocks, but because there is no soil cover for the entire year, the values of SOC stocks are lower than in forests. Another example is the simulation of LUC to olives. The values of crop carbon residue used were the ones from Blasi et al. (1997) and Nieto et al. (2010). Even though these values are the highest obtained in the literature review, we obtain for the CLC class olive groves a loss of more than 3 tC/ha. It would be expected, as it occurred for tomato simulations, that the values remained constant, or approximated the ones from the baseline values. The explanation for the loss is that for permanent crops we do not assume full soil cover during the entire year.

We can see, for all cases, that in the 100-iteration simulation (i.e. Monte Carlo simulation) the values obtained were always lower that the ones obtained for the best estimate case. This means that the Monte Carlo simulation is underestimating the results. Since the best case is equal to the mean of the distribution probability, the standard deviation for each parameter should not influence the mean of the results. Monte Carlo simulations should only allow us to obtain an estimation of the error associated to the simulations. In the next chapter we will make a further analysis of this problem encountered.

6.5 Conclusions

We conclude that some of the values of crop carbon residue are very uncertain and insufficiently characterized by available data to enable a full analysis of the SOC dynamics and its uncertainty. The numbers obtained in the literature review were insufficient for accurate calculations of SOC changes for some LUCs. For cases such as barley, even though we selected the highest available value, the results obtained were below expected. Carbon residues are therefore a crucial parameter and future research efforts should clearly focus on obtaining better quality estimates. Another crucial parameter is soil cover. Independently of the crop carbon residues input given, the percentage of the year when the soil is covered can determine much of the fate of the accumulation of SOC.

For the case of Monte Carlo simulations, the results are all below the best estimate case. A deeper analysis to understand why the Monte Carlo simulations under estimate the results and the influence of the input parameters is done in the next chapter.

7. Estimation of SOC depletion due to land use with RothC - Determination of sensitivity to parameters

7.1 Summary

One of the main determinants of the results of RothC is crop carbon residues ($tCha^{-1}$). In the literature we found some of these values for Portugal and also for Mediterranean regions; we often found multiple values for the same crops and region, but with different magnitudes. For example, in the case of tomato, carbon residues range between 0.76 $tCha^{-1}$ and 64 $tCha^{-1}$, using the yield of tomato for Alentejo obtained from INE (2015) –values shown in Table 17. Climate variables obtained from INE and farmyard manure are also highly variable and influence results significantly. In this section, using the modified version of RothC presented in Chapter 6, we evaluate the role of each variable in results and find plausible domains of acceptable values. We made a statistical analysis, using different UHTUs with different characteristics in order to understand which values should be used for the calculation of CFs. For the case of the Monte Carlo simulation, the results obtained under estimated the expected results. For that reason, also in this chapter, we aimed to find the root of the problem and a possible solution.

7.2 Method

7.2.1 Parameter Sensitivity

After running 100 iterations of the modified RothC model for different regions, we used IBM SPSS 22 to adjust a linear regression model to our data. It was our intention to fit a linear equation where the independent variables were the inputs and the dependent variable was the output of RothC. Linear regression is used when we want to predict a value from a parameter, based on values of other parameters. At its core RothC consists of systems of non-linear equations, and as such the traceability of how each parameter influences results is reduced. The model has a tendency to be looked at as a "black box" and its results are often "just so" explanations. A linear approximation of the results using this statistical procedure was therefore aimed at obtaining a simplified insight on the role of each parameter as a determinant of the results.

The linear regression model, where $x's$ are the independent variables and y is the dependent variable, was defined as

$$y = \beta_0 x_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k + \varepsilon. \quad (12)$$

In the case of this dissertation, the dependent variable is the difference in SOC after 100 years and in the baseline year, after LUC. The independent variables are the inputs that the model takes in, i.e., mean monthly temperature, monthly pan evaporation, monthly precipitation, crop carbon residues, initial SOC and farmyard manure. The equation obtained from this linear regression takes the form

$$\Delta SOC\ [tCha^{-1}] = T \times x_0 + E \times x_1 + P \times x_2 + Res \times x_3 + SOCi \times x_4 + FYM \times x_5, \quad (13)$$

where ΔSOC is the SOC change along the 100 years, i.e. $SOC_{year\ 100} - SOC_{year\ 1}$, T is the mean monthly temperature, E is the monthly pan evaporation, P is the mothly precipitation, Res is the crop carbon residues, SOC_i is the initial SOC and FMY is the farmyard manure. The independent variables $x's$ are the correspondent mean values for the 100 iterations of T, E, P, Res, SOCi and FYM respectively.

After obtaining these linear regressions, it was possible to understand the weight that each RothC input has on the results. This analysis was made obtaining the linear regressions of different UHTUs with different characteristics.

7.2.2 Monte Carlo Simulations

To understand why the Monte Carlo simulations under estimate the expected results, we first ran the simulations for a different number of iterations. These first look lets us understand if 100 iterations are sufficient for the Monte Carlo simulation. First for 100 iterations, second for 200 iterations and then for 1000 iterations. All of these attempts were ran without changing the probability distribution of any parameters.

Next, to evaluate the distribution obtained by the random numbers obtained through Matlab for the normal distribution given, we ran the model several times for different numbers of iterations (100, 200, 300, 400, 500, 750 and 1000 iterations). In this case we programmed the Matlab version of RothC to provide as output not only the SOC changes but also all the values of the parameters obtained using the random numbers for each iteration.

For the last analysis, and for a 100 iteration simulation, we manually reduced the standard deviation of each variable in order to understand how the variability in input data influences the magnitude of final results.

7.3 Results

7.3.1 Parameters Sensitivity

We define the following acronyms used in this section: C is clay fraction in %, E is yearly Pan-Evaporation in mm, T is annual temperature in ºC, Res is the Crop Carbon Residues in $tCha^{-1}$, SOCi is the initial SOC input in $tCha^{-1}$, P is the yearly precipitation in mm, and FMY is the yearly farmyard manure in in $tCha^{-1}$.

In this section we present the results of the analyses made of each input parameter of RothC for three simulated crops (tomato, forage maize and oats). Table 20 and Table 21 describe the inputs of crop carbon residues for each crop, the characteristics of each UHTU simulated, and the goodness-of-fit statistics obtained by the regression model made with the help of IBM SPSS statistics program. The equations represent the regression model obtained for each UHTU and the graphs are a representation of the results of the regression model. The graphs represent the change of SOC content (i.e. $SOC_{year\ 100} - SOC_{year\ 1}$) depending on a particular parameter described: C, E, T, Res, SOCi, P and FMY.

In this first case we present an analysis for LUC to Tomato. The two UHTU used have different values of initial SOC in order to understand the impact of crop residue carbon in two regions that have different behaviours for the same simulation.

Table 20 - Table describing the crop carbon residues values used to simulate a land use change to tomato, the respective characteristics of the UHTU used in the simulation and the goodness-of-fit statistics obtained by the regression model obtained.

LUC TO TOMATO	
Crop Carbon Inputs	
FYM input (tC/ha): $\mathbf{9.9 \times 10^{-3}}$	
Standard deviation FYM: $\mathbf{3.6 \times 10^{-4}}$	
Crop Carbon Residues (tC/ha): $\mathbf{7.6 \times 10^{-1}}$ < tC/ha < $\mathbf{6.4 \times 10^{1}}$	
UHTU	
UHTU 1850 Non-Irrigated Arable Land	UHTU 776 Vineyards
Initial SOC = 80 (tC/ha)	Initial SOC = 39 (tC/ha)
Statistical Analysis	
$\boldsymbol{R^2 = 0.962}$	$R^2 = 0.955$
$\boldsymbol{Standard\ Error = 124}$	$Standard\ Error = 158$

FYM – farmyard manure; UHTU – unique homogeneous territorial units; SOC – soil organic carbon; R^2- coefficient of determination

Starting from the linear regression model described at equation 14 we obtained Figure 16. As we can observe, the values found at the literature review have complete different impacts for our simulations. If we used a value of 64 tC/ha (Ventrela et al., 2012; Ghanem et al., 2011), we would obtain a positive change on SOC values of 750 tC/ha, but if used a value of 0.76 tC/ha (Alves, 1995) we would obtain a loss of SOC of around 10 tC/ha. We can also observe that a change of 1 tC/ha results in a SOC change of 14 tC/ha.

$$\Delta SOC_{1850} = 11.172 * Res - 0.461 * P + 4.252 * E - 35.748 * T + 5.991 * C - 1.364 * SOCi + 40826 * FYM \quad (14)$$

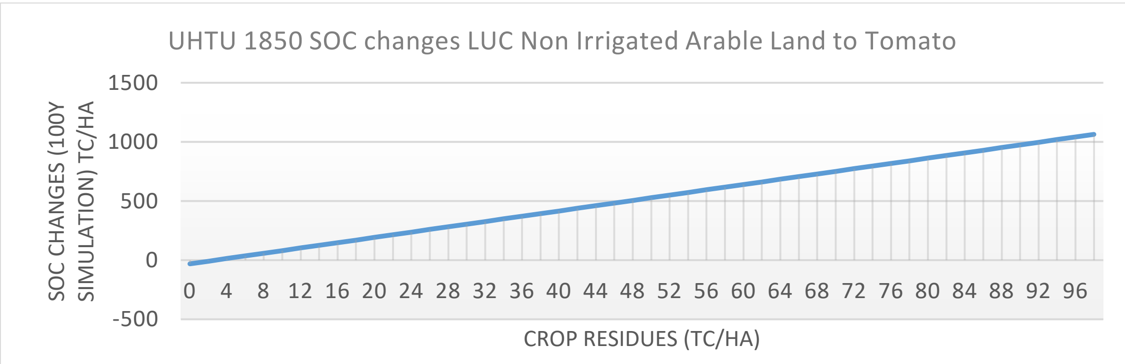


Figure 16- Relationship of SOC content changes for 100 year simulations to the crop carbon residues input. Land use change represented is from irrigated arable land to tomato.

SOC – soil organic carbon; UHTU – unique homogeneous territorial unit

In the case of UHTU 776 described by equation 15 and Figure 16 using a value of 64 tC/ha (Ventrela et al., 2012; Ghanem et al., 2011) would result in a SOC change even higher than the last example, of 800 tC/ha.

$$\Delta SOC_{776} = 14.013 * Res - 0.801 * P + 3.980 * E - 28.278 * T + 9.4 * C \quad (15)$$

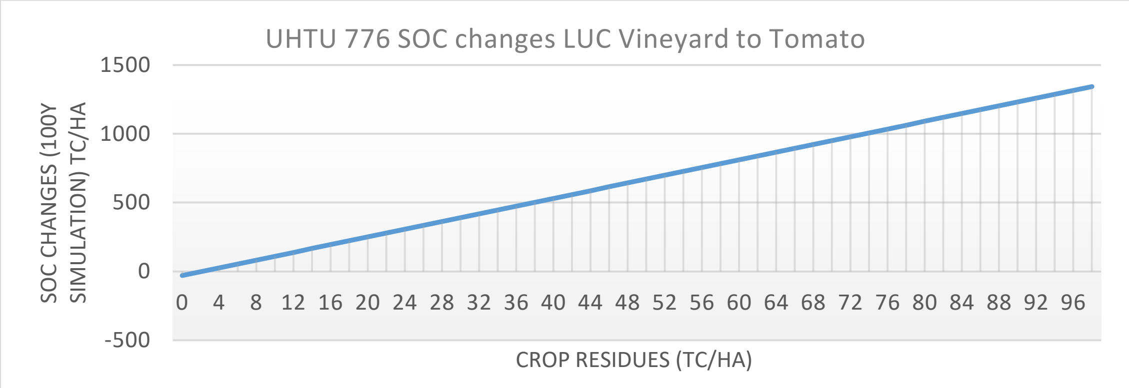


Figure 17- Relationship of SOC content changes for 100 year simulation to the crop carbon residues input. Land use change represented is from vineyard to tomato.

SOC – soil organic carbon; UHTU – unique homogeneous territorial unit

For the case of a LUC to forage maize the range of carbon residues analysed is lower than the previous case of a LUC to tomato.

Table 21- - Table describing the crop carbon residues values used to simulate a land use change to forage maize, the respective characteristics of the UHTU used in the simulation and the goodness-of-fit statistics obtained by the regression model obtained.

LUT TO FORAGE MAIZE	
Common Crop Inputs	
FYM input (tC/ha): $\mathbf{8.8} \times \mathbf{10^{-3}}$	
Standard deviation FYM: $\mathbf{3.2} \times \mathbf{10^{-3}}$	
Crop Carbon Residues (tC/ha): $\mathbf{5.2} \times \mathbf{10^{-1}}$< tC/ha < $\mathbf{4.8} \times \mathbf{10^{1}}$	
Specific UHTU	
UHTU 12 Urban	UHTU 1003 Pasture
Initial SOC = 34 (tC/ha)	Initial SOC = 62 (tC/ha)
Statistical Analysis	
$\boldsymbol{R^2 = 0.978}$	$R^2 = 0.970$
$\boldsymbol{Standard\ error = 42}$	$Standard\ error = 45$

FYM – farmyard manure; UHTU – unique homogeneous territorial units; SOC – soil organic carbon; R^2- coefficient of determination

For UHTU 1003 described by Figure 18 the results obtained verify again that a small change of crop carbon residues input has a major impact on the final results of SOC changes. In this case a change of 1 tC/ha will result in a SOC change of 12.5 tC/ha. If we used a value of crop carbon residue of 48 tC/ha (Berenguer et al., 2009; Vamereli et al., 2003) we would obtain an increase of SOC stocks of almost 600 tC/ha for both UHTU 1003 described at Figure 18 and UHTU 12 described at Figure 19.

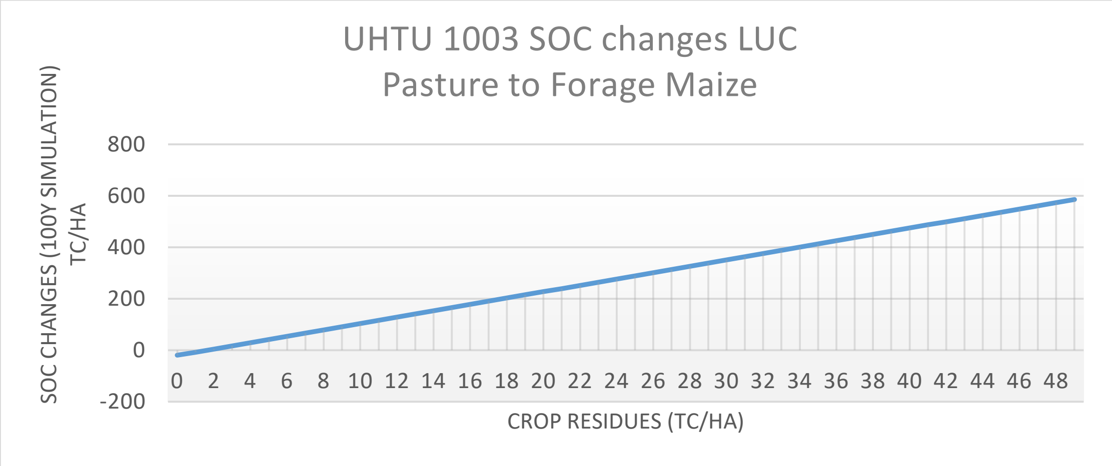


Figure 18 - Relationship of SOC content changes for 100-year simulation to the crop carbon residues input. Land use change represented is from pasture to forage maize.

