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Exploring the Mitigation Potential Role of Legumes in European Agriculture – A Modelling Approach

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June 2015

This thesis is submitted for the degree of Doctor of Philosophy
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“It is the mark of an instructed mind to rest satisfied with the degree of precision which the nature of the subject permits and not to seek an exactness where only an approximation of the truth is possible”

Aristotle 384-322 BC
Greek philosopher, scientist and physician
The increasing atmospheric concentration of greenhouse gases (GHG) has direct consequences on humans and threatens the sustainability of natural and managed ecosystems. The European Union has set high targets for reducing their emissions by 80-95% of the 1990 levels by 2050 and is working progressively to achieve these reductions. Legumes are an important group of crop species as they have the potential to reduce N₂O emissions. Biogeochemical modelling can provide a valuable tool to explore options for mitigating GHG emissions and especially N₂O from European agriculture by simulating novel legume based rotations. UK-DNDC is a process based, biogeochemical model that can be used towards that goal. The model was tested for various regions in Europe and showed that it can
simulate the N dynamics within crop rotations across a range of pedo-climatic zones. It is a useful tool in 1) identifying where and when high emissions occur, 2) highlighting the effects of the management practices on emissions and 3) exploring the impact of alternative managements on emissions. New rotations, which include legumes, have been proposed in order to assess the sustainability of the legumes in European agriculture and the effect that they will have on N₂O production. Five regions in Europe, namely Sweden, Germany, Italy, Scotland and Romania, were selected in order to test the differences between legume based rotations and non-legume based. These regions represent a wide range of pedo-climatic zones in Europe. In most case studies, legumes showed that they can make an important contribution to mitigating N₂O emissions. However, there were cases in which legumes enhanced the production of N₂O. Modelling can help to understand system dynamics and it can also help to explore mitigation options for European agriculture in terms of N₂O production. An important element of environmental modelling is to understand the uncertainty and sensitivity of model parameters in relation to the model outputs. The sensitivity testing of the model showed that clay content, initial soil organic carbon content and atmospheric background CO₂ concentration are three key input parameters Nitrous oxide emissions were one of the results that showed great uncertainty in all the analyses. That highlights the challenges of the modelling activity for accurate N₂O simulations in a dynamic ecosystem.

*Keywords:* UK-DNDC, legumes, European agriculture, Nitrous oxide, novel rotations, modelling.
Lay Summary

The increasing atmospheric concentration of greenhouse gases (GHG) has direct consequences on humans and threatens the sustainability of natural and managed ecosystems. The European Union has set high targets for reducing such emissions by 80-95% of the 1990 levels by 2050, and is working progressively to achieve these reductions. The third most important GHG is N₂O, after CO₂ and CH₄, which is produced largely by agriculture. Legumes are an important group of crops that they have the potential to reduce N₂O emissions. This is due to their distinctive ability to fix atmospheric N in the soil and consequently the inclusion of legumes into the rotation of crops decreases the need for N based fertilisers. However, while the concentration of GHGs has increased over the last 50 years, the production of legumes in European Union has declined. Environmental modelling is a useful tool that can be used in order to find ways to tackle environmental issues and thereby ensure environmental protection. The simulations of the UK-DNDC model were tested against measured data from six sites across Europe and showed that UK-DNDC is capable of simulating the production of N₂O emissions in European agriculture. The environmental sustainability of legume crops incorporated into novel rotations in European agriculture was assessed through UK-DNDC as well as the indirect effect that they will have on N₂O production. The assessment took place in 5 different European regions namely Sweden, Germany, Italy, Scotland and Romania, and showed the positive potential effect legumes can have. An important element of environmental modelling is to understand the uncertainty and sensitivity of model input parameters in relation to the
model results. This activity highlighted to which of the inputs the model showed to be sensitive.
Preface

This Ph.D. thesis is submitted for the fulfilment of the requirements for the Doctor of Philosophy degree from the University of Edinburgh. It illustrates a culmination of a research period of four years (Oct 2010-Sep 2014). This project was a joint collaboration between SRUC (Scotland’s Rural College) and the University of Edinburgh. My supervisors on that project has been Dr Cairistiona F.E. Topp (Head of SRUC’s Modelling Group), Prof Robert M. Rees (Head of SRUC’s Carbon Management Centre) from SRUC and Dr Saran P. Sohi (Leader of Soil Science in UKBRC) from the University of Edinburgh.

This thesis/project is part of a wider European funded project called “Legume-supported cropping systems for Europe”. It is an international research project financed by the EU Framework Programme 7 aiming to develop the use of legumes in cropping systems to improve the economic and environmental performance of European agriculture. This thesis contributed in the biophysical modelling work package.

My primary work has been in the validation, calibration, options assessment and sensitivity analysis of the UK-DNDC model for the European agriculture and it is this work that provides the central theme and content around which this thesis has been constructed. The preparation of this thesis has thus been to extract from these activities a rational and coherent body of work, and one that I can call my own. In chapter 1 can be found more details for the structure of the thesis in section 1.3.
Acknowledgements

I am extremely grateful and I would like to acknowledge all the people who believed on that project and made the completion of this thesis possible. Firstly I would like to thank my two principal supervisors Dr. Cairistiona F. E. Topp and Prof. Robert M. Rees for their constant guidance and endless patience in order to complete this work. I appreciated and benefited greatly from the ease with which we discussed and formulated solutions in all the blind alleyways that arose during the project. I feel really grateful to Dr Bill Spoor who volunteered to proof-read my thesis.

During these years I have met and formulated invaluable friendships. People that their presence helped me with one or another way to complete this project. In particular I would like to thank my office colleagues Dr Emma Tilston, Dr Sarah Buckingham and Dr Davide Tarsitano who assisted me all the way through in so many aspects by improving my English, modelling techniques and work ethics. Here I would like to thank my fellow students and especially Maria Borlinghaus and Marta Piotrowska for brighten up my moody days in the office, my friends Steven Miller, Neil Ramsay, my flatmate François Dussart and all the staff in CSS. I would like to thank all the partners and colleagues from the Legume Futures project and especially Dr Valentini A. Pappa for the fruitful collaboration that we had.

To my family, words cannot really describe of how much support and encouragement they have provided me through these years. Ευχαριστώ Gregory, Sofia and Elisabeth. A big thank you to all my friends back in Greece Marios, Tolis, Vasillis, George, John, Thanos, Michalis, Kostas, and Iris. At the end, thanks to you, reader. If you are reading this line after the others, at least you read more than one page of my thesis. ~ Thank You ~
Declaration

I declare that the present thesis it has been composed by myself and that no part of it has been submitted for any other degree or qualification. The work described is my own unless otherwise stated.

Nikolaos Angelopoulos

…………………………………………………………………………………………………

Date

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Publications

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Chapter 4

The material that is presented in chapter 4 has been used for the needs of the following three publications:

• **European Project (Legume Futures)**
  Legume Futures contract deliverables report


• **Journal Paper (submitted)**

Chapter 5

The material that is presented in chapter 5 has been used for the needs of the following three publications:

- **European Project (Legume Futures)*

  **Legume Futures contract deliverables report**


- **Conference papers (Presentations)**

  Knudsen, M. T., Hermansen, J. E., Olesen, J. E., Topp, C. F. E., Schelde1, K., **Angelopoulos, N.,** Reckling, M. 2014. Climate impact of producing more grain legumes in Europe. 9th International Conference on LCA in the Agri-Food Sector, San Fransisco, USA

*Legume-supported cropping systems for Europe (Legume Futures) is a collaborative research project funded from the European Union’s Seventh Programme for research technological development and demonstration under grant number 245216

www.legumefutures.eu
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Acronyms and Abbreviations

BNF: Biological Nitrogen Fixation
C: Carbon
CH₄: Methane
CO₂: Carbon Dioxide
CO₂eq: Carbon Dioxide Equivalent
DBM: Dynamic Biogeochemical Model
DM: Dry Matter
Eh: Reduction Potential
GHG: Greenhouse Gases
GIS: Geographic Information System
GWP: Global Warming Potential
Ha: Hectare
Hg: Hectogram (10² g)
K: Potassium
LSU: Livestock Units
Mt: Megatonne (10⁹ kg)
N: Nitrogen
NEE: Net Ecosystem Exchange
N₂O: Nitrous Oxide
NH₂_________Amino
NH₃_________Ammonia
NH₄⁺_________Ammonium
NO_________Nitric
NO₂_________Nitrogen Dioxide
NO₃_________Nitrate
NOₓ_________Nitrogen Oxides
Nr_________Reactive Nitrogen
NUE_________Nitrogen Use Efficiency
NUTS_______Nomenclature of Territorial Units for Statistics
O₂_________Oxygen
P___________Phosphorus
R²_________Coefficient of Determination
RMSE_______Root Mean Square Error
SE_________Standard Error
SOC_________Soil Organic Carbon
Tg_________Teragram (10¹² g)
UK-DNDC_____United Kingdom- DeNitrificationDecomposition
USD_________United States Dollars
WFPS_______Water Filled Pore Space
1 Introduction

1.1 The Thesis

Biogeochemical modelling can provide a valuable tool to explore options for mitigating nitrous oxide emissions from European agriculture by simulating a wide range of possible management scenarios. In this study such models have been used to simulate novel legume based rotations. These simulated rotations show that they can influence nitrous oxide concentrations of the emissions. The model used in this thesis was UK-DNDC. The work described in the dissertation demonstrates the use of the model for testing for the European agro climatic zones and the environmental sustainability of the novel legume based rotations. This dissertation looks at the mitigation of nitrous oxide in the European Union and proposes new cropping systems which can be incorporated in European...
Aims and Objectives of the study

The motivation behind this study is the fact that while extensive research has been carried out regarding the ability of legumes to fix atmospheric nitrogen, the differences between a legume-based rotation and a non-legume-based rotation have received little attention. This project aims to contribute significantly towards moving agriculture to a more sustainable future. Modelling new sustainable legume based rotations and the assessment of their environmental impact in terms of greenhouse gases, will aid the design of a more environmentally friendly agriculture in a European perspective. It is essentially this premise, coupled with the objective of developing a better understanding of the mechanisms of the ecosystems that motivates my research.

The increasing atmospheric concentration of greenhouse gases has direct consequences on humans and is creating significant pressures on environmental ecosystems. The European Union has set ambitious targets for reducing such emissions by 80-95% of the emissions by 2050 compared to 1990 levels and works progressively to achieve them (European Commission, 2014). Agriculture is one of the main nitrous oxide emissions sources. Legumes can play an important role in contributing to this goal of reducing emissions due to their N fixing ability and their contribution of high protein content in the final product. Over the last few decades the production of agriculture and can contribute to minimising the dependence of Europe on imported protein.
legumes in Europe has decreased, creating a constant pressure to increase imports of legumes products from other continents and especially South America. European agriculture should start evolving in a more environmental sustainable sector in terms of N₂O production. With the use of UK-DNDC model, novel legume based rotations will be tested in order to assess N₂O emissions in comparison with current practices. By testing new systems and rotations, it may be possible to explore the potential role of legumes in the mitigation of N₂O production in European agriculture in order to reduce the environmental impact of European agricultural systems within a range of agro-climatic zones.

The project has the following objectives in order to fulfil this goal:

i) Validation of the UK-DNDC model using data from six experiments across three different countries in Europe

ii) Perform an options assessment in order to predict nitrous oxide emissions from novel legume based cropping systems compared with non-legume based cropping systems from arable and livestock systems. This has been assessed for a range of different management options across five main agricultural and pedo-climatic zones in Europe for a range of different soils. Assess the effects of the inclusion of legume crops on nitrous oxide emissions in the European agriculture
iii) Perform a sensitivity analysis of the UK-DNDC model (using the built-in function) for nine of the most important input parameters using a Scottish site as a case study.

1.3 The Structure of the Thesis

The thesis is structured as follows. The main components of the thesis are legumes, nitrogen (N) and environmental modelling. The second chapter reviews the current situation in protein production from agriculture in Europe, an analysis of the legumes crops and a review of the cycle of nitrogen with a particular focus in nitrous oxide emissions.

Chapter 3 presents an overview of the environmental modelling. In this chapter the importance of environmental modelling and the biogeochemical models will be discussed with a short review of some of the models. In particular this chapter will review the model that was used during this project the UK-DNDC.

Chapter four presents a sensitivity analysis of the model in a Scottish grassland. A “local” sensitivity analysis was performed for the N fixation index and 5 “global”. The “global” sensitivity analyses focused on the changes of three climate parameters that were default and a combination of the most important soil characteristics. In this chapter the importance of the effect of the changes in these factors on the outputs of the model and more specifically the nitrous oxide emissions, are discussed.
Chapter five presents the calibration and the validation of the model in all the six different sites across Europe with the UK-DNDC model. Here the challenges of applying these modelling activities to legume based rotations will be discussed.

Chapter six presents an options assessment of cropping rotations in the European agriculture. For five different NUTS 2 agro-climatic regions across Europe namely Sweden, Italy, Germany, Scotland and Romania, a number of options were tested for their production of nitrous oxide emissions. The options consisted of two groups of rotations: the legume based and the non-legume (“traditional”) rotations. This test was performed for both forage and arable systems and for a range of the predominant soil types in the study areas.

Finally chapter seven brings together the ideas and the results from the previous three chapters in a discussion of the importance of the results and the actual contribution of the research that took place. In this chapter, ideas are presented and knowledge gaps identified in order to identify future research priorities.