SOC – soil organic carbon; UHTU – unique homogeneous territorial unit; LUC – land use change

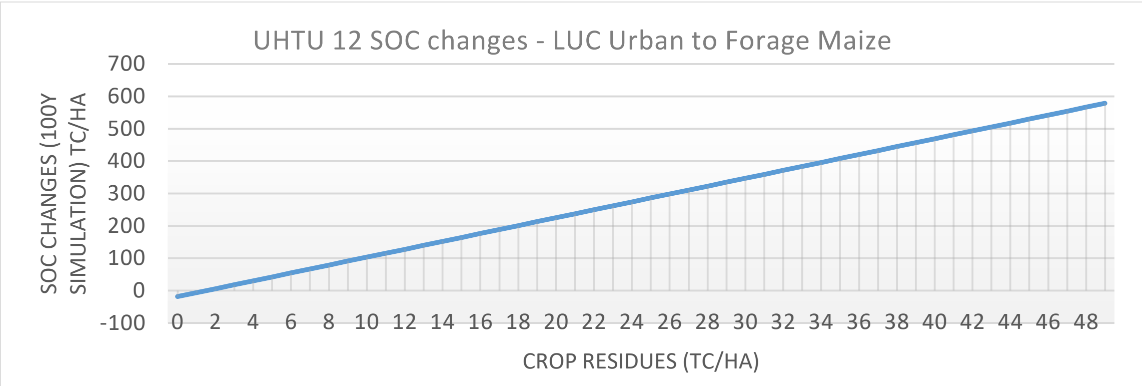


Figure 19- Relationship of SOC content changes for 100-year simulation to the crop carbon residues input. Land use change represented is from pasture to forage maize.

SOC – soil organic carbon; UHTU – unique homogeneous territorial unit; LUC – land use change

For the next cases, instead of analysing the crop carbon residues, we analyse the other input parameters of RothC, i.e., pan evaporation, precipitation, temperature, farmyard manure, SOC initial value and clay fraction. In the first two cases we are in the presence of two parameters that are the opposite of the other. For pan evaporation, we can see that the higher the values, more SOC gains will be obtain. On the other hand, for precipitation, a lower value for precipitation will result in a higher gain of SOC.

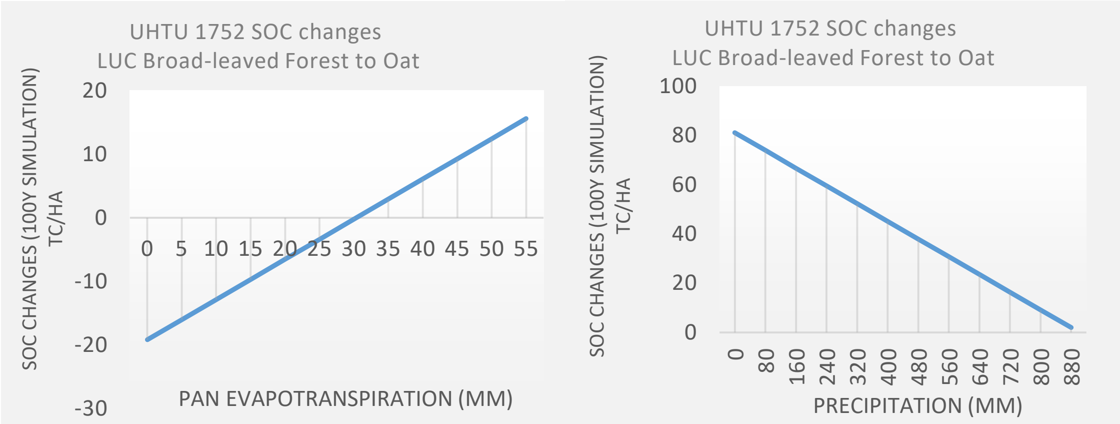
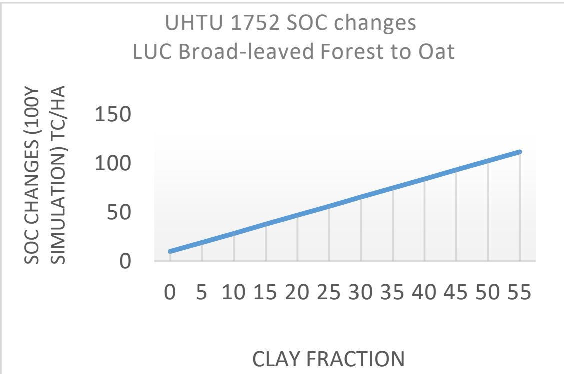


Figure 20- Representation of the effect of the parameters of Pan Evaporation (image on the left) and precipitation (image on the right) to the SOC stocks for a case of LUC from broad-leaved forest to oat – UHTU 1752.

SOC – soil organic carbon; UHTU – unique homogeneous territorial unit; LUC – land use change

Next, for the case of clay fraction and temperature we can see that these parameters have a similar effect to SOC results, where the higher each of the inputs will enable a higher gain of SOC.



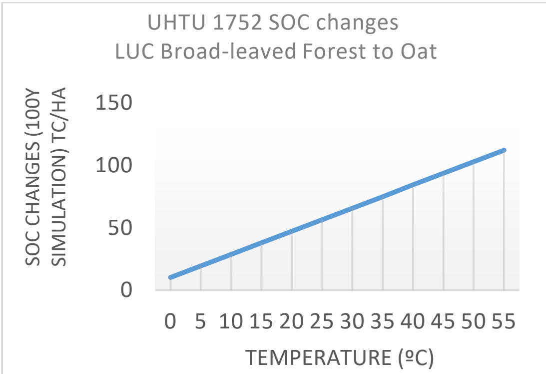


Figure 21- Representation of the effect of the parameters of clay fraction (image on the left) and temperature (image on the right) to the SOC stocks for a case of LUC from broad-leaved forest to oat – UHTU 1752.

SOC – soil organic carbon; UHTU – unique homogeneous territorial unit; LUC – land use change

For the initial SOC input parameter, we can observe that, the higher the value of initial SOC, the lowest gain on SOC will be obtained. On the other hand, farmyard manure has the opposite effect, where a higher value will result in a higher SOC gain.

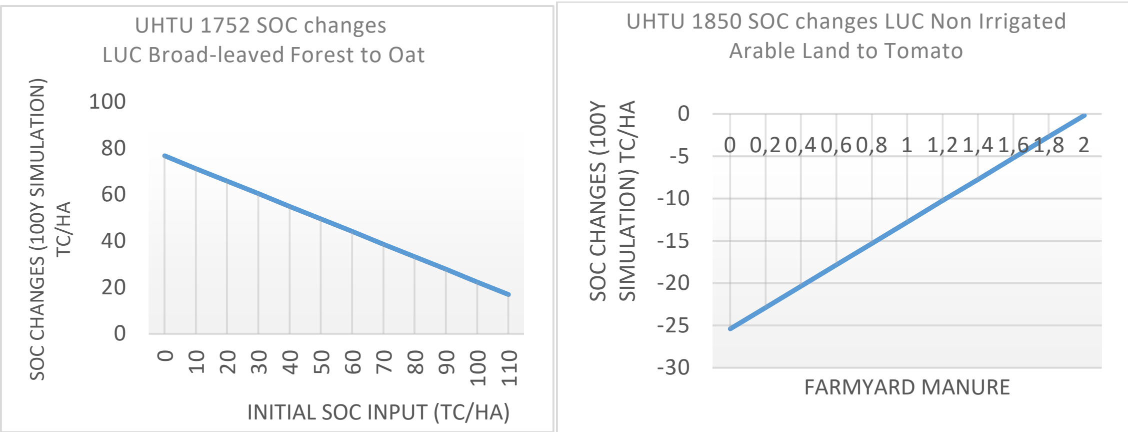


Figure 22 - Representation of the effect of the parameters of initial SOC input (image on the left) and manure (image on the right) to the SOC stocks for a case of LUC from broad-leaved forest to oat – UHTU 1752.

SOC – soil organic carbon; UHTU – unique homogeneous territorial unit; LUC – land use change

7.3.2 Monte Carlo Simulations Sensitivity Analysis

First, in order to understand if 100 iterations for simulations are enough to obtain a Monte Carlo simulation, we ran RothC model for 100 iterations, 200 iterations and 300 iterations. The simulations are for a LUC to wheat. The results are described at Table 22. We can see that, even if we increase the number of iterations, the values do not change significantly. Also, there is no trend visible, i.e., we cannot say that if we run more iterations, all the results will approximate to the best estimate case.

Table 22- SOC change mean values for best case estimate, 100 iterations, 200 iterations and 300 iterations simulations. Land use change to wheat.

SOC changes tC/ha	Best Estimate Case	100 iterations	200 iterations	300 iterations
Artificial Surfaces	-1.39	-6.28	-6.18	-6.08
Non-Irrigated Arable Land	-3.60	-7.90	-7.84	-7.91
Pastures	-9.50	-15.28	-15.26	-15.22
Wetlands	-12.69	-16.39	-16.10	-15.58
Permanently Irrigated Land	0.21	-3.65	-3.55	-3.48
Rice	-0.85	-4.51	-4.30	-4.37
Vineyards	2.75	-2.25	-2.20	-2.40
Fruit trees and berry plantations	2.75	-2.13	-2.25	-2.35
Olive Groves	-0.06	-4.51	-4.45	-4.59
Agro-forestry areas	-6.67	-10.93	-10.93	-10.99
Broad-leaved forest	-13.00	-17.31	-17.17	-17.29
Coniferous forest	-16.40	-20.95	-20.45	-20.57

SOC changes tC/ha	Best Estimate Case	100 iterations	200 iterations	300 iterations
Mixed Forest	-17.31	-21.11	-20.95	-20.96
Forest	-13.90	-18.41	-18.20	-18.21

SOC – soil organic carbon

For this next approach, we made different simulations, with a different number of iterations, in order to understand the distribution of the parameters obtained by the random values equation given to Matlab. The parameter here evaluated is the pan evaporation for January, for UHTU 2. The mean value given was 45.8 mm and the standard deviation was 45.7 mm.

The following histograms describe the distribution of the pan evaporation values for January, for 100 iterations and 1000 iterations. For these simulations, a code line prevented the Matlab random values generate negative values.

Figure 23 shows that the generated values for pan evaporation do not have a regular normal distribution. The values obtained are over estimated. This was due to the large standard deviation, which enabled the selection of very large pan evaporation.

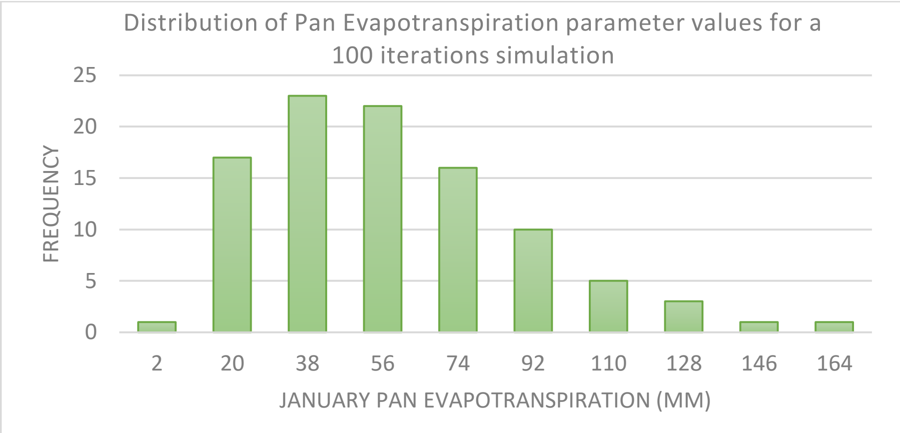


Figure 23- Histogram describing the distribution of pan evaporation parameter values, generated from a random numbers code line on Matlab, for a normal distribution, for 100 iteration simulation.

Figure 24 shows that again the distribution is over estimated and that the values nearer the mean value given are over estimated too, from a range since 30 to 75 mm.

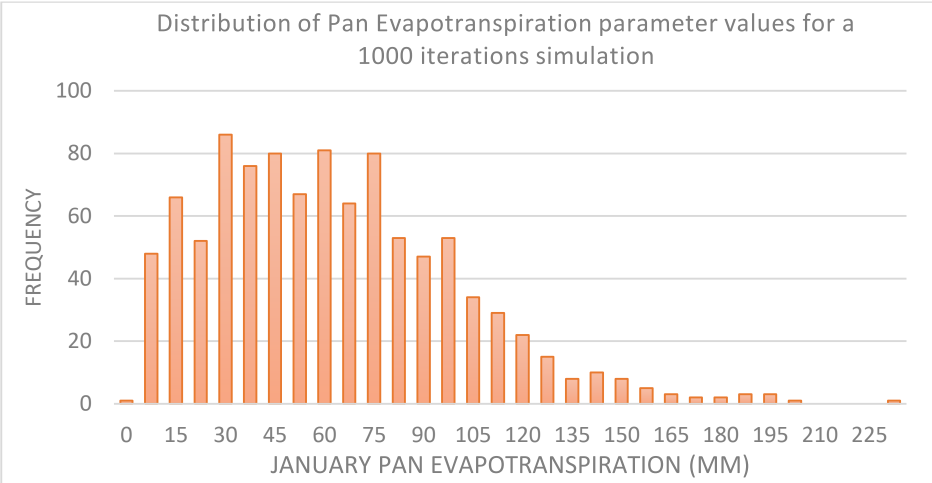


Figure 24- Histogram describing the distribution of pan evaporation parameter values, generated from a random numbers code line on Matlab, for a normal distribution, for 1000 iteration simulation.

Figure 24 shows that the distribution of values will not improve with more iterations for each simulation and there is no trend defined as the number of iterations rise. The value that approximates the mean value given for this parameter is for the case of 100 simulations.

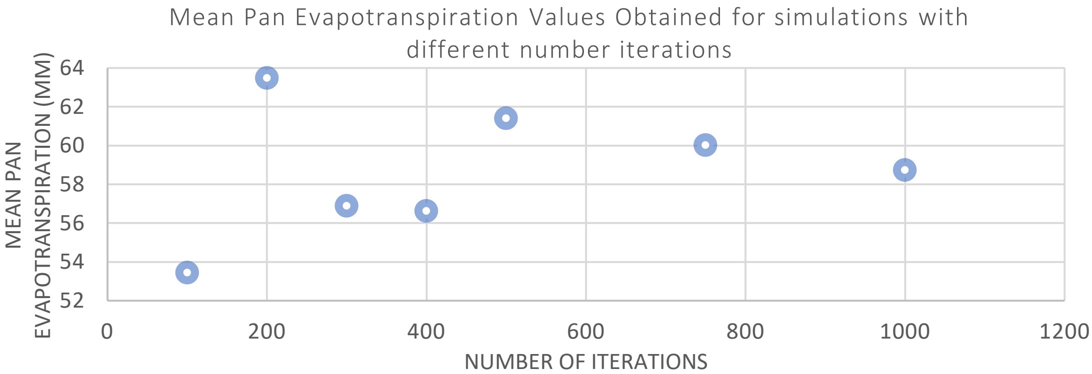


Figure 25 - Mean pan evaporation values generated on the random number code line of Matlab, for a normal distribution, for simulations with different number of iterations.