All the ethical issues that might be matters of consideration have been taken into account. An ethics assessment of the work that has been carried out for this thesis produced according the University of Edinburgh School of GeoSciences guidelines and presented in the Appendix A.
2 Literature review

Caminante, no hay camino. Se hace camino al andar.\(^1\)

Antonio Machado (1912)

2.1 Legumes

2.1.1 Background

There are approximately 250,000 plant species that are known in the world (Wilson, 2001), however only around 10,000 are edible and even less, between 15 to 200 plant species that’s are regularly incorporated into the human diet. Legumes are one of the largest groups of plants and have a great financial importance globally (Lewis et al., 2005). They are very

\(^{1}\) Traveller there is no road. The road is made as you walk.
adaptive, being found in arctic regions (Allen et al., 1964) to tropical regions and deserts (Tadmor et al., 1971). Legumes have played a central role in the diet of humans and animals since prehistory all over the world (Norton et al., 1985). The use of legumes can be traced back to those regions where the first civilisations arose. The earliest signs of legumes are from lentils from 9,500 BC in Persia (Cohen, 1977). Fred et al. (1932) reported the use of legumes from ancient societies of South-western Asia, Egyptians, Romans to Aztec, Indians and Pre-Incas societies and that ancient Greeks worshiped the god of beans, called Kyanites. Currently, legumes are the second most important source of human food and animal forage and also the second most economic important group of plants after cereals. In addition, legumes are one of the most important group of crops in terms of world production (Sathe, 1996; Popelka et al., 2004).

Legumes belong to the family of Leguminosae, which is one of the biggest families in Kingdom Plantae and to the Order of Fabales (Fred et al., 1932). Botanists have recognised up to 740 genera (data of 2011) and almost 19,350 species that belong in Leguminosae family (Lewis et al., 2005; ILDIS, 2006; Royal Botanic Gardens Kew, 2012). It is the third biggest family in the Kingdom Plantae after Compositae and Orchidaceae (NAS, 1979; Corby et al., 1983; Morris, 1997). The name “legumes” originates from Roman times from the verb “legere” meaning ‘gather by hand’ and “legumen” referring to the product that was harvested by hand. The four main subfamilies are namely Pailionoideae, Mimosoideae, Caesalpinioideae, and the smallest being Swartzioideae (Fred et al., 1932; Lim and Burton, 1982; Corby et al., 1983; Polhill and van der Maesen, 1985). The Pailionoideae subfamily has the
majority of genera and species, with almost 65% and 75% respectively (Lewis et al., 2005). The best-known species of the family are chick pea (Cicer arietinum), lupin (Lupins spp.), clover (Trifolium spp.), peanut (Arachis hypogaea), lentil (Lens culinaris), common bean (Phaseolus vulgaris), pea, soybean (Glycine max), and alfalfa (Medicago sativa) (Nwokolo and Smartt, 1996).

One of the most distinctive and common features of leguminous crops is the formation of their seeds inside pods. This is in fact a free pistil occurring before the development of becoming a pod (Fred et al., 1932). The second and most important characteristic that makes this family of crops of particular importance is the ability to fix biological N. Legume seeds are considerably rich in protein, varying from around 17% to approximately 40% of the total dry matter with an average of 26% (Bressani and Elias, 1980; Boulter, 1980; Norton et al., 1985). These percentages are higher than the protein concentration that can be found in cereals (10%-12%) (Adams and Pipoly III, 1980; Shewry and Halford, 2002).

Soybean is the most prominent legume produced globally (Figure 2.1) accounting for almost 70% of total legume production (FAO, 2014b). This is attributable to the fact that soybean contains high concentrations of protein, comprising 37% of total dry matter (Norton et al., 1985) or even up to 43% for some cultivars (Bliss, 1980).

Protein is an essential component of all living organisms and a vital dietary constituent for both animal feed and human food (Voet and Voet, 2004). Legumes are also a significant source of calories, accounting for
almost 11% of the human diet in many countries (e.g. India) that rely primarily on plants as their source of protein. Moreover leguminous crops comprise a range of other nutrients such as oil and polysaccharides (Boulter, 1980). It is noticeable that such crops account for 35% of the world production of processed vegetable oil (primarily from soybean and peanut) (Graham and Vance, 2013). In the United States up to 95% of the production of soybean is dedicated to oil production and feed for livestock (Nwokolo, 1996). Animal feed is heavily reliant on forage legumes (alfalfa, clover and vetches) in many developing countries (Graham and Vance, 2013). The inclusion of leguminous crops in feed for meat and dairy production is essential to have a more balanced diet, enriched with protein (Bliss, 1980).

Legumes are a multi-purpose group of crops, not only in organic agriculture but also in natural ecosystems, agroforestry and even in pharmaceuticals and industry sectors (Graham and Vance, 2013). A study from Arianoutsou and Thanos (1996) showed that legumes can dominate ecosystems that have been heavily disturbed from fires as they showed good adaptation in post fire systems. Following establishment on bare ground they can be a useful group of species in creating suitable conditions for other

Figure 2.1: World production of some of the most important legume crops (Source: own figure based on data from FAO (2014b))
species to grow and also assist with re-establishing damaged ecosystems. Many forage crops are used for improving conditions in ecosystems through offering soil erosion control and wind breaks (Morris, 1997). The spectrum of legume uses extends into industry also, as they can be used for making biodegradable plastics (Paetau et al., 1994), biodiesel fuel, oil lubricant (NBB, 2014; USB, 2010; Morris, 1997), vegetable gum (can be used as thickener and stabiliser for food), indigo dye (Purseglove, 1968), pesticide (Balandrin and Klocke, 1988; Balandrin et al., 1985) and fibre (Abelson, 1994). In the pharmaceutical sector, the use of legumes are quite extensive such as being incorporated into antiflu, antiseptic, anticancer, antigastric, antibiotic, hemostat, hypocholesterolemic and many more products. This is due to the useful phytochemicals properties that legumes have (Morris, 1997; Kennedy, 1995; Molteni et al., 1995).
2.1.2 Biological N fixation

The distinctive feature of leguminous crops is the ability to form symbiotic associations with micro-organisms that are capable of biological nitrogen fixation (BNF). Fixation of nitrogen occurs due to the formation of nodules in the roots of the leguminous crops (Figure 2.2). The first known mention of nodules is attributed to Fuchs who found them in legume crops roots (e.g. Vicia faba) in 1542, without any recognition of their distinct role and who regarded nodules more like a structural part of the plant (Fred et al., 1932). Three centuries later, the agricultural chemist Hermann Hellriegel discovered that the modules accommodated the mutualistic symbiotic relationship with nitrogen-fixing bacteria (Hellriegel, 1886). Due to that distinctive process of biological fixation of atmospheric nitrogen, legumes can be regarded as pioneer plants in soils poor in nutrients (Merkel et al., 1999). Nodules are the point of infection in the host root hair of the crop from a *Rhizobium* bacteria (Lim and Burton, 1982). *Rhizobium* has its origins in Greek as the first part of the word (rhiza) means root (in Greek φίλα) and the second (bios) life (in Greek βίος). The formation of the nodules occurs due to a symbiosis of the bacteria in the root hair of the leguminous crops which follows the root hair infection thread from the bacteria (Dazzo, 1980). *Rhizobium* is a genera which belongs to the
family Rhizobiaceae within the order *Eubacteriales* (Lim and Burton, 1982; Vincent, 1974). According to Vincent (1974) in this genera belong bacteria that have the ability to establish “a morphological defined nodule on the root of a leguminous crop”. Not all legume crops respond the same to all the strains of rhizobia. The symbiosis is heavily dependent on the host leguminous plant (Dazzo and Hubbell, 1982). The two symbionts (*Rhizobium* bacteria and the host root hair) have to be compatible in order to ‘format’ the nodules (e.g. *Trifolium* spp roots susceptible to nodulate from *Rhizobium trifolii*) (Figure 2.3) (Lim and Burton, 1982; Dazzo and Brill, 1979; Dazzo and Hubbell, 1982).

![Figure 2.3: Rhizobium trifolii in a clover root hair tip (examined by scanning electron microscopy x7,500) (Dazzo and Brill, 1979)](image)

The symbiotic relationship can be affected by many different factors that can favour or hinder the infection of the root hair and the growth of the nodule. The main factors that play an important role in the process are mainly soil factors such as calcium concentration, pH (Munns, 1970; Robson and Loneragan, 1970), temperature (Gibson, 1971; Sprent, 1979), soil
atmosphere (Wilson, 1940; Bergersen, 1971; Gibson, 1967), soil moisture (Sprent, 1971) and light (Wilson, 1940). The shape and size of the nodule may vary depending predominantly on the host plant (Kidby and Goodchild, 1966) as they can be spherical, or tubular (Figure 2.4) (Vincent, 1974). Nodule formation can happen either outside the root (exogenous) or very rarely inside the root (endogenous) (Figure 2.4) (Allen and Allen, 1940).

Figure 2.4: Examples of different N fixing nodules. (a) Exogenous elongate nodules on clover. (b) Exogenous globose nodules on soybean. (c) Endogenous semi-globose nodules in peanut. (d) Exogenous elongate short and stubby (coralloid) nodules on guar (Lim and Burton, 1982; Postgate, 1998).
The majority of legumes can fix N but not all. For the two largest subfamilies (Paiionoideae, Mimosoideae) the percentage of the species that fix inert atmospheric nitrogen is around 90% (Vincent, 1974).

2.1.3 Legumes importance

Legumes incorporated into crop rotations can be environmentally beneficial, due to their nitrogen fixing capability. Hence, there are fewer requirements for nitrogen based fertilisers in legume based systems, which can lead to a considerable reduction in the consumption of fossil fuels, greenhouse gas emissions and potential N pollution (Rispail et al., 2010; Jensen and Hauggaard-Nielsen, 2003). Jensen and Hauggaard-Nielsen (2003) have summarised the potential effects of biological nitrogen fixation on different environmental parameters. For pre-cropping periods and during-cropping periods, the ecosystem benefits are decreased N leaching and ammonia volatilisation. During these periods the N uptake remains high, while there are some losses of N from green manure and residue incorporation. For post-harvest and in longer terms, the system benefits from the use of legumes with increased fertility for the soil and N surplus benefit for the subsequent crop. On a longer time-scale there is potentially the negative effect in intensive systems, where additional N in the soil is lost from the system through gaseous emissions or leached in aqueous solution. Nevertheless the presence of legumes and N fixing organisms in the cropping system offers some non-N benefits to the ecosystem. These include the control of soil erosion, deep rooting, the support of the below and above ground biodiversity, contribution to soil structure and enhanced C sequestration. Moreover, there may be reduction in the use of external
inputs like pesticides as some legumes have an ability to control diseases and weeds and to resist insect attacks as they can use water efficiently (Nandasena et al., 2004). The atmospheric nitrogen that is fixed through biological fixation is dominated by the leguminous crops, contributing from 50% to 70% of the total global biological fixation (Delwiche, 1970; Hardy and Holsten, 1972). In Europe the BNF accounts for approximately 1.1 Tg N per year or 4% of the total N input, which is estimated at 23.5 Tg N per year (de Vries, 2011; Leip, 2011).

All these characteristics are crucial in modern agriculture and as a result, make legumes a significant group of crops for rotational and sustainable cropping systems. Legumes can play a critical role in redesigning agriculture with new crop rotations and contribute in low input production systems.

### 2.1.4 Legume Presence in Europe

Although there are significant advantages to utilizing legumes in agriculture, they are not so well represented in Europe. According to FAO (2014b), France (15th) is the only European country in the top 20 countries globally for quantity of pulse (beans, chickpeas, lentils, lupins, peas and vetches) production. Only 6 European countries appear in the top 50 countries ranked for pulse production. In 2011, the amount of European arable land that was occupied by grain legumes reached almost 2%, while in
1961 the figure was around 5%. Alongside the decline of legumes, the area harvested of legumes declined as well (Figure 2.5).

Figure 2.5: Area of harvested legume crops from 1963 to 2011 in EU-27.
(Source: own figure based on data from FAO (2014b))

The actual reduction in cultivated land of protein crops was around four million hectares over the last 50 years in Europe (FAO, 2014b). Around the mid-1970s, cultivated land that was dedicated for soybean and peas, started to increase. This occurred as a result of the European policy for price support being introduced, for the use of soybean and peas as animal feed. There are many drivers that led to the decline in the area which is now used for the cultivation of legumes. One of the main reasons has been agricultural land being used for livestock due to the high demand for meat (beef, pig and poultry), especially pig and poultry which has increased almost three-fold in the last five decades. This increase is a result of dietary changes within the European Union, which nowadays depends more on meat consumption. At the same time, the area of legumes cultivated for human consumption has
dropped by 45% the last 50 years (FAO, 2014b). Livestock feed is based heavily on cereals with around 65% of the total European cereal production used by the livestock sector (European Parliament, 2013). The production of legumes has increased only slightly during the last 50 years (Figure 2.6) in order to accommodate the great increase for meat demand.

![Figure 2.6](image)

**Figure 2.6:** Change in yield production T ha\(^{-1}\) of legume crops from 1961 to 2012 in EU-27. (Source: own figure based on data from FAO 2014)

The yield of legumes has increased (Figure 2.6) between 1961 and 2012. The European Union has a high demand for (mostly for feed), and currently relies heavily on imports. Soybean is primarily used for protein enrichment of the animal feed (European Parliament, 2013). The imports for soybean in particular, are approximately 650 times more than the European production for 2012 and accounts for more than the half of the total net
imports of protein in the continent. The main imports are from South American countries. The net amount of occupied land utilized for soybean that is imported to Europe, relates to the whole territory of Portugal and Austria combined, with almost 17 million hectares estimated for 2008 (von Witzke and Noleppa, 2010).