For the last analysis, we reduced the deviation standards, for all the parameters that had a normal distribution (i.e. pan evaporation, temperature, precipitation, initial SOC content and initial clay fraction). We ran three different times the simulations, each time with different standard deviation values. First, we reduced by half the standard deviation, secondly we reduced by one third of the original standard deviations, and last we divided by 1000 the original standard deviations. Table 22 presents the SOC changes, i.e. $SOC_{year\ 100} - SOC_{year\ 1}$ for a LUC to wheat.

The first and second column presents the values already obtained before for the best estimate case and the 100-iteration simulation, the latter with the original standard deviations. The three following columns represent the results obtained with the reduced standard deviations.

The results depicted in Table 22 show that lower standard deviations will consequently approximate the SOC changes values obtained from RothC simulations to the best case estimate results. This assessment provides validation of the Matlab program and shows that the differences between best estimate scenarios and iterative results was not the result of a computational problem but rather of poor quality input data.

Table 23 – Results obtained through the simulations of RothC for five different usages of the standard deviation.

SOC change (tC/ha)	Best Case Estimate	Original SD	SD/2	SD/3	SD/1000
Artificial Surfaces	-1.39	-6.36	-4.15	-3.46	-1.45
Non-Irrigated Arable Land	-3.59	-7.89	-6.09	-5.44	-3.65
Pastures	-9.50	-15.20	-13.03	-12.06	-9.56
Wetlands	-12.69	-15.99	-13.26	-12.95	-12.73
Permanently Irrigated Land	0.20	-3.68	-2.05	-1.42	0.15
Rice	-0.84	-4.32	-2.73	-2.33	-0.90
Vineyards	2.75	-2.28	-0.12	0.77	2.69
Fruit trees and berry plantations	2.74	-2.28	0.05	0.74	2.69
Olive Groves	-0.06	-4.57	-2.51	-1.87	-0.11
Agro-forestry areas	-6.67	-10.90	-9.23	-8.64	-6.73
Broad-leaved forest	-13.00	-17.39	-15.47	-14.80	-13.06
Coniferous forest	-16.39	-20.36	-18.82	-18.38	-16.45
Mixed Forest	-17.31	-20.94	-19.00	-18.61	-17.36
Forest	-13.89	-18.53	-16.25	-15.78	-13.95

The first results correspond to the best case estimate, i.e., no standard deviation is used. Then the second results are for the original standard deviations obtained from the calculation of the parameters. The last three results correspond to the simulations where we diminish the standard deviation values. SOC – soil organic carbon.

7.4 Discussion

7.4.1 Parameters Sensitivity

For the case of pasture, the mean value of SOC according to LUCAS topsoil data (Brogniez et al., 2015) and the CLC classification (2006) for permanent pastures land is 65 tC/ha and 15.73 clay fraction. This means that, UHTU 3 that has an initial value of 43 tC/ha, will presumably increase its SOC along 100-years. This does not happen in the condition where Crop Carbon Residue is 0.8 tC/ha, that is the only value obtained on the literature review for pasture. For this specific case, to start increasing SOC the monthly crop carbon residue needed to be higher than 1.22 tC/ha. It is expected then, that the values obtained for our simulations for LUC to pasture will be, overall, below expected.

Tomato crops can be included in the permanently irrigated land classes, according to the classification of the CLC (2006). The mean values of the current initial SOC of permanently irrigated land (Brogniez et al., 2015) is 43 tC/ha and a mean of clay fraction of 17. UHTU 1850 that has an initial SOC value of 80 tC/ha, should have its SOC values decreased along the years. For this to happen, its crop carbon residue should be lower than 2.77 tC/ha. If we used a value similar to the one obtained using the harvest index ratios recommended by Ventrela et al. (2012) and a shoot-to-root ratio recommended by Ghanem et al. (2011), we would have obtained an increase of SOC of almost 750 tC/ha in 100-years. Also, analysing UHTU 1062, we would obtain an increase even higher, around 850 tC/ha. Also, any value above 2.77 tC/ha is inaccurate. This value, for UHTU 1850 means that SOC will remain steady in the values of 80 tC/ha, although this value is twice higher the one expected.

Forage maize can also be included in the permanently irrigated land classes (CLC, 2006). For this particular crop, it is expected that the crop carbon residue taken into account, will be a lower value because this type of crop is harvested early and the harvest is complete (no residues are left on the field). For UHTU 1003, it is likely that SOC decreases after conversion to forage maize. For this to happen, crop carbon residues need to be less than 1.58 tC/ha. In the case of UHTU 12, it is expected for the values to remain constant, thereby values around 1.59 tC/ha would be considered. The only value closer to this estimative is 1 tC/ha, which is recommended by Knaber (2002). For instance, a value such as the one recommended by Berenguer et al. (2009) and Vamereli et al. (2003) of 21 tC/ha would lead to an increase of more than 200 tC/ha for the two regions analysed.

Oats can be aggregated into the non-irrigated arable land class (CLC, 2006). The mean value of SOC content is 50 tC/ha. In the case of UHTU 2 it is expected for the values to remain constant. In order for this value not to decrease, the crop carbon residue would have to be 1.62 tC/ha. UHTU 1752 has a forest LU. The most probable for this region is that the SOC content decreases when changing its LU to oat. For this to happened the values of crop carbon residues need to be lower than 3 tC/ha. In order to choose a value lower than 3 tC/ha, the only value gathered in the literature review is 1.354 tC/ha proposed by ISPRA (2016).

Overall, the message of this analysis is that small changes in carbon residues result in over-magnified consequences for SOC loss/accumulation. As we can see in Table 27 of the Appendix, the values obtained in our literature review have different magnitudes, which makes the decisions of SOC modellers critical. For instance, for shrublands the values proposed are 0.68 tC/ha and 4.96 tC/ha. If used alternatively, they will result in completely different SOC dynamic profiles.

An increase in clay fraction, initial SOC, crop carbon residues and manure result in larger SOC gains. Pan evaporation and precipitation are always positive. In the case of pan evaporation, there is a threshold for SOC gains and losses (around 30 mm per month). Values such this are not frequent and happen normally in the months of January and February (INE). In the case of precipitation, it is possible, starting from a value of 880 mm per month, to start depleting SOC stocks, but such precipitation does not occur in the Alentejo region. At most, precipitation in one month is approximately 200 mm. Monthly temperature increases, similarly to pan evaporation, lead to higher SOC gains. A higher value of initial SOC implies that the probability for SOC content increases is lower. Farmyard manure has a limited role in determining SOC increases. It would take a higher value of manure than, for example, crop residues, to enable a similar increase in SOC stocks.

7.4.2 Monte Carlo Simulations

The results obtained and shown in Table 22 demonstrate that increasing the number of iterations does not necessarily approximate the average results of all iterations to the best estimate results, i.e. results obtained using the average of each parameter. When there is more than one option for carbon in crop residues, a parameter with a uniform probability distribution, the two approaches were not expected to lead to the same results necessarily. However, when there is only one estimate available for carbon in residues, since all other variables are normally distributed, the two approaches should result in approximately the same SOC increase/decrease. Our analysis shows that the mismatch is not due to a low number of iterations (long time to converge). As we can see in Figure 23, Figure 24 and Figure 25, the probability distributions for pan evaporation values will not get more accurate while increasing the number of iterations. Also, in Figure 25, the best case that approximates the mean values obtained for pan evaporation is the case where we used less iterations (i.e. 100 iterations).

The results of the two approaches only converge if the standard deviation of input variables decreases. This shows that the root of the problem with our Monte Carlo simulations lies on the high values of standard deviation given to RothC, which in this case are due to low quality data (insufficient number of years and lack of meteorological stations, for example).

7.5 Conclusion

This analysis of the crop carbon residues input explained the main conclusions of Chapter 6 and the magnitude of the results obtained. We conclude that there are critical data gaps for this parameter. We obtained disparate estimates from the literature review conducted. For the generalization of the procedure established in this dissertation, more and better quantifications of the carbon content of plant residues are essential. This is a limitation that we were unable to overcome in this work, so as a tentative solution we opted to limit the values used to the ones that we believe to be more accurate or credible, considering expected results. This is a strong limitation for the application of the analysis in calculations of CFs (Chapter 9), which should therefore only be considered demonstrative.

For the Monte Carlo simulations, we can conclude after our analysis that data limitations for other variables (namely the climate variables) also prevent us from establishing the uncertainty of results. In order to overcome the problems, in the future the input values given to RothC should be recalculated, or obtained from better quality sources with lower deviation standards. Also, another solution for the parameters of initial SOC and clay fraction would be to desegregate the UHTUs even more, i.e., have more UHTUs for the same area. This approach would not result for the climate data because these data were obtained using 12 meteorological stations, which were the only freely available stations with data for several years in the study area. Due to these limitations, we do not present an uncertainty analysis for the CFs in Chapter 9.

8. Estimation of SOC depletion due to land use with RothC - Curve Fitting Equations

8.1 Summary

As explained in the previous section, a Matlab implementation of RothC was one of the outcomes of this thesis in order to fasten calculation time and perform Monte Carlo simulations on input parameters. For the purposes of this dissertation, we ran the modified RothC model for 100 iterations for all the UHTU. The model gives an output of SOC values for each simulated year. Graphically, this represents a curve that can be increasing or decreasing along with the time. This curve is a complex shape, but it can be approximated using simpler curves. Considering that the calculation of CFs shown in the next section requires the calculation of integrals, simplifying the shape of the curve was useful in our work. In this section, in order to calculate the CFs, found the best fit to each SOC curve.

8.2 Method

To find the equations that best fit each curve depicting the changes of SOC during 100 years, we made a routine in Matlab that allows, with the help of the Curve Fitting Application, to estimate the best linear regression fit to each set of data. Matlab is able to adjust different equations. We tried every type of fit with no more than three coefficients to avoid statistical over-specification. The different fits available in the Matlab Curve Fitting Application are described by Table 24.

Table 24- Curve fitting equations available in the Matlab Curve Fitting Application, with three or less coefficients.

Curve Fit	General Formula
Exponential (1st degree)	$f(x) = a\ exp^{(bx)}$ (16)
Fourier (1st degree)	$f(x) = a + bcos(xw) + csen(xw)$ (17)
Gaussian (1st degree)	$f(x) = aexp^{(-\left(\frac{x-b}{c}\right)^2)}$ (18)
Polynomial (1st degree)	$f(x) = p_1x + p_2$ (19)
Polynomial (2nd degree)	$f(x) = p_1x^2 + p_2x + p_3$ (20)
Power (1st degree)	$f(x) = a * x^b$ (21)
Power (2nd degree)	$f(x) = a * x^b + c$ (22)
Rational (1st denominator degree and zero numerator degree)	$f(x) = \frac{p_1}{q_1+x}$ (23)
Rational (1st denominator degree and 1st numerator degree)	$f(x) = \frac{p_1x + p_2}{q_1+x}$ (24)
Sum of Sine (1st degree)	$f(x) = asen(bx + c)$ (25)
Weibul	$f(x) = abx^{(b-1)}exp^{(-ax^b)}$ (26)

We analysed the next goodness-of-fit statistics also obtained in the Matlab Curve Fitting Application: sum of squares due to error (SSE), coefficient of determination (R^2), degrees of freedom, adjusted R^2 and root mean squared error (RMSE). The SSE is used to calculate the total deviation between the observed values in the data set against the predicted values obtained from the fit. A lower value of SSE indicates that the fit presents a lower random error. The R^2 value may be defined as the square of the correlation between the observed values in the data set against the predicted values. It is a value between 0 and 1 and it is used to understand the variation of the data where R^2 closer to 1 represents a better fit. The adjusted R^2 takes into account the degrees of freedom. The degree of freedom is a statistics defined by the number of sample size minus the number of coefficients estimated from the predicted values model. RMSE represents the standard error of the fit. A value closer to 0 represents a better fit. Also, in order to evaluate the goodness of the fits, we made a residual analysis. The residuals obtained from a fit model are defined by the difference of the data given to the model against the predicted values of the fit. The objective of plotting the residues, is to analyse if the values fitted by the model are randomly distributed, i.e. if there is no trend above or below of the observed values and no correlation with the dependent variable (Rawlings et al., 1998).

8.3 Results

We adjusted each dynamic SOC curve of SOC separately for each UHTU and for each simulation. We chose the best three fits to present results in this section: Polynomial 2nd degree, Exponential 1st degree and Power 2nd degree. All other options adjusted worse to the data. For each fit we present results: in Table 25 for a decreasing curve and Table 25 for an increasing curve.

The first curve evaluated was the decreasing curve. The goodness-of-fit results are presented in Table 24. Power 2nd degree has better fit than others, even though every fit has a R^2 approximated to 1. Polynomial 2nd degree presents the highest value of SSE and RMSE.

Table 25- Evaluation on the best fit for an increasing curve obtained in RothC model for UHTU 106.

Curve Fitting Type UHTU 106	**Polynomial 2nd degree**	**Exponential 1st degree**	**Power 2nd degree**
General model	$f(x) = p1 * x^2 + p2 * x + p3$	$f(x) = a * \exp(b * x)$	$f(x) = a * x^b + c$
SSE	29.22	0.65	0.55
R^2	0.9915	0.9914	0.9998
DFE	97	99	97
Adj R^2	0.9913	0.9913	0.9998
RMSE	0.54	0.081	0.075

UHTU – unique homogeneous territorial unit; R^2- coefficient of determination; SSE - sum of squares due to error; adjusted R^2 - degrees of freedom; RMSE - root mean squared error

Figure 25 represents the fit obtained for a Power 2nd degree curve fitting type, where the black points are the sampled values, and the blue line is the curve obtained by the fit. We can see that, even though the blue line adjusts well to the data, the distribution with time of the difference between predicted SOC data by the model and RothC model results (Figure 27) has a distinct pattern. The fitted curve over-estimates and under-estimates the sampled values in diferent regions of the graph. Most importantly, after approximately 90 years, the fitted model underestimates RothC results. At the Appendix we present in Figure 40 and Figure 42 the curve fit and residuals plot for exponential 1st degree and polynomial 2nd degree fit, both for decreasing curves.

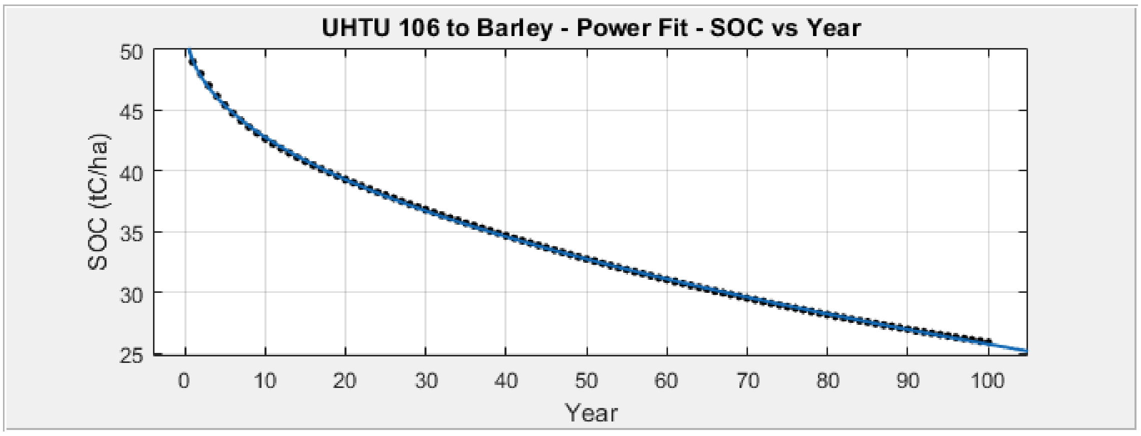


Figure 26- UHTU 106 SOC values through 100 years (points) and respective curve fit (blue line) obtained by 2nd degree Power Equation.

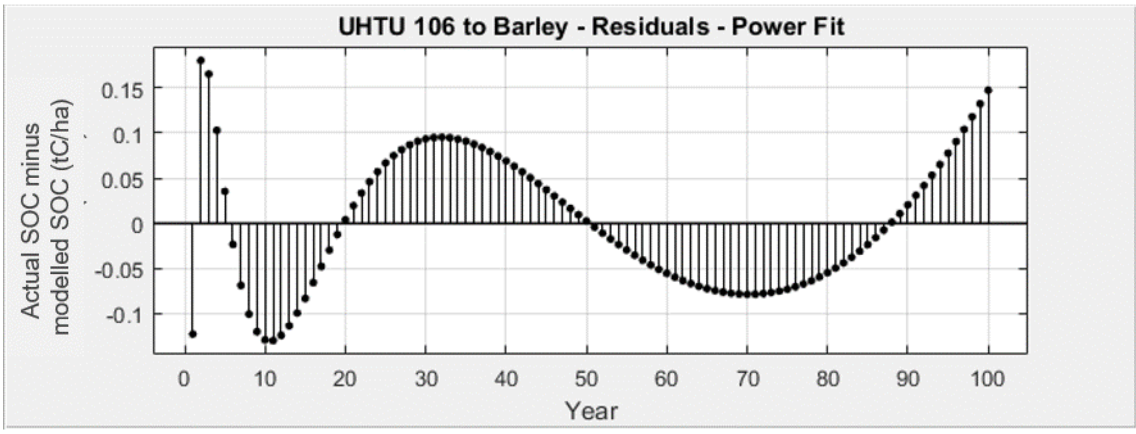


Figure 27- UHTU 106 residuals obtained in the curve fitting described in Figure 26.

In the case of an increasing curve, we can see in Table 26 that all the fits also have high R^2. Exponential fit has the highest values of SSE and RMSE. Also Polynomial fit has a high SSE value.

Table 26- Evaluation on the best fit for an increasing curve obtained in RothC model for UHTU 1.

Curve Fitting Type UHTU 1	Polynomial 2nd degree	Exponential 1st degree	Power 2nd degree
General model	$f(x) = p1 * x^2 + p2 * x + p3$	$f(x) = a * \exp(b * x)$	$f(x) = a * x^b + c$
SSE	3.31	29.92	0.39
$\boldsymbol{R^2}$	0.9930	0.9370	0.9992
DFE	97	98	97
Adj $\boldsymbol{R^2}$	0.9929	0.9364	0.9991
RMSE	0.18	0.55	0.063

UHTU – unique homogeneous territorial unit; R^2- coefficient of determination; SSE - sum of squares due to error; adjusted R^2 - degrees of freedom; RMSE - root mean squared error

The curve fit obtained for Power 2nd degree fit of an increasing curve is shown in Figure 28 and Figure 29 shows us that, even though there is good apparent fit, the temporal distribution of residuals is not random. We can see that the curve is underestimated at the beginning and ending, and overestimated in the middle. The curve fits and residuals plot for the Exponential and Polynomial fits for an increasing curve are depicted in the Appendix in Figure 40 and Figure 41 respectively.

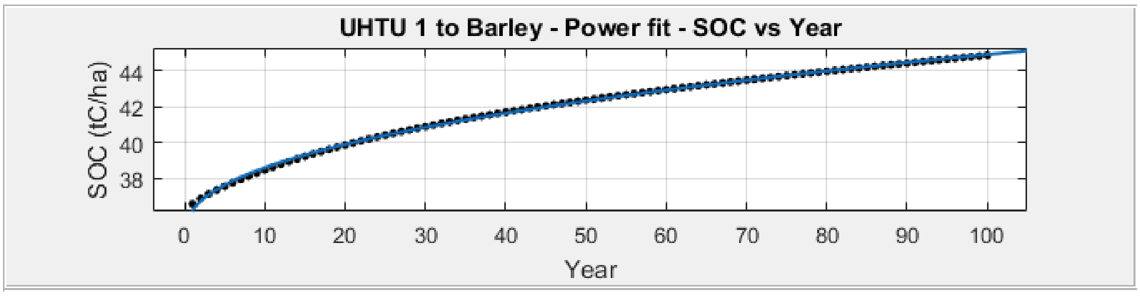


Figure 28- UHTU 1 SOC values through 100 years (points) and respective curve fit (blue line) obtained by 2nd degree Power Equation.

SOC – soil organic carbon; UHTU – unique homogeneous territorial unit

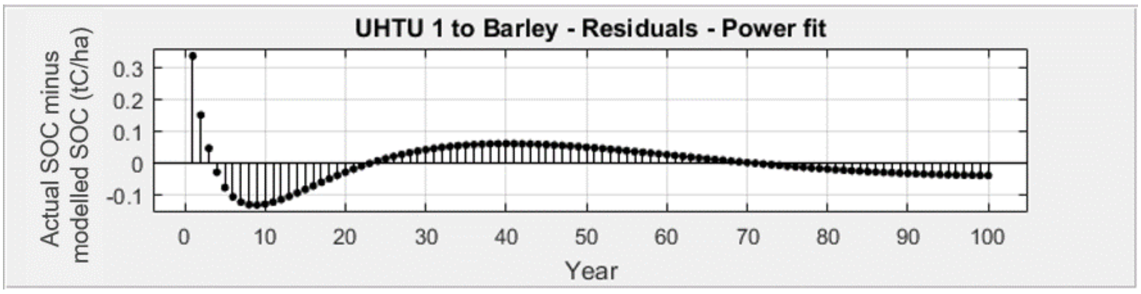


Figure 29- UHTU 1 residuals obtained in the curve fitting described in Figure 28.

SOC – soil organic carbon; UHTU – unique homogeneous territorial unit

8.4 Discussion

The Curve Fitting Application on Matlab has ten different models with three or less coefficients. After trying all of the fit models in a primary analysis of the fit graphs, we concluded that the three best fits were: Polynomial 2nd degree, Exponential 1st degree and Power 2nd degree. Looking at the results presented above in section 8.3 we can observe that $R^2$is insufficient to choose the best fit. On its own, R^2 shows that the three fits are accurate, but when analysing for instance the SSE, we can see that Polynomial is slightly better than the Exponential and Power fits. The curves analysed also have different goodness of fit statistics depending on their orientation (i.e. increasing or decreasing curves). Even though the Power fit was a better option (i.e. lower SSE and RMSE, higher R^2 and adjusted R^2), Exponential fit behaves almost has good as Power fit. This last comparison is not true when assessing an increasing curve. The Power model fits the SOC curve better in both cases (increasing and decreasing) according to the observed values. After the goodness-of-fit analysis, we also assessed the residuals plot for the three fits. Residuals are never randomly distributed as a function of time. There are biases towards under or overestimating the results of the model for earlier or later time. Consequently, no single curve is a fully accurate representation of the results. Overall, the Power fit presents lower residues than the other fits, even though under estimating and over estimating the results in some regions of the curves.

8.5 Conclusions

We can conclude that a simple analysis of R^2 and adjusted R^2 is not enough to evaluate which fit is the most accurate. It is important to take into account a wider analysis with different statistics to make conclusions. Even though for all the cases the R^2 values are approximately equal to 1, we can see that some models do not fit the data as well, presenting high residue values in the cases of Polynomial and Exponential fits.

Also, even though this Power fit is not perfectly fitted to the observed models, we can conclude that it is a good approximation for our intended purposes. As we are calculating CFs in the next Chapter that are the accumulated SOC gain/loss, the regions of the curves that under and overestimate the results of RothC cancel out. We need to take into account that we are trying to fit, in one equation with no more than three coefficients, the behaviour of a complex non-linear model (RothC), thereby the approximations to one equation cannot ever be 100% accurate. We also concluded that even if we chose a fit with more than three coefficients, according to the results, the R^2 value will not ever be better more that 1% of what already is.

9. Calculation of Characterization Factors

9.1 Summary

After running RothC simulations and obtaining an equation that describes the behaviour of each curve, in this final section, we present the method of calculation of the CFs using the curve that fits RothC results best. The model described in this dissertation addresses both land transformation CFs and land occupation CFs. As already explained, to obtain the dynamic curves of SOC change along 100 years, we used RothC to simulate agricultural, shrubland, forest and grassland LU. We model the following biotic LU: 13 agricultural LU classes, 5 forest classes, shrubland and grassland, starting from an initial LU1 that can be each one of the reclassified CLC (as described in Table 6Table 6).

9.2 Method

The CFs determine the accumulated effect of dynamic changes in SOC due to LUC. In order to measure these impacts, we chose two different reference states to evaluate: the current LU before transformation (LU1) and PNV. The first choice of reference state is a historical baseline while the second is a semi-natural baseline. Also, for each reference state we can encounter two different situations: when LU1 is equal to LU2, and when LU1 is different than LU2. These four situations are described in Figure 30, Figure 31, Figure 32 and Figure 33, where LU1 is the current LU, LU2 is the next (intended) LU after the transformation from LU1, PNV is the potential natural vegetation and SOC_{INI} is the initial value (year 1) of SOC in a given LU1. For example, a transformation CF will measure the total depletion of SOC in a “transformation to rainfed barley” in a given UTHU when LU2 is rainfed barley, LU1 is the current LU in that UHTU, and PNV is the natural vegetation in the same region. The PNV of each UHTU was obtained by the overlapping of the UHTU regions with a map of historical estimations in global land cover (Ramankutty and Foley, 1999). Occupation CFs are obtained as the difference between the final SOC value of the reference state minus the final SOC value of LU2. In the case of the transformation CF, this is defined as the difference between SOC stock of the change from LU_{PNV} to LU2 minus the difference between SOC stocks from the change from LU_{PNV} to LU1.

The framework presented here is based on Koellner et al. (2013a) with slight modifications. While Koellner et al. (2013a) compare static situations, our scenario-based model required the adjustments described next.

9.2.1 LU1 as reference state

In the first case, where LU1 is equal to LU2, there is no LUC, and SOC only changes due to the influence of soil, climate and management parameters. The occupation CF will be the last value of SOC for LU1 minus the last value of SOC for LU2. The transformation CF is defined as the area below the curve of SOC for LU1 minus the area of SOC for LU2. In this case, both of transformation and occupation CFs are zero. Equations (27) to (35) for the next four cases describe the CFs of occupation (CFoccupation) and the CFs of transformation (CFtransf). Figure

30 represents the SOC changes when LU1 is equal to LU2. Equations (27) and (28) describe how the CFs are obtained.

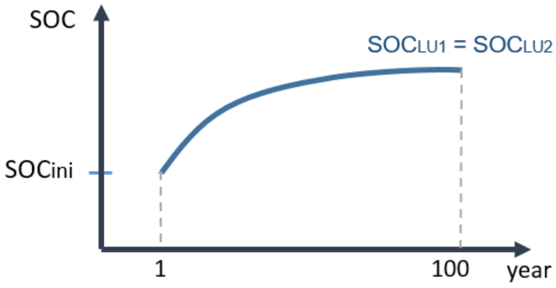


Figure 30- Schematic representation of the calculation of CF when LU1 is equal to LU2 and LU1 is the reference state.

SOC – soil organic carbon

$$CFoccupation = SOC_{100\_LU1} - SOC_{100_{LU2}} = 0 \quad (27)$$

$$CFtransf = \int_1^{100} SOC_{LU1}\, dx - \int_1^{100} SOC_{LU2}\, dx = 0 \quad (28)$$

In this second case, LU1 and LU2 are different and as such there is LUC from LU1 to LU2. The occupation CF is the equilibrium value of SOC (assumed to be SOC after 100 years) for LU1 minus the equilibrium value of SOC for LU2 while the transformation CF is going to be the area below the curve of SOC for LU1 minus the area of SOC for LU2. The CFs are represented in Figure 31 and are obtained according to equations (29) and (30).

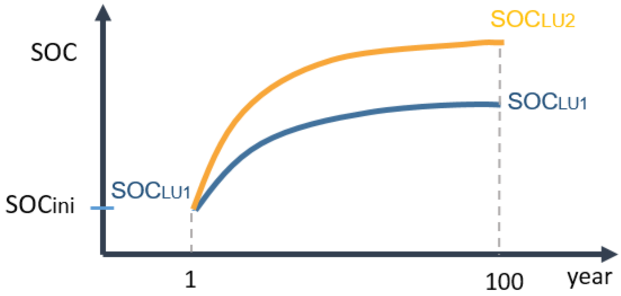


Figure 31- Schematic representation of the calculation of CF when LU1 is different than LU2 and LU1 is the reference state.

SOC – soil organic carbon

$$CFoccupation = SOC_{100\_LU1} - SOC_{100\_LU2} \quad (29)$$

$$CFtransf = \int_1^{100} SOC_{LU1}\, dt - \int_1^{100} SOC_{LU2}\, dt. \quad (30)$$

9.2.2 PNV as reference state

In this third situation, there is no LUC because LU1 is equal to LU2. The occupation CF is going to be the difference of the last SOC for the PNV SOC curve minus the last value of SOC for LU2. The transformation CF is obtained through the difference of the areas below the SOC curve for LU1 against the SOC curve of PNV minus the difference of areas for SOC curve of LU2 against the SOC curve area of PNV. Thereby, as it is possible to see by equations (31) and (32) the transformation CF is zero. Occupation CF is not zero unlike the first case described above.

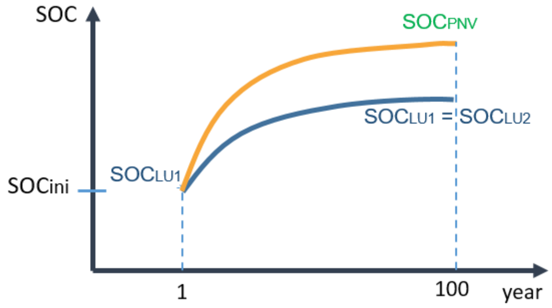


Figure 32 - Schematic representation of the calculation of CF when LU1 is equal to LU2 and PNV is the reference state.