The slow increase in the production of legumes is attributed to farmer choice and uncertainty in yields. Farmers choose to grow more lucrative crops such as cereals with higher yield potential, and with gross margins that are slightly higher than in legume production (European Parliament, 2013). Growing legumes can pose more uncertainties in terms of the amount of the yield achieved as they can demonstrate more delays in maturation and harvesting in comparison with cereals (Flores et al., 2012; von Richthofen et al., 2006).

Agricultural policies have also affected the European production of legumes from 1970 either directly or indirectly. There have been some attempts to tackle this reduction, from a policy perspective but such interventions have failed to have a long term effect, either directly or indirectly, and have only reversed the situation for a short time (e.g. Price support for soya bean, area payment for chickpea, lentil and vetches, McSharry reform) (European Parliament, 2013). The heavy dependence of the European Union on international imports of legumes is recognised and has created debates on whether EU should start producing more home-grown own protein. Over the last decade various changes have led to a more permanent and structural change for legumes in the world markets. Over
the last 20 years, the price of nitrogen fertiliser has more than doubled, thus increasing the cost-effectiveness for the nitrogen fixing legumes (Eurostat, 2014). The producer prices of all legumes have shown (Figure 2.7) a steady increase in the last ten years, which puts legumes in a better position over wheat and other cereals generally in competition for land. Specifically for soybean, the import quantities of soybean from 2002 and onwards have started falling and the price is showing a continuous steady increase, which is likely to continue due to global requirements for feed in an increasing population (European Parliament, 2013).

Figure 2.7: Producer prices of legume crops from 1991 to 2011 from EU-27.  
(Source: own figure based on data from FAO (2014b))
2.2 Global Threats

2.2.1 Human Population Growth

Over the last few decades, the world’s population is constantly increasing. In 2011 the world population (Figure 2.8) broke the 7 billion threshold (United Nations, 2013b). Growth is continuing, at a rate of 4.5 births per second, while at the same time, the mortality rate was recorded at 1.8 deaths per second in 2013. This means that in 2013 alone the net growth of the world’s human population has increased by almost 87 million in comparison with 2012 figures (PRB, 2013).

![Figure 2.8: World’s population from 1950 to 2100. The period after 2010 are estimation based on United Nations estimates while the period before refers to actual data (Source: own figure based on data from United Nations(2013a)](image)

If the current growth rate persists, forecasts suggest that in 2100 the population will reach 16 billion (United Nations, 2013a). These global
population predictions pose pressures on the environment and natural resources, as well as challenges to food security to sustain a growing population. Food scarcity is one of these challenges that is important now and which will become more and more crucial in the future (IFPRI, 2011). Over the last century the population of malnourished people in the world has increased dramatically, exceeding one billion people in 2009 (FAO, 2010).

Reports have indicated that climate change and the higher frequency of extreme weather events globally, will have a negative effect on the agricultural productivity (IPCC, 2013). Traditional agriculture practices will have to change and become more sustainable in both environmental and production terms in order to absorb the increasing pressure of the food scarcity. Global demands for protein increase as income and expectations of the developing world increase. The cultivation of protein-rich crops can accommodate the increasing global needs for animal feed. Crops rich in protein (legumes) can be part of the strategy to minimize or soften some of the pressures that are inevitable in the future.

2.2.2 Climate Change

Planet Earth is experiencing an unusual period of stability, in comparison with the previous periods of dramatic changes, notably the Holocene period. Over the last ten thousand years the naturally developed period of Holocene has created suitable conditions for humans to live and maintain this life on the planet. However, since the industrial revolution in the 1850s, the ecosystem balances have been disturbed (Dansgaard et al.,
A new era of changes pose threats for the system to exceed the limits of the Holocene period. A new driver, the anthropogenic actions, is affecting gradually the natural development of the periods. The new era that has developed was named “Anthropocene” in order to highlight the fundamental influence of human activities in the environment (reference!). This transformation creates pressure to the Earth’s ecosystem as the changes speed up the environmental changes in an unsustainable way and which may last for long period of times or even be irrevocable (Steffen et al., 2007). The question is, how far are we in this change cycle and how much ?? Rockström et al. (2009) identified nine main planetary systems and proposed safe operating limits for each one, shown in Figure 2.9. Climate change and N cycle are two out of three systems that have already exceeded the safety thresholds. Atmospheric CO₂ concentration and radiative force are two parameters that were chosen as indicators for climate change in Rockström et al. (2009). Both CO₂ and radiative force have exceeded the proposed limit by almost 10% and 50% respectively (IPCC, 2013). There are many key indicators that highlight the existence of climate change. These indicators include a number of physical responses to the system changes.
Many researchers have highlighted the extreme increases of indicators such as CO₂ concentration (Etheridge et al., 1996), N₂O concentration (Machida et al., 1995), CH₄ concentration (Blunier et al., 1993), ozone depletion (Shanklin, 2014), temperature anomalies (Mann and Jones, 2003; Mann et al., 1999), central zone N flux (Mackenzie et al., 2002), tropical rainforest and woodland loss (Kates et al., 1990) and extinction of species (Wilson, 2001). Additional indicators include sea level, global and regional surface temperatures, extreme events, ice concentration and ocean acidification (IPCC, 2013).
2.2.2.1 Greenhouse gas (GHG) concentration

Indicators that are playing a central role in quantifying changes and contributing to driving change, are concentrations of the three most important GHGs (Forster et al., 2007). Over the last six decades the concentration of all the three main GHGs are showing an increase rate. Only CH₄ appeared to come into equilibrium around the start of 21st century; however this was only temporary as concentrations continue to increase from 2007 to present.

![Graph showing main GHG concentrations from AD0 until today](image)

Figure 2.10: Main GHG concentrations from AD0 until today (Source: (IPCC, 2013). The black dotted line in the CO₂ graph defines the proposed boundary (Rockström et al. (2009)).
Nitrous oxide concentrations are increasing constantly showing a sharp rise from 1970 until today.

Modern agriculture plays one of the central roles in the formation and acceleration of climate change (Figure 2.11). Agriculture is the main contributor in the generation of GHGs amongst all land uses. Over a period of 20 years (1990-2010) the emissions generated from agriculture, raised by 8% from 4613 Mt CO₂eq to 4983 Mt CO₂eq. In 2011 the highest level of emissions in history from agriculture was recorded with 5335 Mt CO₂eq almost 10% more than the level of the previous decade (FAO, 2014a).

Figure 2.11: Historical global trends of GHG emissions from land use (FAO, 2014a)

Agriculture is one of the main sectors that will be heavily affected and suffer serious losses in crop yields (Figure 2.12) due to climate change. Mitigation options and strategies are crucial in order to minimise the effects of changing weather patterns. Creation of new crop varieties and suitable
sustainable rotations can contribute radically towards a more efficient crop production. The inclusion of biological N fixation plants (e.g. legumes) in novel rotations can be beneficial from the greenhouse gas emissions and sustainability point of view.

![Figure 2.12: Impacts of climate change on crop yield production (IPCC, 2014a)](image)

### 2.2.3 Nitrogen cycle as a global threat

As mentioned in section 2.2.2 the N cycle is one of the three planetary systems that have transgressed the limits set of a safe operating space (Rockström et al., 2009). The amount N$_2$ that has been removed from the atmosphere for anthropogenic use has exceeded the 3.5 times the proposed boundary from Rockström. One of the main reasons for this enormous transgressor is attributed to modern agriculture (Foley et al., 2005). A more detailed explanation of the N cycle is available in section 2.3.1
2.3 Nitrogen

Nitrogen is a major nutrient for biomass production and one of the most abundant elements in the Earth’s atmosphere, comprising 78% of di-nitrogen (N₂) (Sprent, 1979; Sutton, 2011). Although plentiful, nitrogen in the atmosphere is an extremely immobile chemical element which makes it inaccessible to much of the biosphere. The form of nitrogen that is more mobile is called reactive nitrogen (Nr). The main members of the reactive-nitrogen group are nitrate (NO₃⁻), ammonium (NH₄⁺), ammonia (NH₃), nitrogen oxides (NOₓ) and nitrous oxide (N₂O). One of the most common problems that plants meet worldwide is the N deficiency. Plants are unable to use N in the form that exists in the atmosphere, but they need it in specific more reactive forms, in order to be utilised (Erisman, 2011). Consequently, gaseous N is highly susceptible to transformation into forms that can be absorbed and used by plants (Möller and Stinner, 2009). Nitrogen is a main element for the plant as it is present in protein, enzymes and chlorophyll. Therefore, it contributes significantly to human health as it is part of our food diet (Rosswall, 1982). Nitrogen is essential for many biological processes as it is present in the four bases that make up nucleic acids such as DNA and RNA (Pidwirny, 2010). In the bulk majority of soils, N exists in organic form. In agricultural soils the inorganic form of N is significantly higher as it exists in forms such as NH₄⁺ and NO₃⁻. These N forms transform through the processes of nitrification and denitrification (Vinten and Smith, 1993), discussed in section 2.3.1.2 Nitrification.
2.3.1 Global Nitrogen Cycle

One of the most significantly disturbed cycles in the environment is the nitrogen (N) cycle (Figure 2.13), which is one of the most important processes in the environment and especially for the soil component. The main reason for that disturbance over the last century is heavily connected with human actions. Added to the natural sources of N like volcanoes (Reid et al., 2005), oceans (Voss, 2011), soils (Schlesinger, 2009), lighting (Smil, 1997) and weathering of rocks (Holloway and Dahlgren, 2002) there are two main anthropogenic sources which are adding to the global nitrogen budget. Forest fires can be both natural and anthropogenic source of N. Fertiliser manufacture, burning of fossil fuels, principally in industry and transport, are the main anthropogenic ways in which inert nitrogen is transformed into forms which are more prone to be mobile (Sutton, 2011). More specifically the burning of fossil fuels produces emissions of NOx and N2O by the oxidation of N2. The large scale production of N-based fertilisers through the Haber-Bosch process (Haber, 1920) (details for the process in section 2.5) has increased the availability of Nr by the creation of NH₃ and the insufficient use of it is adding extra pressure to the system (Erisman, 2011). All of these activities release different forms of Nr to the atmosphere and as a result, the system becomes unbalanced (Figure 2.13) (Kroeze, 1994). The main two losses of N from the agricultural systems to the environment are from two sources; namely: nitrate (NO₃⁻) from soil to water courses and nitrous oxide (N₂O) from soils, crops and drainage water (indirect losses)

Figure 2.18 presents a simplified version of the N cycle including the inputs, outputs and flows within the system.
2.3.1.1 Mineralisation and Immobilisation

Transforming soil organic N into inorganic mineral forms (NH$_4^+$, NO$_3^-$) occurs via two phases through a process governed by the soil microbial community. The first phase is called mineralisation. This process is completed in two main steps which are called aminisation and ammonification (Verstraete and Focht, 1977). Firstly, soil micro-organisms (mainly heterotrophs) decompose multipart proteins to their simpler compounds such as amines, amides and amino acids. The second step includes the transformation of the amino (NH$_2$) groups to NH$_4^+$ and is performed by heterotroph organisms. Carbon dioxide is also emitted during
this transformation process (Verstraete and Focht, 1977). Immobilisation is the reverse process of mineralisation, which refers to the conversion of NH₄⁺ to organic compounds. In that procedure takes place the consolidation of the inorganic N to the microbial tissue of organic matter (Vinten and Smith, 1993; Addiscott, 2005). Those two processes can take place at the same time depending on conditions (Prakasa Rao and Puttanna, 2000).

### 2.3.1.2 Nitrification

Nitrification is the second phase of the microbial process in which the final compound is NO₃⁻ (Equation 2.1a). Here NH₄ is oxidized to NO₂⁻ and then to NO₃⁻ (Equation 2.1b). This phase is divided in two steps as well. The first includes the conversion of NH₄⁺ to nitrite (NO₂⁻) while in the second, aerobic conditions are required for the transformation of NO₂⁻ to NO₃⁻ from bacteria called nitrifying organisms (Verstraete and Focht, 1977; Addiscott, 2005; Prakasa Rao and Puttanna, 2000).

\[
\begin{align*}
\text{(a)} \quad 2NH_3^+ + 3O_2 + e^- & \rightarrow 2NO_2^- + 2H_2O + 4H^+ \\
\text{(b)} \quad 2NO_2^- + O_2 & \rightarrow 2NO_3^- 
\end{align*}
\]

Equation 2.1: Nitrification process

Nitrification is favoured in oxic (aerobic) conditions and is the main source of N₂O (Prakasa Rao and Puttanna, 2000). The nitrifying organisms taking part in the nitrification are aerobic bacteria such as *Nitrosomonas, Nitrobacter* and *Nitrosospira* which require CO₂, O₂, NH₄ and they are autotrophs. They are rather important in acidic soils and are growing
slowly. Consequently, soil conditions and management can have a big influence in the production of N₂O fluxes (Skiba et al., 1993).

2.3.2 Nitrate (NO₃⁻)

Nitrate is one of the inorganic forms that plants can absorb and plays an important role in plant growth. After the absorption from the plants of NO₃⁻ it will be reduced in NH₄⁺ and then it will be adjusted via glutamate (Prakasa Rao and Puttanna, 2000). Nitrification is really important in the N cycle as NO₃⁻ is extremely mobile and prone to leaching and is regarded as one of the main losses of N (Rosswall, 1982). It is extremely soluble and if it is not acquired by the plant, it will be lost from the soil via leaching or runoff (Prakasa Rao and Puttanna, 2000). The anionic NO₃⁻ cannot be attracted by the clay minerals (negative charged, which highlights the vulnerability to leaching (Tan, 2000). That sets a growing pressure on the quality of the groundwater reservoirs due to the fertilisation use. The percentage of N application to the soil, which is leached to the groundwater, is about 30% (Reay et al., 2003). The factors contributing to leaching are easily displayed by water, high mobility and solubility (Addiscott, 2005). Nitrate leaching is driven by the application and the poor management of N-based fertilisers and it is related with the surplus of N applied. Goulding (2000) has reported though that changes in the management of the field like the change of the time of the fertiliser application can match the crop needs in N and can have noteworthy reductions in the N surplus of up to 65%. More leaching is expected during the autumn and winter months, as the ground remains bare due to land management and the precipitation rate is higher (ADAS, 2003). Soil texture and structure can influence the amount of leachate, as lighter
soils have poor water holding capacity (Addiscott, 2005; Prakasa Rao and Puttanna, 2000). Ferrier and Edwards (2002) have reported that the most considerable issue for the degradation of the water resources for the next 20 years is going to be the agricultural diffuse pollution, as it affects human health and the environmental quality. Unavoidably, through ground water, nitrates are part of the human food diet. Reports have shown that high concentrations of NO₃⁻ in food can create many health issues such as hypertrophy of thyroid (van Maanen et al., 1994), Alzheimer’s disease (Tohgi et al., 1998) and even oral cancer (Badawi et al., 1998). European Union in order to meet the nitrates directive 91/676/EEC targets, there is a need to take measures to reduce high NO₃⁻ concentrations in leachate. This directive, along with the Water Framework Directive (2000/60/EC), put forward that groundwater should not exceed 50mg/l of NO₃⁻ and targets to shield waters from agriculturally derived NO₃⁻ pollution (European Comission, 2009).
2.4 Nitrous oxide (N\textsubscript{2}O)

Nitrous oxide is a main GHG produced by agriculture (Wang and Sze, 1980; Smith, 2010) the third most important (Figure 2.14) after carbon dioxide (CO\textsubscript{2}) and methane (CH\textsubscript{4}) (Smith, 2010).

Figure 2.14: Atmospheric concentrations of the significant GHG’s over the past 2000 years with increases from 1750 attributed to human activities (Forster \textit{et al.}, 2007)

Nitrous oxide accounts for 5% (Figure 2.15) of the total atmospheric greenhouse effect over the last century (Helgason \textit{et al.}, 2005; Bouwman, 1990). It is a potent gas having a substantial lifetime of 120 years (Prather, 1998) and has ca. 300 times greater global warming potential (GWP) than CO\textsubscript{2} over a century (IPCC, 2013). The GWP is a descriptive measure that is used for comparing different gasses in a standardised manner. In the case of GHGs, carbon dioxide is used as the base for which other GHGs are
2.4 Nitrous oxide (N2O)

compared through expressing other gases as carbon dioxide equivalents (1 million metric tonne N2O ≈ 300 million metric tonnes CO2equ). Nitrous oxide has a growth rate of 0.25% per year (Prinn et al., 2000), thus it is expected that atmospheric N2O will significantly increase in the foreseeable future (Randeniya et al., 2002). Compared to CO2, the quantities of N2O are quite low (Figure 2.15) however due to a greater GWP and long lifetime, N2O is a very important GHG. It has also been reported that N2O contributes in the processes of stratospheric ozone layer depletion (Forster et al., 2007; Crutzen, 1970).

![Figure 2.15: Total annual anthropogenic GHG emissions since 1970 to 2010 (IPCC, 2014b)](image)

Europe contributes almost the 11% of the global N2O emissions (Figure 2.16) which equates to 0.8 Mton N2O-N (EDGAR, 2013). The atmospheric concentration is steadily rising from pre-industrial times (1950s)
at approximately 280 ppb to a concentration that exceeds 325 ppb in 2013 (IPCC, 2013).

Figure 2.16: Map of the European emissions of N₂O in 2010 (EDGAR, 2013)

Soil N₂O fluxes are controlled by the microbial-led processes of nitrification and denitrification (Equation 2.1, Figure 2.17), and which are ultimately governed by soil micro-organism communities (Conrad, 1996; Schlesinger and Bernhardt, 2013). Denitrification is the process by which micro-organisms perform the conversion of NO₃⁻ to N₂ and N₂O (Equation 2.2). Nitrous oxide is not a final product but an intermediate one (EFMA, 2003).

\[ 2NO_3^- + 12H^+ + 10e^- \rightarrow N_2 + 6H_2O \]

Equation 2.2: Denitrification process
When there is ample NO₃⁻, there is a strong activity of denitrification process under certain soil conditions. Anaerobic conditions should prevail and soil organic carbon should be present as it acts as a reducing agent (Robertson and tiedje, 1987; Firestone and Davidson, 1989; Prakasa Rao and Puttanna, 2000). The denitrifying organisms are mostly anaerobic and belong to many physiological groups. Enhancement of fluxes occurs when the plant has satisfied its needs for N resulting in a N surplus in the soil as they are favoured by wet conditions (Smith and Conen, 2004).

In order to depict N₂O production, Davidson et al. (2000) introduced the “hole in a pipe” concept (Figure 2.18). Ammonium enters the first pipe and transforms to NO₃⁻ while N₂O and nitric (NO) are emitted from the holes within this first pipe. In the second pipe NO₃⁻ enters and at the end nitrogen gas (N₂) is produced. The losses from each hole are exactly the same as in the previous pipe (N₂O and NO). Increased fluxes are expected if one or more holes are blocked from the rest holes and there is constant needs of oxygen for those processes (Bremner, 1997).
2. Literature review

The main direct anthropogenic source of N₂O is agriculture, animal husbandry, industry and transport. Combined these sources contribute to 64% of total global N₂O production. Undoubtedly agricultural soils are a major contributor to total anthropogenic global N₂O concentration accounting for 47% to 64% of total emissions (Skiba et al., 1998; Mosier et al., 1998; Olivier et al., 1998; Kroeze et al., 1999). This is primarily due to poor land management and in particular the uncontrolled use of fertilisers that contributes to the global greenhouse gas budget (IPCC, 2000). When fertiliser application is combined with favourable denitrification conditions, large quantities of N₂O can be emitted. However, many studies have examined the potential of reducing the N₂O emissions from agriculture through changing management practices. These refer to changes such as shallower tillage depths (or even to no tillage systems) (Oorts et al., 2007; Ball et al., 1999), reduced or more precise application of fertilisers and manures (Meng et al., 2005). “Some additional N₂O is thought to arise in agricultural soils through the process of nitrogen fixation, though the true importance of

Figure 2.18: “Hole in a pipe” conceptual model of N₂O production (Source: own figure based on Davidson et al. 2000)
Nitrous oxide (N$_2$O) remains poorly defined” (Reay, 2011). The work that is presented in this study will aid the investigation of the importance of this source. While there are high levels of uncertainty associated with these values, the fact that the global population is rising and an increased demand for food is expected, 35%-60% higher emissions of N$_2$O are predicted till 2030 (Smith et al., 2008). Nitrous oxide can also be produced indirectly. One of the most important indirect sources is N$_2$O leaching via run off from cultivated soils to aquatic environments such as rivers, lakes, groundwater and estuaries. In estuaries and rivers, nitrifiers and denitrifiers may produce N$_2$O both in the water column and in sediments. Precipitation can leach large quantities on N$_2$O from the soil into rivers, drainage ditches and streams. As a result the N$_2$O, which is lost from the agricultural soils, is going to be emitting as soon as the drainage water is exposed to the atmospheric air (Reay, 2011). There are numerous uncertainties in the way that indirect emissions from managed soils are estimated. These uncertainties are associated with activity data, lack of measurements, leaching factors and natural variability (IPCC, 2000).

2.4.1 Factors Controlling N$_2$O Emissions

Nitrogen production is affected by several factors such as soil O$_2$ concentration (Snyder et al., 2009) water content (Goodroad and Keeney, 1984) organic matter (Pennock et al., 1992), soil temperature (Sarkodie-Addo et al., 2003) and soil pH (Hadas et al., 1989). These factors will be analysed briefly in the following sections.
2.4.1.1 Soil O₂ and water content

Oxygen levels in the soil are generally influenced by water content, microbial activity and temperature, which then control denitrification and nitrification processes (Figure 2.19). Low oxygen pressure can cause pulses of denitrification (Firestone and Davidson, 1989) while N₂O production may be slowed due to aerobic conditions (Davidson et al., 1991). Soils with high moisture content are ideal for denitrification, as it requires anaerobic conditions. The ideal water content for denitrification is 80%-100% (Vitousek et al., 1989; Letey et al., 1981). Under the conditions of waterlogging the denitrification process will be completed and N₂ is the final product with N₂O being the main gas produced, when the soil moisture content is considerably lower. On the other hand during nitrification, when soil O₂ levels increase the ratio N₂O/NO₃⁻ is decreased. At low moisture conditions, the available NH₄⁺ is limited for nitrification, as microbial activity is depressed. It has been observed that the wetting of a dry soil through rain or irrigation leads to N mineralisation, nitrification and large, rapid (but short in duration) NO and N₂O emissions (Scholes et al., 1997) with the peaks of the emissions observed in the first wetting events and decline gradually on the subsequent (Letey et al., 1981).
2.4 Nitrous oxide (N2O)

Figure 2.19: The influence of water-filled pore space on nitrification (grey shaded section) and denitrification (cross-hatched) and contributions of NO, N2O and N2 emissions (Davidson et al., 2000).

2.4.1.2 Temperature

Rates of nitrification and denitrification processes are also affected by temperature. It has been observed that below 5°C, rates are extremely low but they increase significantly when there is an increase in temperature above this level. The optimal temperatures for nitrification and denitrification ranges from 25°C to 35°C and 25°C to 37°C respectively (Flechard et al., 2007). Soils in humid tropics can retain a high level of activation of their processes due to continuous high temperatures and the
cycling of nutrients can be faster in comparison with other regions with colder climates that can hinder these processes. According to Vitousek (1984) the forests that are located in tropic climates cycle two to four times more N in comparison with forests in temperate climates.

During extreme weather events, large amounts of emissions can be produced in only a few days (Otter et al., 1999). Examples of these events are more highlighted especially during winter when there frost weathering in the soil is taking place or in summer period when there is an event of rainfall in dry soils. As a result of the dependency of the N₂O emissions from the temperature the fluxes show a variation according to the season (Flechard et al., 2007).

2.4.1.3 Soil pH

For both nitrification and denitrification there is an optimum pH which ranges from 7.0 to 8.0. At low pH (eg 4.0) the main product of denitrification is N₂O (Eaton and Patriquin, 1989; Brumme and Beese, 1992) particularly with the presence of NO₃. This happens due to the high sensitivity of N₂O reductase to proton activity (Alexander, 1977). According to Ottow et al. (1985), the soil and constituent organisms determine the N₂O ratio rather than decreasing pH. According to Parkin et al. that can be attributed to the adaptation of denitrifiers to acid soils (Parkin et al., 1985). When there are higher values of pH the final product of denitrification is N₂ as N₂O is further reduced (Hadas et al., 1989).
2.4.1.4 Organic Matter

Denitrification can be depended by the presence of organic matter. High availability of organic matter (e.g. organic peat soils) can lead to large N losses from agricultural soils in the form of N₂O fluxes. Moreover, it can induce NO⁻₃ and therefore N₂ emits instead of N₂O. Nitrous oxide losses from the soils can be increased by the addition of organic matter through management like application of organic manure or by the deposition of crop residues. With the presence of organic C the anaerobic conditions prevail as there is an increase of anaerobic microsites and as a result there are ideal conditions for the enhancement of denitrification (Pennock et al., 1992).

2.5 Fertilisers

Fertilisers are a way to supply crops and plants with all the needed nutrients required for growth and to protect against deficiencies. The application of fertilisers by farmers is a practise that has been implemented for many years by using animal wastes or crop residues. It was after 1900 that the human population growth created increased food demands that had to be met. After unsuccessful and costly efforts to develop industrial nitrogen, Carl Bosch and Fritz Haber developed the breakthrough invention of industrial inorganic production of Nr by “synthesizing ammonia from its elements” (Haber, 1920). In the mid of the 20th century the agriculture production was now dependant on industrial made Nr and the nitrogen crisis was soon forgotten (Erisman et al., 2008). This Haber-Bosch invention was proven important as it is one of the main reasons this planet today is hosting more than seven billion people. According to Erisman et al. (2008)
due to Haber’s invention the number of people supported per hectare of arable land was increased to more than double, while the yield production of main crops has increased around 30%-50% (Nelson, 1990) (Figure 2.20).

![Graph showing world population, meat production, and N fertiliser input](image)

**Figure 2.20:** World’s population, meat production and N fertiliser input in the world the last century (Erisman, 2011).

The Haber-Bosch invention in the early 1900s changed the scene of N in the agriculture. It constitutes one of the greatest inventions in the human history by allowing the exponential growth of the population and assuring food security (Sutton, 2011; Erisman, 2011). In 2004 Europe was one of the largest suppliers of meat and cereals accounting for 21% and 20% of the global production (IPCC, 2007). Although the large scale industrial
production of Nr was an achievement that managed to sustain and grow the population, it also resulted in side effects from imbalances in the biological cycle that ultimately pose threats to the ecosystem and wider environment. The main two ways of supplying Nr in the soil is through the application of organic and inorganic fertilisers (Haber-Bosch invention) and the biological nitrogen fixation of protein crops. Fertilisers can be divided generally in two groups: in organic and inorganic or synthetic. The differences between these fertilisers are not to do with the nutrients they contain but from the type of source they originate from.