SOC – soil organic carbon; PNV – potential natural vegetation

$$CFoccupation = SOC_{100\_PNV} - SOC_{100\_LU2} \tag{31}$$

$$CFtransf = \left(\int_{1}^{100} SOC_{LU1}\,dt - \int_{1}^{100} SOC_{PNV}\,dt\right) - \int_{1}^{100} SOC_{LU2}\,dt - \int_{1}^{100} SOC_{PNV}\,dt = 0. \tag{32}$$

The last case is the most complex and it involves more than a 100-year simulation. While all other cases are a direct adaptation of Koellner et al. (2013), this case is a departure because the authors of the reference model consider instantaneous transformations while, in the case of our approach, even when there is no LUC there are still SOC changes. The framework devised here was a tentative approach of dealing with this issue.

First, the line in blue in Figure 33 represents no LUC but just the SOC changes over 100 years if LU1 remained LU1. The green line represents the change of LU1 to PNV, for a simulation of 200 years.

Finally, the line in orange is divided in two parts. The first part (from year 1 to year 100) is the change from LU1 to LU2. The second part (from year 101 to 200) is the change from LU2 to PNV. The occupation CF will be obtained simply by the difference of the last SOC value for PNV at year 200 minus the last SOC value for LU2 at year 100.

The transformation CF is calculated using the area between the SOC curve for PNV for years 100 to 200 and the SOC curve of LU2 for years 100 to 200 plus the area between the SOC curve for PNV for years 1 to 100 and the SOC curve of LU2 for years 1 to 100. This area is then subtracted from the area obtained by summing the area between the curve of SOC of PNV for years 1 to 100 and the of SOC of LU2 for years 1 to 100 plus the area between SOC curve of LU2 for year 1 to 100 and SOC curve of LU1 for year 1 to 100. Equations 33, 34 and 35 show the calculation necessary for the CFs.

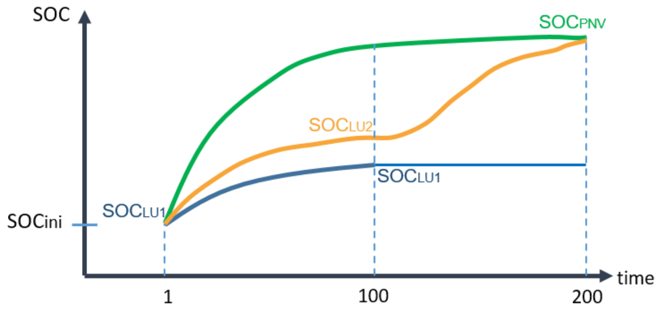


Figure 33 - Schematic representation of the calculation of CF when LU1 is different than LU2 and PNV is the reference state.

SOC – soil organic carbon; PNV – potential natural vegetation

$$CFoccupation = SOC_{200\_PNV} - SOC_{100\_LU2} \tag{33}$$

$$\begin{aligned} CFtransf = & \left(\int_{1}^{100} SOC_{PNV}\, dt - \int_{1}^{100} SOC_{LU2}\, dt\right) + \left(\int_{101}^{200} SOC_{PNV}\, dt - \int_{101}^{200} SOC_{LU2}\, dt\right) \\ & - \left(\left(\int_{1}^{100} SOC_{LU2}\, dt - \int_{1}^{100} SOC_{LU1}\, dt\right) \right. \\ & \left. + \left(\int_{1}^{100} SOC_{PNV}\, dt - \int_{1}^{100} SOC_{LU2}\, dt\right)\right) \end{aligned} \tag{34}$$

Equation (35) is equivalent to:

$$CFtransf = \left(\int_{101}^{200} SOC_{PNV}\, dt - \int_{101}^{200} SOC_{LU2}\, dt\right) - \left(\int_{1}^{100} SOC_{LU2}\, dt - \int_{1}^{100} SOC_{LU1}\, dt\right). \tag{35}$$

9.2.3 Undefined integral for Power 2nd degree fit

As described at section 8, Power 2nd degree fit is the curve fitting type chosen to adjust the results of our simulations. The undefined integral for this equation fit is

$$\begin{aligned} \int f(t) &= \left(t \left(\frac{at^{b}}{b+1} + c\right) + cte\right)\Big|_{t_1}^{t_2} \\ &= \left(t_2 \left(\frac{a{t_2}^{b}}{b+1} + c\right) + cte\right) - \left(t_1 \left(\frac{a{t_1}^{b}}{b+1} + c\right) + cte\right). \end{aligned} \tag{36}$$

The integral defined from t = 1 to 100 is

$$\int_{1}^{100} (ax^{b} + c)\, dt = \frac{a(100^{b+1} - 1)}{b+1} + 99c. \tag{37}$$

Equation (37) was the basis for implementation of the calculation procedure of CFs. We developed a Matlab routine, which was appended to the RothC implementation, to calculate all CFs for each UHTU. All results presented here are CFs that are defined as a depletion of SOC. This means that a positive CF represents a loss of SOC.

9.2.4 Comparison with other models

We compared the results of the approach in this dissertation with three different models for the calculation of CFs. One is for the occupation CFs and the last two are for transformation CFs. The first map was obtained from the method proposed by Morais et al. (2016b). The other two methods for transformation CFs are respectively based on Milà i Canals et al. (2007) and Brandão and Milà i Canals (2013) and were retrieved from Teixeira et al. (2016). All three are proxy-based models that use SOC depletion as the indicator for LU impact assessment. The main distinctions are the regeneration times assumed. Milà i Canals et al. (2007) uses a constant regeneration time of 50 years for the LUC to agriculture, while Brandão and Milà i Canals (2013) and Morais et al. (2016b) use a constant second regeneration time (20 years for LUC between LU2 and PNV) and the first regeneration time (conversion from LU1 to PNV) is adjusted according to the second assuming constant regeneration rates.

9.3 Results

The full results obtained for the CFs for each LU assessed are available at: https://fenix.tecnico.ulisboa.pt/homepage/ist172997/supplementary-materials. In this section we present only an analysis of the results obtained for tomato and compare them to the CFs obtained using proxy-based models. The model for conversion to tomato provides good results and as such was selected for demonstration of CFs.

9.3.1 Characterisation Factors Results

Figure 34 shows the spatial distribution of transformation CFs to tomato for the case where the reference state is LU1. The range of values goes from approximately -1 ktC/ha to 5 ktC/ha. These CFs depend on the present LU before conversion. Conversion from LU similar to tomato generates less aggregated impacts over 100 years (left bound), and conversion from forest uses generates higher impacts (higher bound). Higher values CFs are then found on the north of Alentejo.

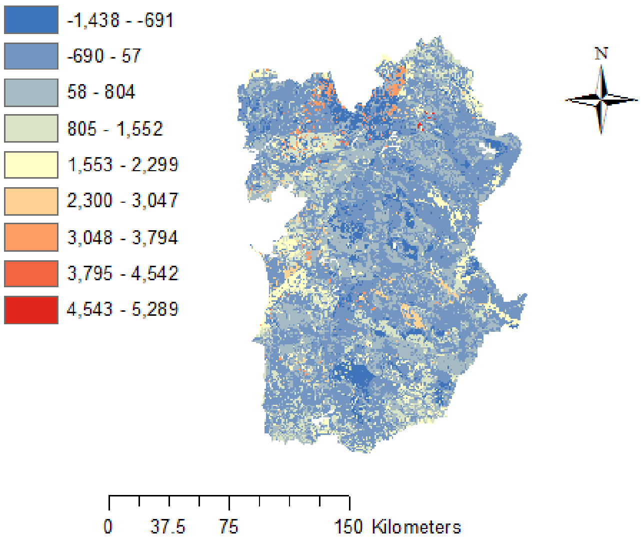


Figure 34- Transformation characterization factors for a land use change to Tomato crop (tC/ha) for LU1 as a reference state.

Figure 35 shows the spatial distribution of the transformation CFs for the case where PNV is the reference state. The range of CFs is higher than in Figure 34, going from approximately -2 ktC/ha to almost 10 ktC/ha. This is due to the fact that the change is compared with a semi-natural state and aggregated over a longer period. Once again it is possible to see that at north of Alentejo we can find the highest CFs, consequence of a conversion from forest uses to tomato crops.

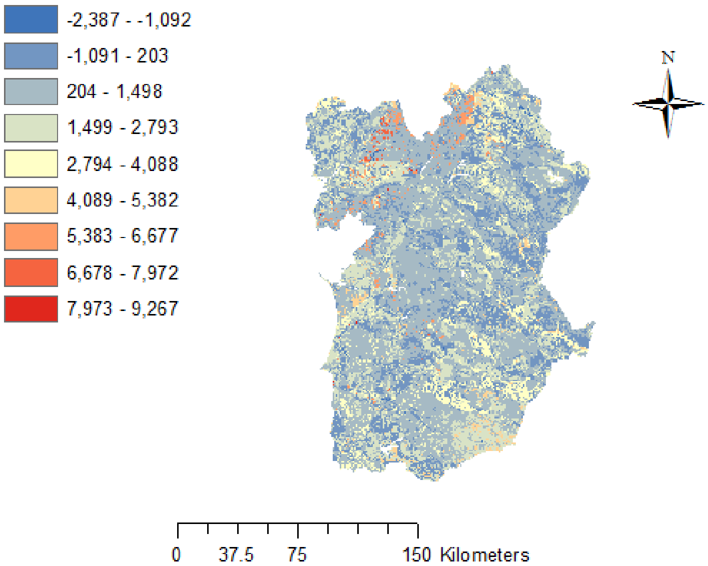


Figure 35- Transformation characterization factors for a land use change to Tomato crop (tC/ha) for PNV as a reference state.

Figure 36 depicts the distribution throughout Alentejo of occupation CFs, for LUC to tomato with PNV as a reference state. We can see a pattern with larger areas with lower values, i.e. with larger gains of SOC stocks (i.e. lower CF values), in blue zones east of the region. The other zones of the region present higher gains of SOC (i.e. higher CF values), where south of Alentejo we have the highest values of CF.

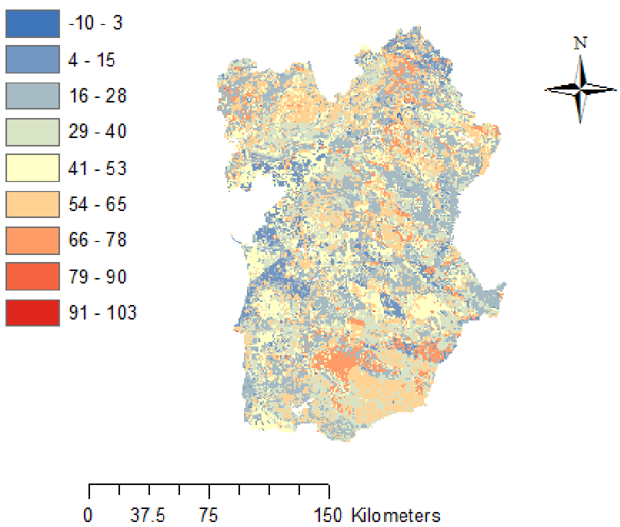


Figure 36 – Occupation characterization factors for a land use change to Tomato crop (tC/ha year) for PNV as a reference state.

9.3.2 Comparison of CFs with other models

The map in Figure 37 depicts the distribution of occupation CFs obtained by Morais et al. (2016b). This layer for Alentejo was retrieved from a European map of CFs. Morais et al. (2016b) do not disaggregate agricultural LUs. As such, the map depicts LUC to agriculture (the class that would be used to assign a land use CF to transformation to tomato) with PNV as a reference state. Their approach is not as regionalized as the approach suggested in this dissertation, having only 4 levels of desegregation for this region. There is no gain of SOC (i.e. no negative CFs) after occupation, only losses. The method for calculation of occupation CFs is not dependent of any regeneration time, and assumes that SOC stocks are constant.

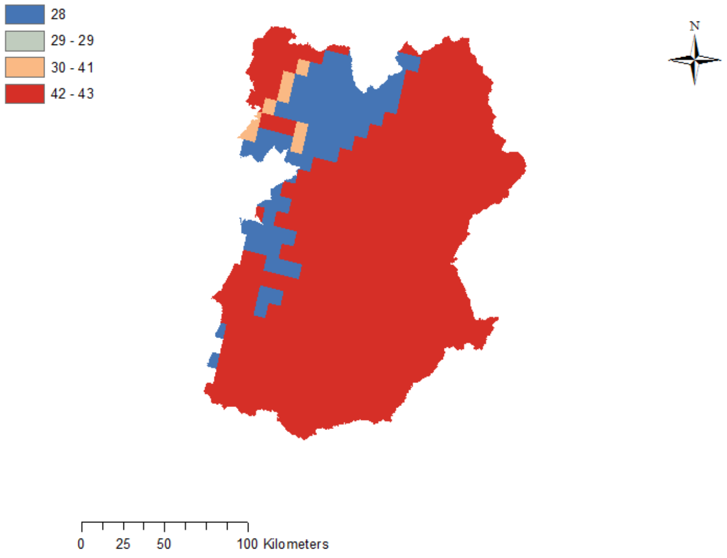


Figure 37 – Occupation characterization factors for a land use change to agriculture crop (tC/ha.year) for PNV as a reference state, based on the methodology proposed by Morais et al. (2016b).

Figure 38 shows the distribution of transformation CFs obtained using the method of Morais et al. (2016b). It depicts LUC to agriculture also, with PNV as a reference state. Again in this case, there is no negative CF, i.e., there are only gains or null changes in SOC. It would be expected that for some regions (e.g. urban areas) we encounter a gain of SOC during the occupation phase. The comparison clearly shows the value of adding additional LU classes – if all agricultural classes are aggregated, then it is impossible to take into account possible gains from particular crops (such as tomato).

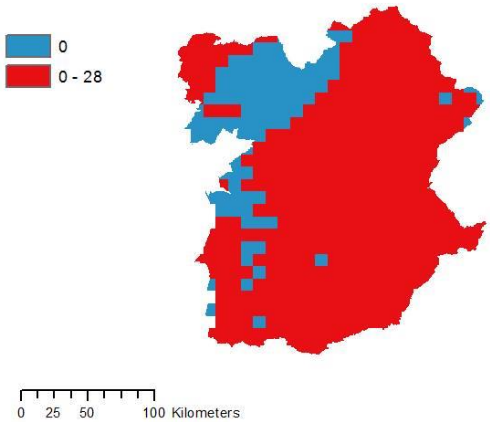


Figure 38- Transformation characterization factors for a land use change to agriculture (tC/ha) for PNV as a reference state and based on the methodology proposed by Morais et al. (2016b).

Figure 39 shows the distribution of transformation CFs calculated according to the method of Brandão and Milà i Canals et al. (2013). It depicts LUC to agriculture with PNV as a reference state. This map shows no regionalization of the assessments within the area of Alentejo. The CFs were established per climate region and therefore the entire region of Alentejo is given only one CF. The fact that there are no negative CFs once again shows, as in our assessment, that it is crucial to disaggregate agricultural classes as much as possible because specific crops impact soils differently. In terms of absolute value, the CFs in Morais et al. (2016b) are of the same order of magnitude of the CFs obtained in this dissertation. The CF of Brandão and Milà i Canals et al. (2013) is relatively lower.

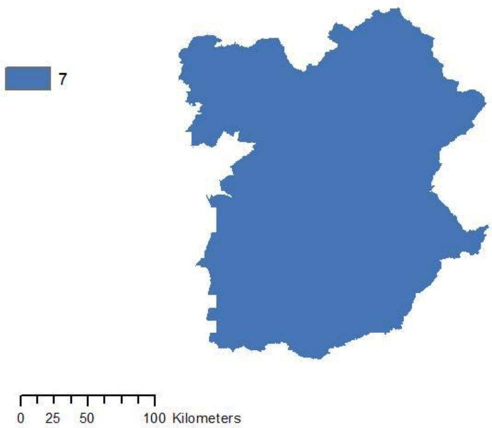


Figure 39 - Transformation characterization factors for a land use change to agricultural crop (tC/ha) for PNV as a reference state based on the methodology proposed by Brandão and Milà i Canals (2013).

Another method that can be used as a comparison in this dissertation is the methodology of Milà i Canals et al. (2007). In this case, the transformation CF is 485 $kgC.m^{-2}$ for the entire globe. This means that the model was not regionalization and as such it is difficult to consider it relevant for the region of Alentejo. The difference in absolute values, however, highlights that using global

CFs is a pitfall that should be avoided in LCIA as global factors – particularly for aggregated LU classes – are irrelevant to the regional crop production.

9.4 Discussion

We found that results obtained using different reference states have different ranges and geographical distributions of CFs. It is then important to establish a common methodology on which reference state to be used in order to compare results of different assessments. The most important distinction found was, however, the disaggregation of LU classes. Only the CFs obtained in this dissertation considered specific agricultural LU sub-classes – tomato – while a broader category (agriculture) is used by Morais et al. (2016b), Brandão and Milà i Canals (2013) and Milà i Canals et al. (2007). We focused on this example of tomato here as demonstration, but similar results would be obtained if any other LU classes were considered.

Comparing the results obtained using PNV as reference state in this dissertation with the results obtained using other models, we can see that in the case of occupation CFs the results have the same order of magnitude. The spatial distribution is not equal; in the case of this dissertation, the higher CFs values are on the southeast of Alentejo while in the case of Morais et al. (2016b) the highest values found are east and northwest. This is explained by the fact that Morais et al. (2016b) only provides CFs for aggregated agricultural uses, and does not discriminate for tomato (or any other crop). Another different aspect from the two maps obtained is the disaggregation of regions, which is much less detailed in the case of Morais et al. (2016b).

Brandão and Milà i Canals (2013) and Milà i Canals et al. (2007) provide CFs with different orders of magnitude when compared to the results calculated.We can also understand that assuming different regeneration times or simulation times will have an impact on the results, as it is the case of Brandão and Milà i Canals (2013), but the determinant for results are the number and disaggregation of LU classes and the regionalization of the CFs. The spatial distribution of CFs proposed by Brandão and Milà i Canals (2013) is homogeneous at the scale of Alentejo.

In this models, regionalization takes into account parameter averages per biome (e.g. ecoregion, climate region) only. In the case of Milà i Canals et al. (2007) there is no regionalization. In our method, we used a more specific and disaggregated regionalization in order to identify homogenous regions within the biomes of Alentejo.

9.5 Conclusions

We were able to calculate CFs for occupation and transformation based on scenarios obtained from the RothC model. Our implementation of RothC can calculate CFs automatically, which will assist any future developments of this work. The occupation CFs are a good approximation in terms of magnitude to the values calculated according to Morais et al. (2016b). In the case of transformation CFs, the results proposed by this dissertation do not have similar magnitude values when compared to Milà i Canals et al. (2007) and with Brandão and Milà i Canals (2013) due to the different regeneration times assumed, the aggregation of LU classes and the regionalization level of CFs. We can conclude that, a factor that limits the comparability of results is the time used for regeneration or simulation. One solution to this issue is to use RothC simulations results directly and calculate the regeneration times according to the intensity of the changes along the years. Looking at dynamic SOC curves, it would be possible to assume that SOC stabilizes not after 100 years but when the difference between SOC in year *t+1* and *t* is lower than a given threshold. The regeneration time would then be *t*. This way it is possible to perform the same calculations described in this dissertation independently for each LUC in each region, with the most accurate regeneration times possible.

At the moment, it is premature to claim that the CFs obtained in this thesis show that proxy-based models lead to misleading results. Given all limitations in this implementation of our method, the CFs we show here should not yet be used in LCIA. What they do show is the value of the procedure we established here – since it can facilitate the inclusion of more land use classes than proxy-based models, and the disaggregation of LU classes is crucial, this method should be further explored.

10. Conclusions

The main objective of this dissertation was to understand the viability and accuracy of an LCIA application of process-based models to determine the impacts of LU and LUC. We developed one LCIA midpoint method of LU impacts using SOC as an indicator on soil quality. We wanted to test if process-based models can help obtain more accurate CFs and what are their limitations. This is a paradigm-shifting method, so far virtually untested, in which the CFs are calculated based on scenarios. This approach enabled a dynamic and regionalized assessment of soil quality. Process-based models also enable a regionalized assessment of soil dynamics based on scenarios that is less data-constricted than proxy-based models. Proxy-based models such as Morais et al. (2016b), who also use SOC depletion as the indicator, require large datasets on SOC distribution. They rely on statistically processed data and thus typically fail to include more than 4-7 LU classes. Process-based models, on the other hand, are limited by data only in what regards input variables and parameterization. Despite promising, as shown in this dissertation, these are also a number of significant limitations to point out next.

Due to the computational limitations of the process-based models (i.e. running time) the region in study was Alentejo, Portugal, used as a proof of concept. This dissertation includes not only the implementation of the process-based models, but also a sensitivity analysis of the model RothC. In the end, we present a methodology that allowed the calculation of CFs based on the results obtained from the simulations of RothC. This dissertation presented a method that can be used globally, for the assessment of regionalized CFs for LU impacts, using SOC as a midpoint indicator for LCIA application. We were unable to implement successfully the DNDC simulations for Alentejo's region. The first problem encountered was that the data required for DNDC was not always available, so we resorted to data that was non-region specific generalization for each crop. This by itself introduces uncertainty in calculations. Also, the running time for this model was extremely large. A simulation for all UHTUs would take 5 days to run. Using only one UHTU, we tested whether, despite limitations on running time, the results of the simulations were promising. The example UHTU showed that since the model was not correctly calibrated for the region of study, results were unusable. This unsuccessful experience with DNDC led us to focus on RothC.

DNDC requires much more specific data then RothC, and consequently its implementation was harder. Also, the running time was higher than expected, and because we did not have access to the code, we could not re-write it in a different programming language as we did with RothC. This is an important comparison, because even though there is a need to regionalize LCIA and make assessments based on scenarios, we can see that a more complex model will carry practical limitations. We can conclude than that the frontier design at Figure 9 has a deep relevance when choosing a model to work with for a LCA study. In our case, we also concluded that, for the time available to do the study and the computational limitations that we had, RothC is a more balanced model, that can be computationally doable and the same time sufficiently complex to be a step forward from proxy-based models. Additionally, the implementation of RothC in Matlab should from now facilitate the calculations involved due to a lower running time. This may, in the future, allow studies such as this one to increase the spatial range, i.e. Europe and the entire world.

Another main limitation encountered in this dissertation was the data quality for carbon in crop residues. This is a crucial input variable necessary in RothC. This input value has a major impact in the results, as we could understand in the sensitivity analysis, since the values available in the literature have different orders of magnitude for the same region and the same crop. To make these simulations the more accurate possible, it is important to have better information of these values. Having more regionalized data accessible would be a great improvement since, as mentioned before, process-based models are also limited by data, albeit less, than proxy-based models – in this case data for input variables.

When making regionalized assessments as was the case here, rather than site-specific implementations of the models that often resort to measured data, it is challenging to access all the data needed. We often resorted to assuming for instance validity of data originally obtained for other regions. These assumptions added to the uncertainty of results.

Another problematic aspect encountered in the data were the values of SOC from the LUCAS Topsoil database. When overlapping the CLC map of LUs with LUCAS Topsoil database we found that there were values for the artificial areas much larger that for forest areas. This may be due to sampling – "urban" areas are often assumed to be "artificial" areas but a large proportion of these are vegetated. The difference in SOC between natural and artificially vegetated areas may in effect not be as high as expected. It may also mean that the uncertainty in the measurements are high. In any case, initial SOC is another crucial parameter whose determination at regional levels ignores many of the site-specific natural variability.

For the case of RothC simulations, we were unable to successfully implement a Monte Carlo simulation that estimates the uncertainty associated with the simulations. This problem was due to the high standard deviations of some input data. This is a consequence of low availability and/or quality of climate and crop data, i.e. lack of longer time series and stations. The solutions proposed to overcome this limitation in the future are to recalculate the input values using a different method, obtaining the values from different sources (although by this time, the most regionalized sources freely available were the ones used in this dissertation), or to desegregate our UHTUs in order to diminish the standard deviation associated to the initial SOC and clay fraction input parameters. If this problem would be successfully resolved, then it would be possible to perform a Monte Carlo simulation for our assessments. This approach should be explored in the future as it will enable the calculation of error of the CFs (which proxy-based models rarely indicate). For the purpose of this dissertation, to overcome this specific limitation, we used a best estimate approach to calculate CFs based on SOC curves. This approach simply takes the average/most likely values of the input parameters for the simulations with RothC. This is an important limitation that reduces the usability of the CFs obtained in the end, but it allowed us to proceed and obtain the conclusions described next.

After running al the simulations, the Matlab implementation of RothC enabled us to fit the curves obtained on the simulations. This fit was successful even though it had some error associated. It is important to consider that RothC is a non-linear and complex model, and being able to fit the results to one equation with only three coefficients was an only a simplification to facilitate the calculation of CFs. This step was necessary only to simplify the calculation of CFs.

We were able in the end to calculate CFs for occupation and transformation. Given all the limitations associated with their calculation and the demonstrative goals of this dissertation, we believe the CFs cannot yet be used in LCIA before the future additional work indicated before to solve each issue. However, their calculation provided additional important insights. The comparison of the results with other proxy-based model CFs proposed in literature was the number and disaggregation of LU classes. In our example, we showed that models that aggregate all agricultural crops will not capture the spatial distribution of the impacts of particular crops, such as tomato. Additional factors are the regeneration time and simulation time. Our transformation CFs were higher than the CFs of Brandão and Milà i Canals (2013). This is a consequence of the higher regeneration time assumed in this dissertation. This will then lead, according to our model, to an accumulation of the gains and losses of SOM over the years. We propose as future work to obtain more accurate regeneration times using the results obtained from RothC. One important limitation of this dissertation is the use of a fixed time horizon of 100 years used for the simulations of DNDC and RothC, as well as for regeneration time in CF calculations. This was a simplification that can be corrected in the future. The correct approach for their calculation would be to use the regeneration time for each crop, i.e., the time that takes for the SOC curve to stabilize. This regeneration times can be obtained by finding the saturation points that indicate when the curve of SOC stabilize, thereby indicating how many years it takes for the regeneration of the LU. This fact influences directly the calculation of the transformation and occupation CFs. Using a fixed regeneration time results in an over or under-estimation of the CFs for each LU class. With our proposed fix it is possible to calculate CFs based on regeneration times that will be dependent not only on the LUC but also on the specific characteristics of each region. This approach of the regeneration times calculation can be used not only for the method proposed in this dissertation but also for proxy-based models.

As additional further work, we suggest LCIA model developers work with process-based models and better and data. Monte Carlo simulations are a powerful tool to calculate error distributions for CFs, but only if probability distributions for all input variables can be rigorously defined. Another recommendation for further work is to determine regeneration times in models such as RothC, and then use them in proxy-based models. As mentioned, this requires abandoning the assumption of a 100-year time frame, which was used in this dissertation, and determine regeneration times for each LU class depending on the shape of the SOC dynamic curve. More efficient computational models are also required to enable these assessments for the entire world. It is also important to have models that allow a specific parameterization made by the user. This will enable accurate results dependent on the specific region, preventing situations like the one here presented for DNDC. For the specific case of LCA, it is also important to have simple models that can accurately simulate the dynamics of soils at regional rather than plot level, that require input parameters that are freely available and that are easy for the user to run. A standardized method on how to draw the specific UHTUs is also needed in order to compare process-based and proxy-based models. It is also important to keep assessing CFs using detailed LU classes like the ones of this dissertation (e.g. tomato, orange and others), and not only broad categories.

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Appendix

Table 27- Crop Carbon Residues values with respective References and Methodologies of calculation. Where Res/Crop is the ratio of Residues and Crop Productivity; Res is Residues amount; HI is harvest index; S:R is shoot to root ratio.

Crop	Type Values	Values	Reference	tC/ha
Tomato	Res/Crop	0.3	Blasi et al. (1997)	9.7
		0.3	ISPRA (2016)	9.7
		1	SEMA (2016)	32.368
		0.07	Dias and Azevedo (2004)	2.265
	Res (t/ha)	1.69	Alves (1995) in Dias (2002)	0.76
	HI	0.415	Ventrela et al. (2012)	64.198
	S:R	4.2	Ghanem et al. (2011)	
Oats	Res/Crop	0.86	Dias and Azevedo (2004)	6.65
		1.3	SEMA (2016)	10.06
		0.175	ISPRA (2016)	1.354
		1	Dias (2002)	7.739
		1.3	APA (2011)	10.06
		0.7	Blasi et al.(1997)	5.417
	HI rainfed	0.44	Fuentes et al. (2014)	9.853
	S:R rainfed	4.12	Jebari (2016)	
Barley	Res/Crop	1.2	APA (2011)	0.991
		0.8	Blasi et al. (1997)	0.661
		0.86	Dias and Azevedo (2004)	0.710
		0.2	ISPRA (2016)	0.165
Wheat	Res/Crop	0.86	Dias and Azevedo (2004)	0.707
		1.3	SEMA (2016)	1.068
		0.1725	ISPRA (2016)	0.141
		1.3	APA (2011)	1.068
		0.7	Blasi et al. (1997)	0.575
	S:R rainfed	4.12	Jebari (2016)	0.702
	HI rainfed	0.67	Vleeshouwers and Verhagen (2001)	
		0.44	Fuentes et al. (2014)	1.499
	S:R irrigated	7.66	Fuentes et al. (2014)	1.689
	HI irrigated	0.37	Erice et al. (2014)	
		0.43	Dauden et al. (2004)	1.339
Pasture	Res (tC/ha)	0.8	Knabner (2002)	0.8
Maize Forage	Res/crop	0.72	Dias and Azevedo (2004)	17.377