Figure 2.21: Human made Nr creation from 1850 to 2005 (IPCC, 2013)

Despite the fact that the industrialised form of food production is dating back to 1900s, the inorganic fertiliser usage has shown an enormous increase since 1960s worldwide (Figure 2.21).
There are huge energy demands in the fertiliser production, as discussed by Jensen and Hauggaard-Nielsen (2003). Estimates suggest that approximately 1% of the total world’s energy consumption has to be used in order to manufacture N-based fertilisers consumed (Snyder et al., 2009). During the manufacture of fertilisers, it has been observed that greenhouse gases are emitted, approximately 1 kg of N fertiliser normally produced 2500 g of CO₂, 10 g of N₂O and 1 g of CH₄ (Haag & Kaupenjohann, 2001).

The use of N-based fertilisers is constantly increasing worldwide (Alexandratos and Bruinsma, 2012). Europe is the largest consumer of N-based fertiliser over the last decades (Jensen and Hauggaard-Nielsen, 2003) (Figure 2.22).

Figure 2.22: Total N fertiliser nutrient consumption in EU-27 for the period from 1927 to 2009 (EFMA, 2009a)
The decline observed between 1990 and 1995 occurred due to the economic collapse of eastern European countries and introduction of the new Common Agricultural Policy (CAP) that was brought into effect in 1990.

Nowadays the current levels of N-based fertiliser consumption in the EU-27 varies from 42 kg ha\(^{-1}\) and is going up to 243 kg ha\(^{-1}\) while the average stands at about at 90 kg ha\(^{-1}\) of agricultural land (Jensen and Schjoerring, 2011). Consumption within the whole European Union has stabilised at around 11 Tg however, it is expected to rise in the next decade by about 0.5 Tg (EFMA, 2009b). The use of the fertilisers is dominated by almost 80% of the N based fertilisers while the N compounds hold approximately the remaining 20% (EFMA, 2003). Global N inputs from artificial fertilisers in comparison with biological nitrogen fixation and animal manure have been shown to be considerably higher (Mosier et al., 2004).

Over the last years 50 years there has been an attempt by the European Union through CAP to reduce the uncontrolled supply of nitrogen in the agricultural production. Surplus nitrogen is not absorbed by plants/crops and can create imbalances and pressures to the system resulting in nitrogen compounds being leached, lost in runoff or even emitted. The nitrogen use efficiency (NUE) is important to minimise pressures to the ecosystem and can be defined as the ratio between the nitrogen in the crop leaving the agricultural land with the nitrogen that was applied in that land for the production of the crop. The NUE varies in European Union from less than 50% to 70% depending on the amount of N surplus of each country (OECD, 2004).
2.6 Conclusions

During the last century the environment has received constant pressures from anthropogenic activities. A perpetual need to increase available food and protein alongside with the application of modern agricultural management activities are playing an important contribution to these pressures. Legumes are an important group of crops mainly due to their high content of protein and the ability of fixing N. There is a crucial need to maximise yields while reducing the use of inorganic fertilisers and limit N₂O production. The adoption of legume crops into crop rotations could be a mutually beneficial choice. The representation of legumes in European Union has declined over the last decades while global issues like human growth population, climate change and nitrogen cycle are enhancing the existing pressures. Nitrogen based fertilizers have increased the last 50 years and consequently N₂O emissions are following the same trend. The above literature review has identified these issues and will be researched further the potential effect of legumes in European agriculture through environmental modeling which is expanded in the next chapter.
3 Environmental Modelling

*Everything should be made as simple as possible but not simpler*

Albert Einstein (1879-1955)

3.1 Background

One of the most important and potent elements that has been in widespread used, and in many cases not used in an efficient way, is nitrogen and associated compounds (Sutton, 2011). Soils play an important role in the production and the storage of \( \text{N}_2\text{O} \) (Bowden, 1986). For several decades agricultural practices have contributed to the disturbance of the ecosystems and have created pressures on the environment. Atmospheric pollution through \( \text{N}_2\text{O} \) and \( \text{NH}_3 \) emissions and the contamination of ground water
through nitrate leaching are the main concerns for the protection of the environment (Rosswall, 1982). Environmental modelling is a useful tool that can be used in order to find ways to minimise these environmental issues and ensure environmental protection (Qin et al., 2013). Modelling can be defined as a mathematical approach that conceptualizes from our understanding of natural environment, and it is a description which can focus on a specific research questions in relation to the ecosystem (Aral, 2014). Environmental modelling is not used in order to replace observed data and measurements. However, models can be used as a powerful tool that can help the scientific community better understand the measurements and can help in the interpretation of the details of the mechanisms behind them. One of their main potential benefits in research is their ability to simulate aspects of reality and the predictions can be a valuable additional tool for decision making and testing different scenarios for various mitigation options. In order to resolve environmental issues they need to be fully understood (Wainwright and Mulligan, 2013). There are two main scientific tools that are available in order to understand and identify the physical processes and balances within the environment that can help us address any environmental issue. Those are field or laboratory experiments and environmental modelling. Both have advantages and disadvantages in their use and in the way they perceive and try to address the problem. They can show as well, a different degree of complexity in individual aspects. It is well established that field measurements can have a high level of difficulty both in execution and in analysing results. Both aspects are important and necessary. Necessary because field observations are important scientific tools in the stage of identifying the problem and understanding it in depth.
When it comes to the resolving the problem, experimental set ups and field observations are not always the most thorough tool that can be used towards the assessment and the choice of the best remedial strategy. One of the main difficulties in field observations is that observations in a specific site may only be applicable for that specific site and provide no information of the implications of those strategies in fields with different characteristics. Furthermore spatial, time and cost limitations can be a considerable hindrance to conducting a comprehensive field experiment. A well validated model can be a very worthwhile tool in decision making and can in some cases replace field based experiments (Jørgensen and Fath, 2011b). Modelling gives the opportunity to test different scenario approaches for various mitigation options. It is more cost effective and the experiments can undergo many changes and even be re-designed following the results of earlier simulations. On the other hand the field measurements are showing a higher level of complexity in that respect because of their inherent structure do not allow such easy flexibility within a season or even between seasons.

Models are not new, as they have been used for many years in order to give a representation of real life and have been used extensively in biological and physical sciences (Jørgensen and Fath, 2011d; Smith and Smith, 2007). Models are in fact an abstraction of reality. In order to be effective and regarded as good, they should describe the most vital details that are needed in order to depict reality but not all the details because then they tend to be the reality itself (Wainwright and Mulligan, 2013; Jørgensen and Fath, 2011d). There should be a balance between the amount and the
complexity of the parameters needed and the greatest representation of reality in order to achieve an effective and the least complex model. That means using the least amount of complexity that is needed but without leaving important aspects of reality outside the modelling activity. Natural ecosystems by definition are complex and dynamic (Mulligan and Wainwright, 2013). Models are not trying to simplify that complexity. They rather try to describe this complexity under a certain focus. They focus on the aspects that are relevant to the main hypotheses of the goals of the model while excluding unrelated details. There are many environmental models that describe dynamics within the environment focusing on different matters of interest (Jørgensen and Fath, 2011d).

The rise of environmental/ ecological modelling started in the 1970s, mainly due to the needs of science and the invention of computers, with the development of three main types of models namely the population dynamics, bioenergetics and the biogeochemical. During the preceding years, important scientific questions had emerged from all the different aspects of the ecosystem. The scientific community responded in that urgent need for ways to tackle the issues with more types of models, namely Spatial, Structurally dynamic, Artificial Neural Networks, Ecotoxicological, and Dynamic biogeochemical model (DBM).

This range of models can address most scientific questions, however there are constant endeavours to create new models that can include or focus on more detailed environmental questions. In environmental modelling the nature of certain issues requires a combination of two or more models in
order to find a suitable answer. These types of models are called hybrid models. The most popular type of models the last 40 years is the dynamic biogeochemical models (Jørgensen and Fath, 2011a) and the following analysis will focus on this type of model.

3.2 Dynamic biogeochemical models (DBM)

Since the early 1970s there has been a number of DBMs developed. Biogeochemistry is the science which includes the definition and the understanding of the movement of the chemical elements which influence the relationship of life and the environment (Vernadsky, 1994). The DBMs are the mathematical interpretation of the movement and the transportation of different chemical elements in the terrestrial ecosystems which describes biogeochemistry (Li, 2007). These models are crucial when there is a need to attempt to describe the complex dynamics and cycling of various biogeochemical compounds of the environment. The construction of these types of models needs comprehensive databases of field (and crop) measurements in order to clarify and describe all these dynamics and processes that are taking place in an ecosystem. That means a good and sophisticated knowledge of the system dynamics are required so the model can capture all the details in a comprehensive way. Due to the nature and the level of complexity that these models are expected to deliver, the requirement for sophisticated knowledge of the system can be regarded as a disadvantage for that type of models (Jørgensen and Fath, 2011a; Jørgensen and Fath, 2011c). Until now there have been many attempts to develop environmental models (almost 4000), with the first complete attempt in 1925
with the first environmental biogeochemical model built by Lotka-Volterra and Streeter-Phelps (ref). The accumulated experience in developing modelling tools combined with our increasing knowledge of the physical reality of managing soil C and N, has contributed to environmental protection and management (Jørgensen, 1999).

The main processes of nitrogen cycle which are defined by most of the models are namely surface application of organic and inorganic fertilisers, nitrification, denitrification, plant uptake, mineralization and nitrate leaching (McGecham and Wu, 2001). There are many research teams that they have produced many field scale simulation models during the last four decades that can simulate the dynamic processes of different compounds in the environment but with a particular focus on nitrogen, and some examples are given in Table 3.1.: These models all describe the effect of weather, human activities on the soil C and N cycles. A short description of these models is described in the following section.
Table 3.1: Examples of environmental field scale models that can simulate nitrogen processes

<table>
<thead>
<tr>
<th>Environmental Models</th>
<th>SOILN (KTH, 2013)</th>
<th>DayCent (Parton et al., 1994)</th>
<th>ECOSYS (Grant, 1989)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>DAISY (Hansen et al., 1991)</td>
<td>ANIMO (Wageningen, 2013)</td>
<td>CANDY (Franko et al., 1995)</td>
</tr>
<tr>
<td></td>
<td>CERES EGC (Jones and Kiniry, 1986)</td>
<td>FASSET (Berntsen et al., 2004)</td>
<td>APES (Donatelli et al., 2006)</td>
</tr>
<tr>
<td></td>
<td>SUNDIAL (Bradbury et al., 1993)</td>
<td>NDICEA (Burgt et al., 2006)</td>
<td>DNDC (Li et al., 1992)</td>
</tr>
<tr>
<td></td>
<td>EPIC (Williams et al., 1984; Williams, 1990)</td>
<td>APSIM (Keating et al., 2003)</td>
<td>CropSyst (Stockle et al., 2003)</td>
</tr>
</tbody>
</table>

SOILN model was developed by the Royal Institute of Technology in Sweden. It has now been incorporated into COUP, which fully describes the soil N and water cycle in one model. SOILN before incorporation into COUP had to be run separately the water module. It is a model that simulates the water, heat, nitrogen and carbon processes (KTH, 2013). It can support a wide range of crops. In the latest versions of the model the C:N ratio of the microbial biomass can be determined and quantified whereas in the earlier versions that ratio was assumed. However, the plant uptake of N is based on an empiric calculation that depends on the root distribution (McGechan and Wu, 2001).
The Royal Veterinary and Agricultural University in Denmark developed the mechanistic simulation model DAISY (Hansen, 2013). The model can simulate dynamics of soil water, crop production and nitrogen (Hansen et al., 1991). One of the main characteristics of DAISY model is the wide range of options of crops (McGeocham and Wu, 2001) and the ability of the model to simulate successfully arable (Smith et al., 1997). Generally, it provides a really detailed treatment of plant uptake as there is a weather-driven plant growth sub model which interacts with the dynamic processes of nitrogen. Another advantage of the model is its representation of volatilization from fertiliser at the time of application but this also means that the model does not describe volatilization from the ammonium pool (McGeocham and Wu, 2001). The main disadvantages of DAISY include the inability to simulate woodland sites; it does not include a mechanism (estimation?) of root turnover and the level of difficulty to be parameterised (Smith et al., 1997; Hansen et al., 1991).

The CERES model is a model for the soil and crop interactions (Jones and Kiniry, 1986) that was developed to the CERES-EGC by adding a soil nitrogen component (Gabrielle et al., 2006). The model was developed by INRA/AgroParisTech Environment and Arable Crops Joint Research Unit (EGC). The model can simulate dynamics of soil water, carbon and nitrogen production (INRA, 2011) and crop growth (Wattenbach et al., 2010) in agro ecosystems. CERES-EGC shows some difficulties regarding the simulations of NEE and latent heat fluxes (Wattenbach et al., 2010).
CropSyst (Cropping Systems Simulation Model) is a multi-year, multi-crop model developed by the University of Washington in 1990s. The model can simulate soil water processes (included erosion from water), nitrogen budget, crop, root and canopy growth, decomposition and salinity. The model actually consists of five main components and three utility programs. One key feature of the model is the inclusion of the GIS-CropSyst which facilitates GIS based simulations from polygons that they come from the ArcView (Stockle et al., 2003).