		1 0.13 0.09	SEMA (2016) ISPRA (2016) APA (2011)	24.134 3.137 0.521
	Res (tC/ha)	1	Knabner (2002)	1
	HI irrigated	0.48	Berenguer et al. (2009)	48.897
	S:R irrigated	2.21	Vamereli et al. (2003)	
Maize	Res/crop	0.72 1 0.13 1	Dias and Azevedo (2004) SEMA (2016) ISPRA (2016) APA (2011)	3.5 4.87 0.633 4.87
	Res (tC/ha)	1	Knabner (2002)	1
	HI irrigated	0.48	Berenguer et al. (2009)	21.929
	S:R irrigated	2.21	Vamereli et al. (2003)	
Rice	Res/Crop	0.7 1.4 0.1675 1.4 1.7	Dias and Azevedo (2004) SEMA (2016) ISPRA (2016) APA (2011) Vlyssides et al. (2015)	1.929 3.858 0.46 3.858 4.685
	HI	0.56	Carreres et al. (2010)	
Peach Tree	Res/Crop	0.41 0.16 1 0.2	Dias and Azevedo (2004) SEMA (2016) APA (2011) Blasi et al. (1997)	2.536 0.989 6.185 1.237
Orange Tree	Res/Crop	0.15 0.07 1 0.1	Dias and Azevedo (2004) SEMA (2016) APA (2011) Blasi et al. (1997)	0.59 0.275 3.934 0.874
Grape	Res/Crop	0.4 0.39 0.43 1	Blasi et al. (1997) Dias and Azevedo (2004) SEMA (2016) APA (2011)	0.979 0.954 1.052 2.447
	Res (t/ha)	3.58	Velazquez et al. (2011)	1.305
Olive	Res/Crop	0.47 1.13 1 2.6	Dias and Azevedo (2004) SEMA (2016) APA (2011) Blasi et al. (1997) in Vlyssides et al. (2015)	0.311 0.749 0.662 1.723
	Res (t/ha)	1.22 3.8	Aguilera et al. (2015) Nieto et al. (2010)	0.549 1.71
Potato	Res/Crop	0.4	SEMA (2016)	3.035

		0.4 0.4	Blasi (1997) in Vlyssides et al. (2015) APA (2011)	3.035 3.035
Pine	Res (t/ha)	0.271 1.63	Dias and Azevedo (2004) Dias and Azevedo (2004)	0.12195 0.7335
	Res (tC/ha)	2.96	APA (2015)	2.96
Eucalyptus	Res (t/ha)	0.546	Dias and Azevedo (2004)	0.2457
	Res (tC/ha)	2.04	APA (2015)	2.04
Cork	Res (tC/ha)	1.85	APA (2015)	1.85
Holmoak	Res (tC/ha)	2.04	APA (2015)	2.04
Oak	Res (tC/ha)	1.85	APA (2015)	1.85
Shrublands	Res(tC/ha)	0.68 4.96	Roura et al. (2011) Rosa (2009) in APA (2015)	0.68 4.96
Grasslands	Res(tC/ha)	0.8 0.41	Roura et al. (2011) APA (2015)	0.8 0.41

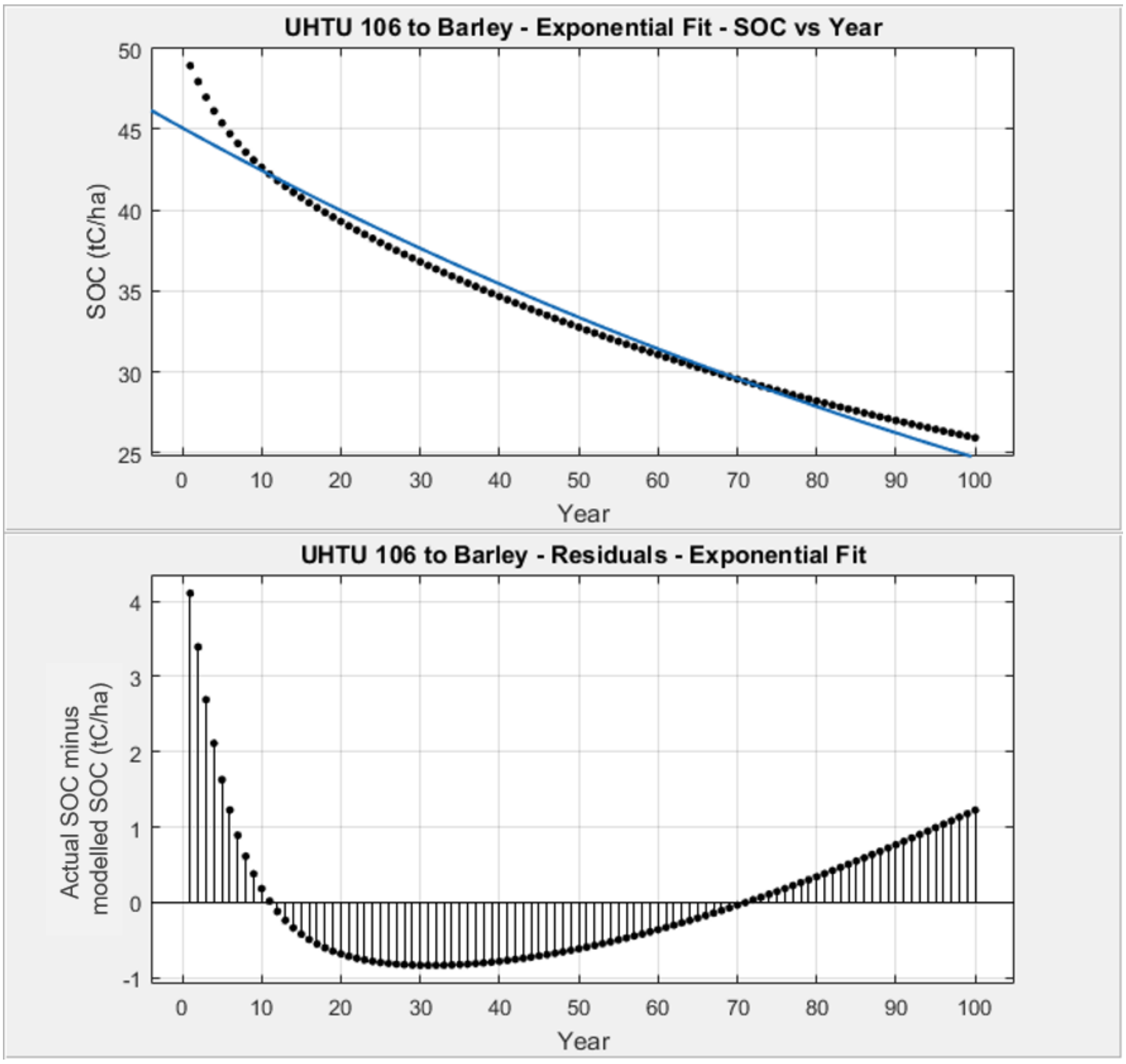

Figure 40- UHTU 106 SOC values through 100 years (points) and respective curve fit (blue line) obtained by Exponential 1st degree equation (first graph). Residuals Plot obtained from the fit represented above (second graph).

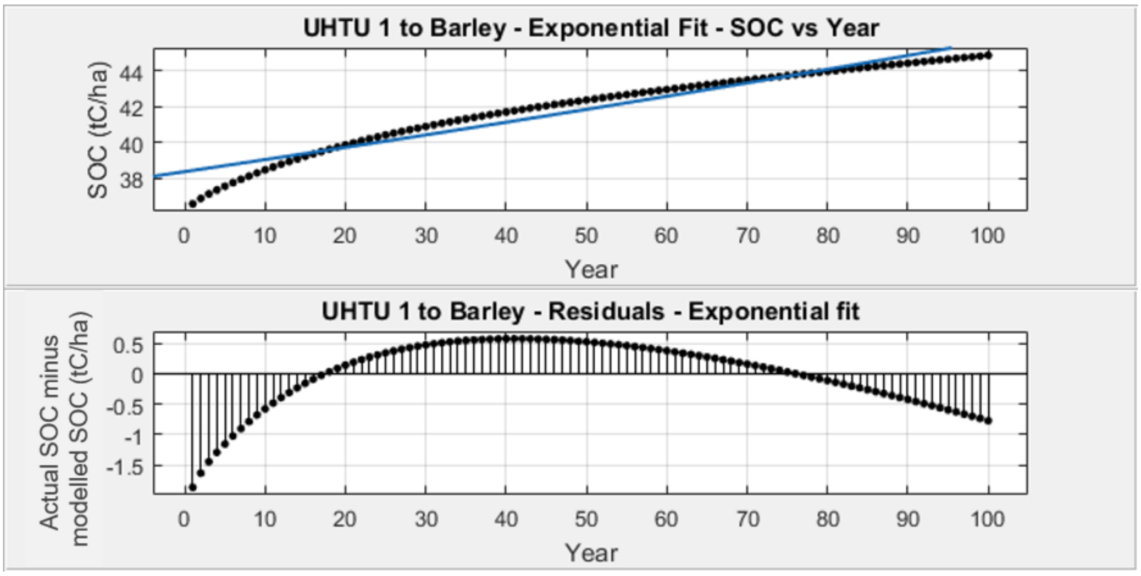

Figure 41- UHTU 1 SOC values through 100 years (points) and respective curve fit (blue line) obtained by Exponential 1st degree equation (first graph). Residuals Plot obtained from the fit represented above (second graph).

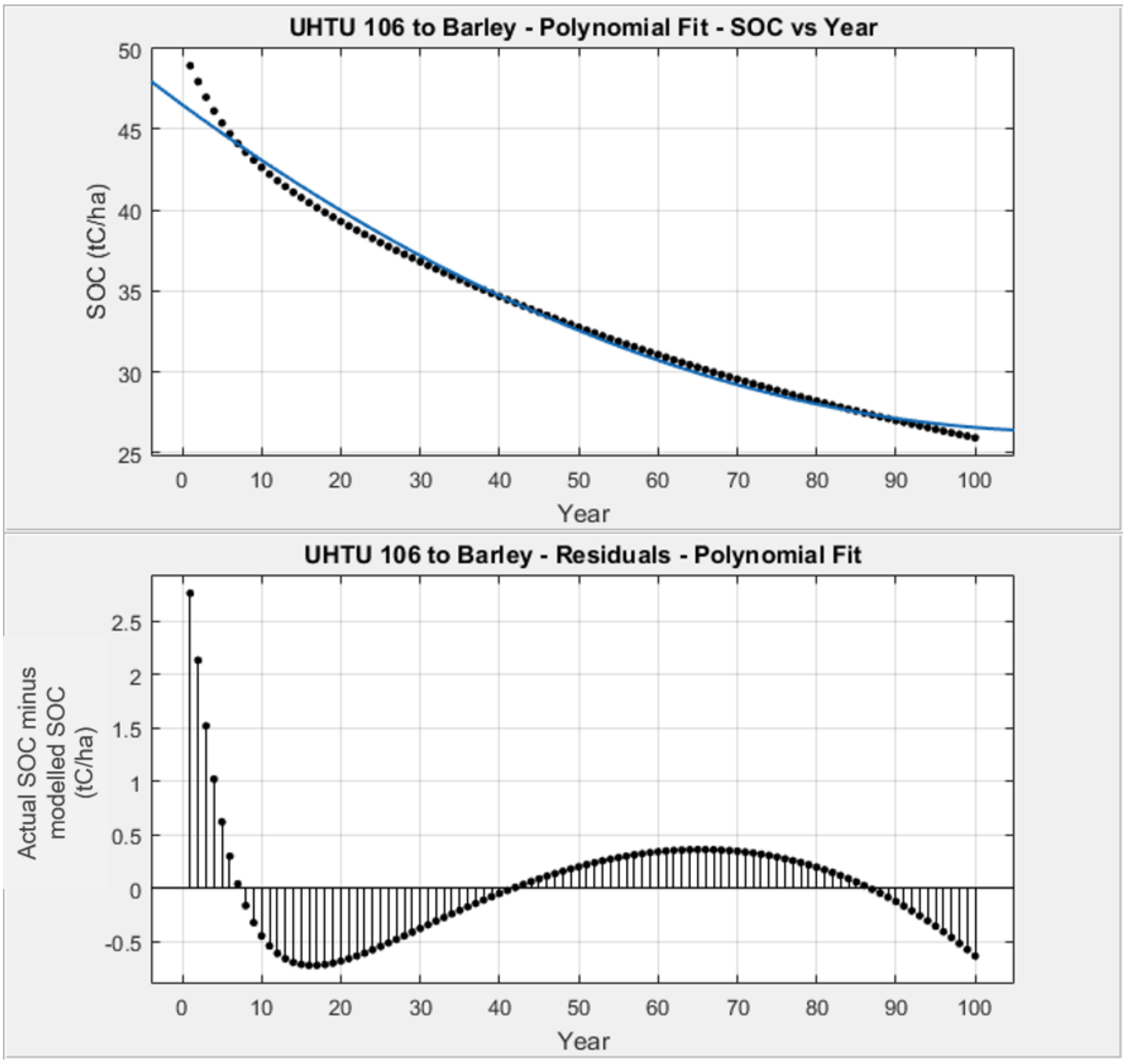

Figure 42- UHTU 106 SOC values through 100 years (points) and respective curve fit (blue line) obtained by Polynomial 2nd degree equation (first graph). Residuals Plot obtained from the fit represented above (second graph).

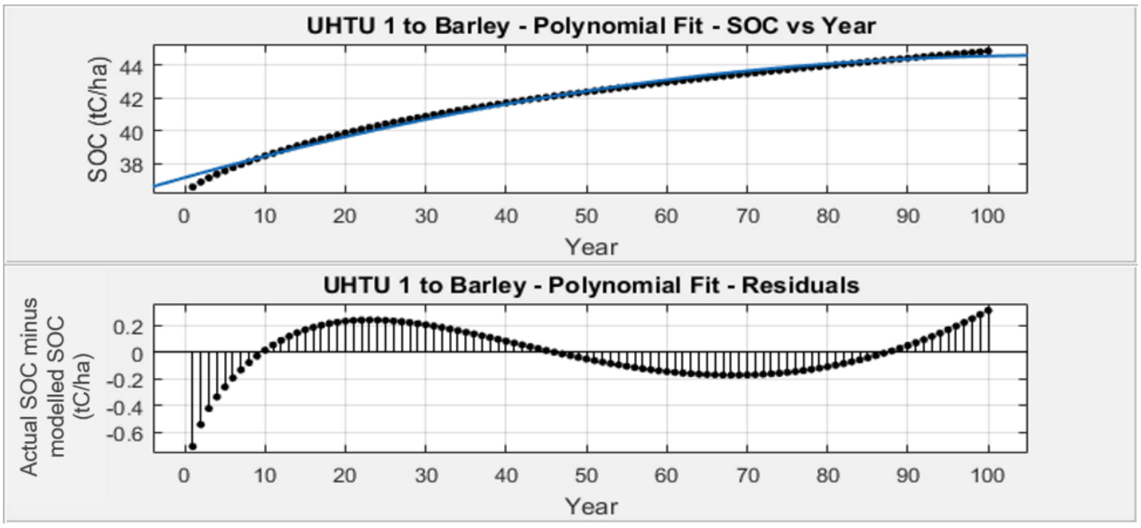

Figure 43- UHTU 1 SOC values through 100 years (points) and respective curve fit (blue line) obtained by Polynomial 2nd degree equation (first graph). Residuals Plot obtained from the fit represented above (second graph).

Table 28- SOC change ($SOC_{year\ 100} - SOC_{year\ 1}$) mean values for best estimate and 100 iterations and respective standard deviation for the last case. Land use change to oat.