The SUNDIAL (SimUlation of Nitrogen Dynamics In Arable Land) model was developed by Sustainable Soils and Grassland Systems Department Rothamsted Research in the United Kingdom. It is a dynamic process-based model which describes the turnover of C and N in the soil and crop systems (Rothamsted, 2013). One of the strengths of the model is the sophisticated volatilization of the plant litter (McGecham and Wu, 2001) and the fact that it can simulate more crop rotations for several years (Rothamsted, 2013). One of the main disadvantages of the model is that it uses weather data with a weekly interval. As a result, there is a loss of accuracy in the results and eventually the ability to represent reality. The above weakness is more noticeable when it comes to processes that are influenced by the pattern of rainfall as they cannot depict in detail the variety of the events of the rainfall over a weekly period, and rainfall tends to be more variable on a day-to-day basis than temperature.

In the early 1980s the USDA (United States Department of Agriculture) started developing a model to assess the effects of management
activities and especially of soil erosion in the soil productivity on the U.S. soils (Williams, 1990; Xiong et al., 2014). The result was the EPIC (Erosion Productivity Impact Calculator) model (Williams, 1990). The model is focused more on the implications of the management decisions (tillage, pesticide and fertiliser applications, change of cropping systems) on soil and its loss, the soil water quality and the crop production (Williams, 1990). The advantage of the model can be the same time its disadvantage. The model provides a simplified but effective crop growth approach that in the same time is generic and due to its uncomplicatedness of the described biogeochemical processes the model shows that there are limitations on its use (Stockle et al., 2003).

ANIMO (Agricultural Nitrogen Model) was developed by Wageningen University in the Netherlands. It is a computer simulation process oriented model which can predict nitrogen, carbon and phosphorus loads in watercourses (Wageningen, 2013). The model shows some strength which relates to the ability of the model to represent the processes associated with the application of animal slurry. The fact that it is considering ammonia volatilization after the slurry application and the process of anaerobiosis are also identified as strengths of the model. At the same time, the fact that ANIMO provide a complex animal slurry treatment has been proven to be a barrier for using the model, as it requires a substantial amount of field measurements for the application of the slurry data to be collected. The poor representation of denitrification can be listed as one of the weaknesses of the model (McGecham and Wu, 2001).
3.2 Dynamic biogeochemical models (DBM)

CANDY (CArbon and Nitrogen DYnamics) was developed by Helmholtz Research centre (UFZ) in Germany (Helmholz, 2012). CANDY is a model that can simulate carbon, nitrogen, water and temperature either in field or at a regional scale (Smith et al., 1997). One of the main strengths of the model is the fact that there is a choice of up to six different categories of applications of organic matter (manure, slurry, plant litter etc.). The main drawback of the model is that the empirical relationships that are used to describe the soil water content submodel (McGeacham and Wu, 2001).

There are models that could be used for the needs of this project as they could respond in an acceptable way in most of the needs of the project. These models are Day-Cent, DAISY and UK-DNDC. All these models can simulate the C, N dynamics in the soil and express the relationships between them. The model that was selected for this project was the UK-DNDC which is based on the biogeochemical model of DNDC. There were many reasons which led to that decision. The DNDC model is a well-established model used by a number of research groups across the globe for predictions of N\textsubscript{2}O emissions with a long list of published papers for more than 20 years. Another main reason for the selection of this model was the personal communication and close collaboration I had with the developing team of the model and especially with the leader of the team Prof. Changsheng Li. This collaboration made possible the constant improvement of the model according to the project needs. The expertise that was available in the group that I am part of (Modelling Group of Crop and Soils in SRUC) made the choice of the model to be used in this project a relatively easy decision.
3.3 DeNitrification-DeComposition

DNDC is a dynamic and deterministic simulation model of carbon and nitrogen biogeochemistry in agro-ecosystems (Li, 2013). DNDC can simulate several processes related to the nitrogen and carbon cycle (Smith et al., 2010) and it predicts crop growth, soil carbon dynamics, nitrogen leaching, and emissions of trace gases (Li, 2013). The model creates a bridge between the N and C biochemical cycles and four main ecological drivers (weather, soil, vegetation, human activities) (Li, 2007). Initially the model was developed for predicting carbon sequestration and trace gas emissions from upland agro-ecosystems in the United States (Li et al., 1992). As Li described in his paper (1992), the model is heavily driven by rain events and generally from the water input to the system as it has been observed that it is one of the main drivers for the production of N₂O (Mosier et al., 1986; Sexstone et al., 1985). The model is driven by two main equations of soil biogeochemistry, namely the Nerst (basic thermodynamics) (Stumm and Morgan, 1981) and Michaelis-Menten (kinetics of microbial growth with nutrients) (Paul and Clark, 1989) equations.

The first DNDC model, developed in 1992, consisted of three main sub-models: specifically (i) the thermal-hydraulic flows, (ii) the decomposition and (ii) the denitrification. The soil thermal-hydraulic sub-model predicts the soil temperature and the soil water content while the decomposition sub-model simulates the carbon and nitrogen pools in the soil. The denitrification sub-model uses the outputs from the previous sub-
models to determine the quantities of N₂O and N₂ produced from the field (Figure 3.1) (Li et al., 1992).

Figure 3.1: Structure of the primary version of the model highlighting the relationships between the main three submodels (Li et al., 1992).

In the later versions of the model, there were many additions and improvements. One of the major changes was the addition of the crop growth sub-model (Li et al., 1994) in which the relationships of C and N between plant and soil are simulated (Gilhespy et al., 2014). In 2000, there was the addition of another two key sub-models to the model which describes the nitrification and the fermentation processes (Gilhespy et al., 2014). The nitrification in the previous versions of the models in 2000 was upgraded in a sub-model so it can accommodate NO and N₂O production (as part of the nitrification) as a function of the nitrification rate and temperature.
in order to adequately simulate predictions. In the fermentation sub-model, all the processes were included to describe CH$_4$ production (Li, 2000; Li et al., 2000). It can be used for both site and regional simulations. The main difference between the two is the scale of the simulation. The site simulation refers to field scale while the regional to regions or even larger geographical areas.

The model has been validated for a range of agricultural systems all over the world. Some examples of countries for which the DNDC has been well tested are Canada (Smith, et al., 2010), China for potato, rice and corn, and for crop rotations which include winter wheat-maize, winter wheat-rice millet and winter wheat-corn (Qiu et al., 2009; Wang et al., 2008), Thailand (Frolking et al., 2004) and India (Babu et al., 2006) for rice. The model has since been developed further by many research groups for wider applications to studies of C and N cycling in agro ecosystems across the world (Giltrap et al., 2010a). The model been modified by many researchers to make it suitable for relevant production systems or even for specific crops (Giltrap et al., 2010b; Giltrap et al., 2010a). DNDC has also been combined with economic models (e.g. Leip et al, 2008). In the following table (Table 3.2) lists all the models that have been produced based on DNDC.
Table 3.2: Models-members of the family DNDC with a short description

<table>
<thead>
<tr>
<th>Models based in DNDC</th>
<th>Short Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>UK-DNDC</td>
<td>Modifications in order to fit local conditions of the UK (Brown et al., 2002)</td>
</tr>
<tr>
<td>NZ-DNDC</td>
<td>Modifications in order to fit local conditions of New Zealand (Saggar et al., 2004; Saggar et al., 2007)</td>
</tr>
<tr>
<td>PnET-N-DNDC</td>
<td>Combination of two models PnET and DNDC. Predicts GHG forest soils (Li et al., 2000).</td>
</tr>
<tr>
<td>Wetland-DNDC</td>
<td>Predicts CO₂ and CH₄ from wetlands (Zhang et al., 2002a)</td>
</tr>
<tr>
<td>Forest-DNDC</td>
<td>Predicts forest production and GHG from upland and forested wetlands (Li et al., 2005)</td>
</tr>
<tr>
<td>Forest-DNDC-Tropica</td>
<td>Predicts N₂O from tropical rainforests (Kiese et al., 2005)</td>
</tr>
<tr>
<td>Landscape-DNDC</td>
<td>Predicts C and N cycles in forest arable and grasslands(Haas et al., 2013)</td>
</tr>
<tr>
<td>Mobile-DNDC</td>
<td>Addition of an empirical model to provide climatic information for canopy layers (Grote et al., 2009)</td>
</tr>
<tr>
<td>Manure-DNDC</td>
<td>Calculate the GHG and the NH₃ emissions from livestock. Production and handling of manure from feedlot systems (Li et al., 2012).</td>
</tr>
<tr>
<td>Crop-DNDC</td>
<td>A model that combines detailed crop growth algorithms with soil biochemistry (Zhang et al., 2002b)</td>
</tr>
<tr>
<td>DNDC-Rice</td>
<td>Predicts GHG from rice production systems (Li et al., 2004)</td>
</tr>
<tr>
<td>DNDC-Europe</td>
<td>Combination of two models CAPRI and DNDC. Assess the effect of agri-environmental policy on GHG in Europe (Leip et al., 2008)</td>
</tr>
<tr>
<td>EFET-DNDC</td>
<td>Combination of two models EFET and DNDC for the region of Baden-Württemamber, Germany. GIS economic ecosystem model (Neufeldt et al., 2006)</td>
</tr>
<tr>
<td>NEST-DNDC</td>
<td>Combination of two models NEST and DNDC. Predicts CH₄ emissions from permafrost conditions (Zhang et al., 2012)</td>
</tr>
<tr>
<td>BE-DNDC</td>
<td>Regional model modifications for Belgium (Beheydt et al., 2007)</td>
</tr>
<tr>
<td>DNDC-CSW</td>
<td>Addition of a submodel to fit the to the needs of the Canadian Spring Wheat (Kröbel et al., 2011)</td>
</tr>
</tbody>
</table>
3.4 UK-DNDC

3.4.1 Background

In 2002, a new version of DNDC was developed in order to estimate emissions from the UK agriculture (Brown et al., 2002). UK-DNDC was based on the 7.5 version of DNDC with modifications to allow the model to run on a regional scale linked to UK relevant databases. The main changes were focused on soil characteristics, crops, daily climate, livestock, management and in the irrigation library file. These changes in the libraries affected the regional mode of the model. In 2006, the model was updated and the second version was made available. The model now is written in windows based visual C++ from turbo C which makes the incorporation of the updates easier. One of the main changes was the improvement of the carbon allocation and the biomass values as an enhancement to the model at the time. At the same time DNDC keeps developing and improving in many aspects creating a gap in performance for the two models (DNDC and UK-DNDC). This gap was addressed in 2011, when the two models merged. The new UK-DNDC combined all the updates of the DNDC model (version 9.4) and the updated regional databases for the UK. The improvements of the newer version of DNDC were focused more in the crop growth sub-model, extended choice in farm management practices, soil climate, the N and the CH₄ production. The site specific mode was the same as the latest version of DNDC.
3.4.2 UK-DNDC structure description

3.4.2.1 Input data

The structure of the UK-DNDC is identical to the structure of DNDC. First of all the model is driven by four main factors namely weather data, human activities (management practices), soil properties and crop details (Li, 2007). As mentioned before, the model can run in two modes, site and regional. Depending on the mode selected, the model will require different corresponding input data. For the regional mode, the model uses a database that has to be prepared by the user containing all the spatial information which describes the main drivers. For the needs of this project, the mode that was used was the site mode. The required input details are described in Table 3.3. In order to have precise simulations, it is necessary to ensure the provision of accurate input data to the model.
Table 3.3 : Input data for DNDC

<table>
<thead>
<tr>
<th>Climate</th>
<th>Soil Properties</th>
<th>Vegetation</th>
<th>Human activities</th>
</tr>
</thead>
<tbody>
<tr>
<td>Latitude</td>
<td>Land type use</td>
<td>Texture</td>
<td>Tillage</td>
</tr>
<tr>
<td>Climate data</td>
<td>Field capacity (wfps)</td>
<td>Soil pH</td>
<td>Fertilisation</td>
</tr>
<tr>
<td>• temperature (°C)</td>
<td>Hydro Conductivity (m/hr)</td>
<td>Porosity (0-1)</td>
<td>Manure application</td>
</tr>
<tr>
<td>• precipitation (cm)</td>
<td>Wilting point (wfps)</td>
<td>SOC top 5 cm (kg C/kg)</td>
<td>Crop type</td>
</tr>
<tr>
<td>• radiation (MJ/m²/day)</td>
<td>Soil structure</td>
<td>Slope (0°-90°)</td>
<td>Irrigation</td>
</tr>
<tr>
<td>• wind speed (m/s)</td>
<td>Microbial activity index (0-1)</td>
<td>Bulk Density (g/cm³)</td>
<td>Flooding</td>
</tr>
<tr>
<td>• humidity (%)</td>
<td>Initial concentration at surface soil for NO₃ and NH₄ (mg N/kg)</td>
<td>Fraction of leaf and stems left in the field after harvest</td>
<td>Plastic</td>
</tr>
<tr>
<td>N concentration in rainfall (mg N/l or ppm)</td>
<td>Atmospheric background concentration in • NH₃ (ug N/m³) • CO₂ (ppm)</td>
<td></td>
<td>Grazing or cutting</td>
</tr>
</tbody>
</table>

Any change to any of these key drivers can cause a change to a number of environmental factors such as soil temperature, radiation and soil moisture. These factors can cause changes to biogeochemical processes like denitrification, nitrification and decomposition and consequently determine the amount of the emissions from the soils. All these interactions make clear the challenge in order to express them in a mathematical framework that can produce reliable outputs from a dynamic system such as the ecosystem (Li, 2007).
The climate data can be in different formats depending on the availability and the details of the data. The data that the model requires in order to be able to make simulations are the temperature and the precipitation of the site or the area. The temperature can be in two formats: either as a daily mean value or as daily minimum and maximum values. If the wind speed is not available for the area, the model uses the default value of 2 m/s in order to create to calculate the transpiration rates for the site. If radiation data are not available, the latitude value and the temperature are used from the model in order to calculate the amount of radiation the area is receiving. For the atmospheric background concentrations of NH$_3$ and CO$_2$ the model provides default values if the measurement data are not available (NH$_3$: 0.06 ug N/m$^3$, CO$_2$: 350 ppm).

The soil properties are really important as they define all the details of the soil profile. For UK-DNDC, the soil profile consists of 5 soil layers of 10 cm each. Is worth noting that many of the soil default values, for example field capacity and the wilting point, are expressed according the US soil standards and not the UK. Moreover all the input parameters that are inserted in the model are referring to the top layer of the soil. The soil organic carbon (SOC) in the model exists in 4 main pools: namely microbial biomass, passive humus, humads and litter. These pools consists of more pools that they have different rates of decomposition. The SOC value refers to the surface value of the soil (0-5 cm).

The third main driver (vegetation) describes the details relating to the rotation and the managements of the crops within the rotation. A list of pre-
set crops, including default values which describe the growth of the crop are provided. It is important to note that the crop model is empirical and the default values do not necessarily predict the crop yields that are observed in the UK. There is the possibility of changing all of the crop parameters of each crop manually, and therefore there is the feasibility of setting the parameter values to obtain more realistic crop yields. The main eight parameters that can be defined for each crop are:

- Maximum biomass production (kg C/ha) (for grain, leaf and stem and root)
- Biomass fraction (for grain, leaf and stem and root)
- Biomass C/N ratio (for grain, leaf and stem and root)
- Annual N demand (kg N/ha)
- Thermal degree days for maturity
- Water demand (g water/g DM)
- N fixation index
- Maximum root depth

The maximum biomass production refers to the maximum potential production for a crop which is not subjected to any water or N stress. The thermal degree days describes the accumulative daily average air temperature from seeding to maturity for the crop. Only the temperatures above 0°C are calculated for that parameter as there is no crop growth at below 0°C. The N pools in the soil are regarded as inactive at that temperature. The parameter value for the N fixation represents the ratio between the total N content in the plant and the plant N taken from the soil. If the crop is not a fixing nitrogen crop this value is equal to 1. The model
gives the opportunity to the user to create a new crop if it is not in the list by defining all the parameters manually through the crop creator option.

The last main driver of the model is the human interactions through the rotation choice and the management of the field. For all the human management events, information on the day in the year that the exact activity took place has to be provided. Management practices like fertiliser and manure application have to be described with the exact type, depth, and the amount in kg per ha of the application. For the manure application the user can manually define the C/N ratio of the product of the application. For tillage the most important detail is the depth of the tillage as this defines how many soil layers have been disturbed. For forage systems, there is the opportunity to define the grazing events over the year in the field and the timing of grass cuts and the proportion of the sward removed. Grazing and nitrogen excretion for dairy cow, beef/veal, sheep, horse and pig are described within the model. In case of different livestock types (for example lambs) grazing on the field, the livestock units (LSU) conversion factor can be used to determine stocking densities (SRUC, 2013). There are extra options for describing additional feed which fed in the field, and the handling of the excreta. The latter was added to the model so that the effect of emission arising from the return of excreta at grazing could be separated from those arising from the soil. The last management event that can be defined is the irrigation which has to be selected the method (flood, sprinkler, dip) the amount and the number of events. Although the use of plastics can be described in DNDC, this feature has not been added to UK-DNDC.
3.4.2.2 Sub-models

The whole model consists of two main components which are each divided into 3 sub models (Figure 3.2). The first component is split into the following sub-models: soil climate, plant growth and decomposition sub-models. Li et al (1992) describes that component thoroughly in their paper.

The soil climate sub-model predicts the soil temperature and moisture and the soil reduction- oxidation reaction (redox, Eh). The model divides it into five main horizontal layers of 10 cm each. Input data for the soil properties are regarded to be uniform across all the layers while the predictions of the sub-model are not, as the values for the outputs may vary within layers (Giltrap et al., 2010a). The soil texture and the soil water regulate the changes in water and soil temperature (Brown et al., 2002).
Figure 3.2: How is the DNDC (v9.4) model structured (Source: own figure based on (Li, 2007; Li, 2013))
The crop growth sub-model is an empirical model. The sub-model uses as a reference point the maximum potential yield and depresses the growth according to the availability of water and N in the soil. The demands of the crop are modelled based on the C/N ratio and the potential maximum yield. The N that is available to the plant is through the N pools (NH$_4^+$ and NO$_3^-$) in the soil. The demand of N from the soil by the crop varies according to the depth. According to Molz and Remson (1970), the demand is proportional to the biomass of the root in the soil. The top quarter part of the root holds the vast majority of the biomass (40%) while the rest (60%) is distributed in the remaining three-quarters. The water demand is based on the crop water requirement parameter, while the thermal degree days are driving the growth from seeding to maturity.

The third sub-model of the first component is the decomposition. The soil microbes break down C into dissolved organic carbon (DOC) compounds in order to survive and satisfy their needs in energy. In oxic conditions the activity of soil microorganisms is enhanced, the decomposition is dominant and there are losses of C as CO$_2$ to the atmosphere with the help of oxygen as a dominant oxidant. Those three sub-models compose the first component of the model. The outputs of that component are namely soil temperature and moisture, Eh and substrates of C and N.

Depending on the soil redox potential and the dominant oxidant there are different reactions occurring in the soil and therefore there is either
production or consumption by the microorganisms of CO₂, N₂O and CH₄ (Figure 3.3).

The outputs from the first component feed the second component which essentially is a link between the environmental factors and the production of GHGs. It consists of three sub-models, namely denitrification, nitrification and fermentation. The nitrification and denitrification sub-models performance was improved by the deployment of the concept of the “anaerobic balloon” by simulating the soil aeration status. This is described by calculating - oxygen diffusion and consumption. This simple kinetic scheme was introduced to the model in 2000 and it was part of the upgrades to the PnET-N-DNDC version (Gilhespy et al., 2014). The anaerobic balloon can be “defined as the volumetric fraction of anaerobic microsites in a soil” (Li, 2007). This scheme integrates the main two equations of Nerst (Stumm and Morgan, 1981) and Michaelis-Menten (Paul and Clark, 1989) equations (Li, 2007). The balloon can either swell or shrink with values that vary from 0 (aerobic condition) to 1 (anaerobic condition). UK-DNDC uses the Nerst equation in order to calculate the Eh, which determines the size of the balloon, and divides the anaerobic and aerobic parts of the soil layers. In the aerobic parts the nitrification process is taking place while in the anaerobic phase denitrification is occurring. Once the balloon inflates, the substrates that are allocated to the anaerobic parts of the layer will contribute to the reductive reactions in each layer and as a result the denitrification and CH₄ production will be enhanced. On the other hand, when the anaerobic balloon deflates, it is stimulating the nitrification process and the CH₄ oxidation by the contribution of the substrates that are distributed in the
aerobic parts of the soil layers to the oxidative reactions. The rates of these reactions that occur within the balloon, are calculated by the Michaelis-Menten equation (Li, 2007). The model creates a series of anaerobic balloons, all with different dominant electron acceptors (O₂, NO₃⁻, Mn⁴⁺, Fe³⁺, SO₄²⁻) that are used by the soil microorganisms. In the case of the prevalence of oxic conditions, the balloon is deflated and O₂ is the dominant electron acceptor until it is exhausted completely and then the balloon erupts as it reaches its maximum size. Soon after the balloon erupts, the model creates a new balloon in which the dominant electron acceptor is NO₃⁻ until it depletes completely. After the depletion of all the major electron acceptors the Eh has reaches a low value of -150 mV or even lower. At that point the fermentation sub-model will be activated and the role of the electron acceptor will be played by hydrogen (H₂) and there will be enhanced CH₄ production (Figure 3.3) (Li, 2007; Li, 2013).
During the run of the simulation, the model provides the user with the opportunity to have a visual perception of the run with seven different information windows, on the same screen. This information provides a demonstration of the dynamics of the simulated climate conditions, soil climate and chemistry, the crop growth and the gas emissions.

The outputs of the model are produced from both components of the model. The model produces 10 different output files for each year of the simulation and a multi-year summary (Table 3.4). The main outputs of the model are the soil climate data (moisture, temperature, Eh), and concentrations of SOC, NO3⁻, NO2⁻, NH4⁺, urea, NH3, total denitrification and nitrification and the emissions of CO2, NO, N2, N2O, CH4 and NH3.
Table 3.4: Outputs from the model

<table>
<thead>
<tr>
<th>File name</th>
<th>Time step</th>
<th>Short description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Annual soil report yr No¹</td>
<td>Annual</td>
<td>Quick summary of the inputs for the run</td>
</tr>
<tr>
<td>Climate yr No</td>
<td>Daily</td>
<td>Summary of the inputs and simulations of the data that was not available</td>
</tr>
<tr>
<td>Field Crop yr No</td>
<td>Daily</td>
<td>Modelled crop growth data for all the crops planted</td>
</tr>
<tr>
<td>Field Manage yr No</td>
<td>Daily</td>
<td>Summary of the management practices that were followed</td>
</tr>
<tr>
<td>Graze yr No</td>
<td>Daily</td>
<td>Summary of the grazing events and predictions for the C and N in meat products and livestock emissions</td>
</tr>
<tr>
<td>Soil C yr No</td>
<td>Daily</td>
<td>Modelled data for the C pools in the soil and the CH₄ and CO₂ production from the system</td>
</tr>
<tr>
<td>Soil Climate yr No</td>
<td>Daily</td>
<td>Modelled data for the soil temperature, moisture, oxygen and Eh for depths of 1, 10, 20, 30, 40 and 50 cm</td>
</tr>
<tr>
<td>Soil N yr No</td>
<td>Daily</td>
<td>Modelled data for N pools and fluxes in different depths.</td>
</tr>
<tr>
<td>Soil Water yr No</td>
<td>Daily</td>
<td>Modelled data for the water budget in the site.</td>
</tr>
<tr>
<td>Soil P yr No</td>
<td>Daily</td>
<td>Modelled data for P pools and fluxes from the site</td>
</tr>
<tr>
<td>Multi-year summary</td>
<td>Annual</td>
<td>A multi-year report for main outputs in an annual time step</td>
</tr>
</tbody>
</table>

¹ yr No: refers to the number of year in the simulation

3.4.3 Improvements to the model

During this project, UK-DNDC has undergone many changes and updates and there have been a total of three versions. During the period of research of this project some errors and flaws were identified either in the actual code of the model or in the perception of some of the relations in the
biogeochemistry cycles. There were three main improvements that were incorporated in the model due to that research project. Once it was identified a flaw or a bug in the model there was communication with the developer of the model Prof Changsheng S. Li in order to find a solution and discuss the problem that had emerged.

The first one that was identified early in the project was a bug in the code of the model in relation to planting and harvest date. In this case, there was a discrepancy between model output and input of two days. The second most important was the correction of the crop creator function in the model. The model provides the opportunity to the user to create a new crop from the beginning with parameters that the user can define. During the experiments for this project this function was used but it was recognised that the model was keeping the previous parameters that had been defined for the “empty” crops. These “empty” crops were part of earlier tests of the model so even if they were “empty” their parameters were filled with values. As a result of that, the model was running the simulation with these values and was not replacing them with the new values that the user had defined in the user interface box. In the actual interface box the new user values were saved but the code was keeping the model’s default values from the “empty” crops.

The third issue that was identified emerged from the use of the model in mixed systems of grasslands and arable fields. By the time the user selected the option perennial for the planted crop (most of the times grassland) the model was keeping the same crop for all the years the rotation was in the field so there is no need from the user to introduce the crop in
each year of the rotation. In mixed systems of arable and grasslands there was the need to stop the model after some years of the perennial grassland and continue the rotation with an arable crop. After that identification of the absence of that ability in the model the developer Prof Changsheng S. Li released an update in which he included one more option in the menu of the tillage events. This option is called “Terminating till” and its role was to stop the growth of the perennial crop and remove it so the rotation could continue without the presence of the perennial crop.
4 Sensitivity Analysis and Uncertainty of UK-DNDC in relation of the grassland site at Easter Bush

*Il n’est pas certain que tout soit incertain*²

Blaise Pascal (1669)

### 4.1 Introduction

An important element of environmental modelling is to understand the sensitivity of the model outputs in relation to the uncertainty of the model parameters (Warmink *et al.*, 2010; Refsgaard *et al.*, 2007a; Pogson *et al.*, 2012). According to Refsgaard *et al.* (2007a), an essential part of the last step

² *It is not certain that everything is uncertain.*
4. Sensitivity Analysis and Uncertainty of UK-DNDC in relation of the grassland site at Easter Bush

of the modelling process is the evaluation of the model with the uncertainty assessment.

4.1.1 Uncertainty

Uncertainty is a situation in which the information provided are inaccurate, inadequate or not known. In a modelling activity there are different sources of errors that lead in the uncertainty. These can arise either as part of the development stage of the model (e.g. built-in parameters, equations) or during the use of it (input parameters) (Walker et al., 2003). In relation to uncertainty associated with model development, uncertainties may arise because by definition a model is a simplification of the dynamics of reality and key processes may not be adequately represented through the mathematical algorithms and conjecture errors may be present. One other category that can create inconsistencies is the conceptual errors of the context on which the model will focus. This may occur in the design and development stage of the model. Other possible errors can emerge from definition of the parameter values. These errors propagate through the model and they have unavoidable effects on the actual predictions of the model outputs and create the propagation of uncertainty. It is important to quantify the uncertainty in the model to understand the sensitivity of the outputs of the model. In biogeochemical models, the site characteristics are described in the input variables (Hastings et al., 2010). These input variables can be categorised into three main groups: the meteorological data of the area (e.g. precipitation, temperature and radiation), the soil characteristics of the study field and the management of the rotation (e.g. fertiliser application,
ploughing, grazing). The collection of all these data through measurements has an associated uncertainty due to various reasons including external driving forces that can prove challenging to control (time and spatial), instrument imprecision, and human factors. The uncertainty that will be tested in this chapter focuses only to the input parameters of climate and soil properties.