Final land use (tC/ha)	Oat Best Estimate	Oat 100 iterations	Standard Deviation
Artificial Surfaces	-3.7	-8.5	9.3
Non-Irrigated Arable Land	-6.5	-10.5	10.3
Pastures	-12.5	-18.0	12.1
Wetlands	-15.6	-18.9	14.0
Permanently Irrigated Land	-2.4	-6.1	9.4
Rice	-3.7	-6.9	9.3
Vineyards	0.1	-4.7	9.1
Fruit trees and berry plantations	-0.1	-5.1	8.9
Olive Groves	-2.9	-7.1	10.0
Agro-forestry areas	-9.4	-13.7	10.6
Broad-leaved forest	-16.0	-20.0	12.2
Coniferous forest	-19.6	-23.3	12.1
Mixed Forest	-20.5	-24.0	13.1
Forest	-16.9	-20.9	12.8

Table 29- SOC change ($SOC_{year\ 100} - SOC_{year\ 1}$) mean values for best estimate and 100 iterations and respective standard deviation for the last case. Land use change to potato.

Final land use (tC/ha)	Potato Best Estimate	Potato 100 iterations	Standard Deviation
Artificial Surfaces	15.4	9.9	13.9
Non-Irrigated Arable Land	10.9	7.0	14.5
Pastures	5.1	-0.9	16.7
Wetlands	1.0	-1.1	17.3
Permanently Irrigated Land	15.6	12.1	13.8
Rice	14.4	11.3	13.5
Vineyards	19.2	14.0	13.8
Fruit trees and berry plantations	19.1	13.5	14.2
Olive Groves	15.4	11.2	14.5
Agro-forestry areas	7.4	3.2	14.8
Broad-leaved forest	-0.4	-4.0	16.0
Coniferous forest	-4.4	-7.8	16.2
Mixed Forest	-5.5	-7.9	17.2
Forest	-1.1	-5.0	16.7

Table 30- SOC change ($SOC_{year\ 100} - SOC_{year\ 1}$) mean values for best estimate and 100 iterations and respective standard deviation for the last case. Land use change to maize irrigated.

Final land use (tC/ha)	Maize Irrigated Best Estimate	Maize Irrigated 100 iterations	Standard Deviation
Artificial Surfaces	-9.1	-13.0	8.3
Non-Irrigated Arable Land	-10.3	-14.1	9.3
Pastures	-16.6	-21.7	11.3
Wetlands	-18.8	-21.7	13.1
Permanently Irrigated Land	-6.5	-9.8	8.3
Rice	-6.9	-10.3	8.2
Vineyards	-4.2	-8.5	8.0
Fruit trees and berry plantations	-4.4	-8.9	7.8
Olive Groves	-7.2	-11.0	8.8
Agro-forestry areas	-13.1	-16.9	9.9
Broad-leaved forest	-19.2	-23.3	11.1
Coniferous forest	-22.2	-26.4	10.9
Mixed Forest	-23.3	-26.6	12.4
Forest	-20.2	-24.3	11.8

Table 31- SOC change ($SOC_{year\ 100} - SOC_{year\ 1}$) mean values for best estimate and 100 iterations and respective standard deviation for the last case. Land use change to forage maize.

Final land use (tC/ha)	Forage Maize Best Estimate	Forage Maize 100 iterations	Standard Deviation
Artificial Surfaces	-12.5	-16.2	7.7
Non-irrigated Arable Land	-13.7	-17.1	8.9
Pastures	-20.0	-24.7	10.7
Wetlands	-22.0	-25.1	12.4
Permanently Irrigated Land	-9.9	-12.7	7.9
Rice	-10.3	-13.3	7.8
Vineyards	-7.8	-11.6	7.5
Fruit trees and berry plantations	-8.0	-11.8	7.1
Olive Groves	-10.7	-14.1	8.2
Agro-forestry areas	-16.4	-19.9	9.1
Broad-leaved forest	-22.5	-26.2	10.7
Coniferous forest	-25.3	-29.1	10.8
Mixed Forest	-26.4	-29.6	11.8
Forest	-23.5	-27.0	11.5

Table 32- SOC change ($SOC_{year\ 100} - SOC_{year\ 1}$) mean values for best estimate and 100 iterations and respective standard deviation for the last case. Land use change to rice.

Final land use (tC/ha)	Rice Best Estimate	Rice 100 iterations	Standard Deviation
Artificial Surfaces	-6.4	-12.1	8.9
Non-Irrigated Arable Land	-7.8	-13.3	9.9
Pastures	-14.0	-21.1	11.8
Wetlands	-16.3	-21.8	13.2
Permanently Irrigated Land	-4.0	-8.8	8.9
Rice	-4.3	-8.9	9.0
Vineyards	-1.4	-7.1	8.7
Fruit trees and berry plantations	-1.6	-7.7	8.4
Olive Groves	-4.6	-10.1	9.3
Agro-forestry areas	-10.7	-16.2	10.2
Broad-leaved forest	-16.9	-22.9	11.6
Coniferous forest	-20.1	-25.7	11.8
Mixed Forest	-21.3	-26.6	12.8
Forest	-17.9	-23.9	12.5

Table 33- SOC change ($SOC_{year\ 100} - SOC_{year\ 1}$) mean values for best estimate and 100 iterations and respective standard deviation for the last case. Land use change to vineyards.

Final land use (tC/ha)	Vineyards Best Estimate	Vineyards 100 iterations	Standard Deviation
Artificial Surfaces	-5.1	-9.8	9.7
Non-Irrigated Arable Land	-6.4	-11.0	10.4
Pastures	-13.6	-19.9	12.3
Wetlands	-15.4	-19.9	13.4
Permanently Irrigated Land	-2.0	-5.9	9.5
Rice	-3.4	-6.6	9.2
Vineyards	0.8	-4.3	9.5
Fruit trees and berry plantations	1.3	-4.5	9.6
Olive Groves	-2.1	-7.3	10.2
Agro-forestry areas	-9.9	-14.5	10.8
Broad-leaved forest	-17.5	-22.0	12.1
Coniferous forest	-21.5	-25.3	12.3
Mixed Forest	-22.5	-26.1	13.0
Forest	-18.5	-23.1	12.9

Table 34- SOC change ($SOC_{year\ 100} - SOC_{year\ 1}$) mean values for best estimate and 100 iterations and respective standard deviation for the last case. Land use change to orange.

Final land use (tC/ha)	Orange Best Estimate	Orange 100 iterations	Standard Deviation
Artificial Surfaces	4.1	-1.6	10.5
Non-Irrigated Arable Land	2.7	-2.6	11.5
Pastures	-3.2	-9.9	13.5
Wetlands	-6.7	-11.5	14.6
Permanently Irrigated Land	6.6	1.7	10.6
Rice	6.1	1.5	10.4
Vineyards	9.4	3.2	10.4
Fruit trees and berry plantations	9.3	3.1	10.1
Olive Groves	6.1	0.7	11.1
Agro-forestry areas	-0.3	-5.6	11.9
Broad-leaved forest	-6.8	-12.1	13.2
Coniferous forest	-10.2	-15.3	13.5
Mixed Forest	-11.3	-16.1	14.2
Forest	-7.6	-13.1	13.8

Table 35- SOC change ($SOC_{year\ 100} - SOC_{year\ 1}$) mean values for best estimate and 100 iterations and respective standard deviation for the last case. Land use change to peach.

Final land use (tC/ha)	Peach Best Estimate	Peach 100 iterations	Standard Deviation
Artificial Surfaces	5.5	-0.3	10.7
Non-Irrigated Arable Land	4.0	-1.2	11.8
Pastures	-1.9	-9.1	13.6
Wetlands	-5.5	-8.7	15.3
Permanently Irrigated Land	7.9	3.1	10.8
Rice	7.4	2.6	10.8
Vineyards	10.8	4.7	10.7
Fruit trees and berry plantations	10.7	4.4	10.7
Olive Groves	7.5	2.0	11.3
Agro-forestry areas	1.0	-4.6	12.1
Broad-leaved forest	-5.5	-11.2	13.4
Coniferous forest	-8.9	-14.0	13.5
Mixed Forest	-10.0	-14.8	14.4
Forest	-6.4	-12.1	14.0

Table 36- SOC change ($SOC_{year\ 100} - SOC_{year\ 1}$) mean values for best estimate and 100 iterations and respective standard deviation for the last case. Land use change to olive irrigated.

Final land use (tC/ha)	Olive Irrigated Best Estimate	Olive Irrigated 100 iterations	Standard Deviation
Artificial Surfaces	-5.1	-10.9	9.5
Non-Irrigated Arable Land	-8.0	-12.7	10.2
Pastures	-15.1	-21.4	12.1
Wetlands	-17.2	-21.5	13.4
Permanently Irrigated Land	-3.3	-7.7	9.4
Rice	-4.3	-8.6	9.2
Vineyards	-0.7	-6.4	9.2
Fruit trees and berry plantations	-1.0	-6.6	9.2
Olive Groves	-4.1	-8.8	9.9
Agro-forestry areas	-11.3	-16.2	10.5
Broad-leaved forest	-18.8	-23.6	11.7
Coniferous forest	-22.3	-27.5	11.6
Mixed Forest	-23.5	-27.9	12.7
Forest	-19.8	-24.6	12.3

Table 37- SOC change ($SOC_{year\ 100} - SOC_{year\ 1}$) mean values for best estimate and 100 iterations and respective standard deviation for the last case. Land use change to pasture.

Final land use (tC/ha)	Pasture Best Estimate	Pasture 100 iterations	Standard Deviation
Artificial Surfaces	-8.5	-12.5	7.7
Non-Irrigated Arable Land	-10.6	-13.8	9.0
Pastures	-16.2	-20.7	10.8
Wetlands	-17.3	-20.6	12.7
Permanently Irrigated Land	-7.0	-9.9	8.0
Rice	-7.6	-10.5	7.8
Vineyards	-5.0	-8.7	7.5
Fruit trees and berry plantations	-5.3	-9.0	7.2
Olive Groves	-7.7	-11.1	8.4
Agro-forestry areas	-13.1	-16.5	9.3
Broad-leaved forest	-18.8	-22.3	10.8
Coniferous forest	-21.3	-24.9	10.7
Mixed Forest	-22.2	-25.6	11.7
Forest	-19.7	-23.2	11.7

Table 38 - SOC change ($SOC_{year\ 100} - SOC_{year\ 1}$) mean values for best estimate and 100 iterations and respective standard deviation for the last case. Land use change to oak.

Final land use (tC/ha)	Oak Best Estimate	Oak 100 iterations	Standard Deviation
Artificial Surfaces	17.4	9.6	12.7
Non-Irrigated Arable Land	13.7	7.5	13.4
Pastures	9.0	0.7	15.6
Wetlands	6.0	1.4	18.1
Permanently Irrigated Land	17.5	11.4	12.4
Rice	16.6	11.0	12.3
Vineyards	20.8	13.2	12.3
Fruit trees and berry plantations	20.6	12.9	12.2
Olive Groves	17.4	10.5	13.0
Agro-forestry areas	11.0	4.5	13.8
Broad-leaved forest	4.5	-1.5	15.0
Coniferous forest	1.5	-4.7	14.9
Mixed Forest	0.5	-5.0	15.9
Forest	3.9	-2.3	15.8

Table 39- SOC change ($SOC_{year\ 100} - SOC_{year\ 1}$) mean values for best estimate and 100 iterations and respective standard deviation for the last case. Land use change to eucalyptus.

Final land use (tC/ha)	Eucalyptus Best Estimate	Eucalyptus 100 iterations	Standard Deviation
Artificial Surfaces	17.4	12.8	13.4
Non-Irrigated Arable Land	13.7	10.7	14.1
Pastures	9.0	4.1	15.9
Wetlands	6.0	4.1	17.9
Permanently Irrigated Land	17.5	14.7	13.2
Rice	16.6	14.3	13.2
Vineyards	20.8	16.6	13.2
Fruit trees and berry plantations	20.6	16.3	13.6
Olive Groves	17.4	14.1	13.7
Agro-forestry areas	11.0	7.7	14.2
Broad-leaved forest	4.5	1.6	15.6
Coniferous forest	1.5	-1.3	15.7
Mixed Forest	0.5	-1.8	16.6
Forest	3.9	0.8	16.5

Table 40- SOC change ($SOC_{year\ 100} - SOC_{year\ 1}$) mean values for best estimate and 100 iterations and respective standard deviation for the last case. Land use change to holmoak.

Final land use (tC/ha)	Holmoak Best Estimate	Holmoak 100 iterations	Standard Deviation
Artificial Surfaces	17.4	12.8	13.4
Non-Irrigated Arable Land	13.7	10.7	14.1
Pastures	9.0	4.1	15.9
Wetlands	6.0	4.1	17.9
Permanently Irrigated Land	17.5	14.7	13.2
Rice	16.6	14.3	13.2
Vineyards	20.8	16.6	13.2
Fruit trees and berry plantations	20.6	16.3	13.6
Olive Groves	17.4	14.1	13.7
Agro-forestry areas	11.0	7.7	14.2
Broad-leaved forest	4.5	1.6	15.6
Coniferous forest	1.5	-1.3	15.7
Mixed Forest	0.5	-1.8	16.6
Forest	3.9	0.8	16.5

Table 41- SOC change ($SOC_{year\ 100} - SOC_{year\ 1}$) mean values for best estimate and 100 iterations and respective standard deviation for the last case. Land use change to shrublands.

Final land use (tC/ha)	Shrublands Best Estimate	Shrublands 100 iterations	Standard Deviation
Artificial Surfaces	30.4	21.4	14.4
Non-Irrigated Arable Land	26.3	18.9	15.1
Pastures	21.9	12.4	17.0
Wetlands	18.3	11.7	18.9
Permanently Irrigated Land	30.2	23.1	14.4
Rice	29.2	22.5	13.8
Vineyards	33.9	25.1	14.4
Fruit trees and berry plantations	33.7	25.1	14.5
Olive Groves	30.3	22.5	14.9
Agro-forestry areas	23.2	15.7	15.4
Broad-leaved forest	16.5	9.7	16.7
Coniferous forest	13.1	6.3	16.2
Mixed Forest	12.2	5.8	17.4
Forest	16.0	8.8	17.2

Table 42- SOC change ($SOC_{year\ 100} - SOC_{year\ 1}$) mean values for best estimate and 100 iterations and respective standard deviation for the last case. Land use change to grassland.

Final land use (tC/ha)	Grassland Best Estimate	Grassland 100 iterations	Standard Deviation
Artificial Surfaces	-10.2	-13.2	7.6
Non-Irrigated Arable Land	-11.2	-14.1	8.9
Pastures	-17.0	-21.1	10.7
Wetlands	-17.7	-19.5	13.5
Permanently Irrigated Land	-7.8	-10.3	7.9
Rice	-8.6	-10.8	7.6
Vineyards	-5.8	-9.1	7.4
Fruit trees and berry plantations	-5.6	-9.3	7.0
Olive Groves	-8.1	-11.3	8.3
Agro-forestry areas	-13.8	-17.1	9.2
Broad-leaved forest	-19.6	-22.7	10.8
Coniferous forest	-22.4	-25.3	10.5
Mixed Forest	-23.2	-25.7	11.9
Forest	3.9	0.8	16.5