### 4.1.2 Sensitivity analysis

Sensitivity analysis allows the uncertainty to be quantified (Qin et al., 2013; Caswell, 1978). It assesses the impact of the values for a given input on the variation of the model’s results. Therefore, it identifies the inputs that have the greatest influence on the model outcomes. As a result of the sensitivity analysis, the strengths and the limitations of the model can be identified (Hamby, 1994). Modelling can therefore contribute to experimental design by identifying key parameters to which the model is sensitive, and hence where more robust information would be beneficial in understanding the biological processes which are being modelled.

Sensitivity analysis can either be performed for one variable at a time or number of input variables. In the case of one variable, the analysis is called “local” and allows the value associated with the variable to change within a defined range while the remaining variables are held constant (Saltelli et al., 1999). Unlike “local” sensitivity analysis, the “global” sensitivity analysis (SA) allows the values associated with a range of variables to change simultaneously (Sun et al., 2012). This is giving a great advantage to the global in comparison to the local analysis. Hence, “global”
SA considers the interactions between the different variables and the effect of the combination of changes on the outputs (Qin et al., 2013).

4.1.3 Monte Carlo analysis

The Monte Carlo method is based on the selection of random numbers in order to mimic the conditions of a random physical process and test the effect that these random values have on the results (Hammersley and Handscomb, 1964). The approach that was used was the probabilistic approach of Monte Carlo analysis. It can be defined as the intentional selection of random values in a stochastic process of events (Kalos and Whitlock, 2008; Hammersley and Handscomb, 1964).

4.1.4 Focus

This chapter focuses on the uncertainty perceived from input sources which creates a stochastic uncertainty due to inherent variability of the variables. The objective of this chapter was to investigate the sensitivity of the UK-DNDC model through an experimental grazed grassland site in south-east of Scotland. This required a “global” sensitivity approach which assessed the sensitivity of the input parameters on seven outputs namely: grazed biomass C, the dissolved SOC, N₂O, NO, N₂, NH₃ and N leaching.
4.2 Materials and Methods

4.2.1 The Uncertainty in UK-DNDC model

The model that was used is the UK-DNDC (see more information for the model in Chapter 3). The UK-DNDC model offers a built-in Monte Carlo simulation (Figure 4.1). For each selected input parameter, a default of eight random values within the specified range is selected. The user can change the number of values selected. The range in the input is defined in the interface as a proportion (0-1) of change from the base value, which is specified by the user. The proportion that is defined is symmetrical. The Monte Carlo test that is incorporated in the UK-DNDC model performs a discrete prior distribution of 50 samples within a given range. A uniform distribution of the parameter values within the given range is assumed by the Monte Carlo approach incorporated into UK_DNDC.
Figure 4.1: Table of the input parameter that the user in UK DNDC can define the variation range.
For a single simulation, the user can select up to five different input parameters to change. When more than one parameter is selected, the number of runs required increases exponentially. This is because the model was run for all the possible combination of values of all the selected input parameters. Hence, as the number of input parameters assessed increases, the time required to run the model also increases exponentially. The output that is produced is a yearly summary for each year simulated for each of the 12 main outputs. In this study, five of these outputs were not assessed namely: grain C, shoot C, root C, cut biomass C, and CH4. The first two outputs are relevant for arable rotations while this analysis was focussed on a grassland field. In the field experiment root C was not measured and therefore it was not used as an output from the model in the sensitivity analysis. The cut biomass C was not included in the assessment as there was only one cut on the first year of the 10 year experiment and would not give significant data for the assessment. Methane was not part of the assessment as it is outside the focus of this study. The seven outputs that their uncertainty will be assessed are the grazed biomass C, the dissolved SOC, N2O, NO, N2, NH3 and N leaching.

4.2.2 Sensitivity study of input variables

The sensitivity analysis focussed on a long term (10 years) heavily grazed grassland in the south-east of Scotland. More details for the site details and input parameters can be found in section 4.2.2.2. The sensitivity analysis of the model that was conducted was “local” and “global”. One
“local” and five different “global” analyses with combinations of the selected input parameters were performed. The selection of four input parameters for the Monte Carlo and not five was due to the fact that the number of runs required for the combination of the five parameters was prohibitive in terms of the time required to run the simulation (32,768 runs x 10 years rotation = 320,768 years in total). For the first and the last “global” analyses, three input parameters were selected and thus the possible combinations was 512 ($8^3$ runs=512 runs, 512x 10 years rotation = 5120 years in total). For the remaining three analyses the model executed 4,096 runs (possible combinations) for each ($8^4$= 4,096 4,096 runs x10 years rotation = 40,960 years in total).

The “local” analysis was focused on the change of the N fixation index. The first “global” focused on the change in the default values that were used for three of the atmospheric input parameters. The second until the fourth analyses focused on the effect of the changes of the most important soil input parameters on the specified outputs. From the results of these analyses the most important variables were identified. The final “global” analysis focused on assessing the sensitivity of the outputs of those variables (Table 4.1).
Table 4.1: The three different sensitivity analyses that were performed with the input parameters that changed in each

<table>
<thead>
<tr>
<th>Input parameters</th>
<th>1st global</th>
<th>2nd global</th>
<th>3rd global</th>
<th>4th global</th>
<th>5th global</th>
</tr>
</thead>
<tbody>
<tr>
<td>Atmospheric CO₂ concentration</td>
<td>Soil clay</td>
<td>Soil clay</td>
<td>Field Capacity</td>
<td>Atmospheric CO₂ concentration</td>
<td></td>
</tr>
<tr>
<td>Atmospheric NH₃</td>
<td>SOC content</td>
<td>SOC content</td>
<td>Wilting Point</td>
<td>Clay</td>
<td></td>
</tr>
<tr>
<td>Atmospheric N deposition</td>
<td>Hydro conductivity</td>
<td>Field Capacity</td>
<td>Hydro conductivity</td>
<td>SOC content</td>
<td></td>
</tr>
<tr>
<td>pH</td>
<td>Wilting Point</td>
<td>pH</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

For the atmospheric data (located in the climate input screen) a sensitivity analysis was performed for three of the total five available input parameters (atmospheric CO₂ concentration, atmospheric NH₃, atmospheric N deposition). Data was not available for the whole period of the experiment and the default values were used instead. Air temperature and precipitation were the two input parameters that were not selected from the list of the climate parameters. Both of these parameters are associated with a daily value, while the outputs that are produced from the model are referring to an annual accumulative value. Due to this, the results cannot depict the day by day change of the outputs and therefore could possibly lead to misconceptions for the sensitivity of the model.

Six of the most important input soil parameters were selected to be tested through the built-in Monte Carlo. By performing three analyses, with
three different combinations, it was possible to identify the relative importance of the parameters selected within each subset. The range of the change for the input parameters defines the possible values that the Monte Carlo method will pick the values for the sensitivity analysis (Table 4.2).

The bulk density and the porosity were not selected as they are directly related parameters. In relation to the Monte Carlo simulation in UK-DNDC, it was not possible to define this relationship as they are entered independently into the UK-DNDC interface. For the 1st “global” analysis, the percentage change assumed for the three atmospheric input parameters was 100%. This meant for the atmospheric CO$_2$ concentration were the lowest value that was selected of the range was 280 ppm, the preindustrial concentration of the gas (IPCC, 2007). This was because there was no available data for these input parameters and the purpose was to examine their effect on the outputs. Some of the values that were selected may are an extreme representation of reality but is important to include them in these analyses to check the response of the model in a range of even extreme values. With respect to the soil parameters the range selected was ±20% while holding others fixed (Li et al., 1992) (Table 4.2). This percentage reflects the range of the clay fraction for sandy clay to silty clay loam. The soil type at grassland site was a sandy clay loam.
### Materials and Methods

Each rotation was run for 10 years. This created challenges in the comparison between runs. The effects of differences in the input parameters were assessed on the total value of the outputs over 10 years. This avoided confounding the changes of management events and weather variability within the period of the rotation with the sensitivity of the outputs to

<table>
<thead>
<tr>
<th>Input Parameter</th>
<th>Base Value</th>
<th>Range</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Atmospheric CO₂ Concentration</td>
<td>380</td>
<td>0-760</td>
<td>100%</td>
</tr>
<tr>
<td>Selected values</td>
<td></td>
<td>280-760</td>
<td></td>
</tr>
<tr>
<td>Atmospheric NH₃ (ug N/m³)</td>
<td>0.06</td>
<td>0-0.12</td>
<td>100%</td>
</tr>
<tr>
<td>Atmospheric N deposition (mg N/l)</td>
<td>0.5</td>
<td>0-1</td>
<td>100%</td>
</tr>
<tr>
<td>Soil clay (Clay fraction)</td>
<td>0.27</td>
<td>0.21-0.33</td>
<td>20%</td>
</tr>
<tr>
<td>Hydro Conductivity (m/hr)</td>
<td>0.02268</td>
<td>0.018144-0.027216</td>
<td>20%</td>
</tr>
<tr>
<td>SOC content (kg C/kg soil)</td>
<td>0.0516</td>
<td>0.04128-0.06192</td>
<td>20%</td>
</tr>
<tr>
<td>pH</td>
<td>5</td>
<td>4-6</td>
<td>20%</td>
</tr>
<tr>
<td>Field Capacity (wfps)</td>
<td>0.52</td>
<td>0.416-0.624</td>
<td>20%</td>
</tr>
<tr>
<td>Wilting Point (wfps)</td>
<td>0.24</td>
<td>0.192-0.288</td>
<td>20%</td>
</tr>
</tbody>
</table>
uncertainty of the inputs parameters. The only variability in the results was due to the changes of the input parameters.

The Spearman’s rank correlation coefficient, a nonparametric measure of statistical dependence between variances, was used to assess the correlation between the input and the outputs. For the statistical analyses GenStat (16th edition, Release 16.1, VSN International Ltd., Oxford) was used.

4.3 Results

4.3.1 N fixation “local” analysis

In the “local” analysis was tested how sensitive the model is in the N fixation crops when the N fixation index is changing. This analysis showed that change on the N fixation is affecting by 75% the NH₃ while the N leaching is affected by almost 40%. Nitrous oxide and NO emissions show a dependence on the changes of the N fixation index by 32%. The values that are associated with C were not highly affected by the change of the N fixation index as it was limited to a 6% effect.
Figure 4.2: Results from the “local” sensitivity analysis of the N fixation index.

4.3.2 Default atmospheric data analysis

Due to limitations of the analysis, as mentioned before, a sensitivity analysis was performed to three out of five input parameters located on the climate screen (atmospheric background NH$_3$ concentration, N concentration in rainfall, atmospheric background CO$_2$ concentration). According to the results (Figure 4.3) from the sensitivity analysis it is clear that the influence of the changes in the atmospheric background NH$_3$ concentration and N concentration in rainfall are insignificant as they did not show any contribution to the main seven outputs. However, the model showed high sensitivity to atmospheric background NH$_3$ concentration for the NH$_3$ outputs. This is because both the input parameter and result refer to the same compound of N. In that analysis, the most influential input parameter is the atmospheric background CO$_2$ concentration which shows a strong
contribution to all the outputs considered. In N leaching and NH\textsubscript{3} this influence has a negative response on the results.

![Figure 4.3: Coloured correlations between the selected input parameters and the outcomes. Table of the contribution of each of three of the main climate input parameters in seven main outputs of the model (1st “global”).](image-url)
4.3 Results

4.3.3 Soil characteristics data analyses

4.3.3.1 Second “global” analysis

For the three analyses of the soil characteristics input parameters, 6 of the main input parameters were tested in 3 different possible combinations. For the first analysis, the sensitivity of the model for four of the inputs namely pH, SOC, hydroconductivity and clay fraction (Figure 4.4) was tested. According to the correlation of the inputs with the outputs, hydroconductivity shows no influence on the outputs and the outputs affected by pH were NO, N₂ and NH₃. Similarly, SOC also affected N₂ and NH₃. SOC also affected the dissolved SOC. However, as clay content increases, grazed biomass C declines. Clay content also influences the N leaching and the NO production. According to the sensitivity test N₂O and N₂ seems to be dependent on the concentration of SOC.
4. Sensitivity Analysis and Uncertainty of UK-DNDC in relation of the grassland site at Easter Bush

Figure 4.4: Coloured correlations between the selected input parameters and the results. Table of the contribution of each of four of the main soil input parameters in seven main outputs of the model (2nd “global”).

4.3.3.2 Third “global” analysis

The second sensitivity test of the soil characteristics (Figure 4.5) is showing almost the same results with the first as they share two common input parameters, namely clay and SOC. However, wilting point has little influence on the seven outputs considered. Increasing field capacity had a positive effect on N₂O and a negative effect on NO.
4.3 Results

Figure 4.5: Coloured correlations between the selected input parameters and the results. Table of the contribution of each of three of the main climate input parameters in seven main outputs of the model (3rd “global”).

<table>
<thead>
<tr>
<th>Clay</th>
<th>Grazed Biomass C</th>
<th>Dissolved SOC</th>
<th>N₂O</th>
<th>NO</th>
<th>N₂</th>
<th>NH₃</th>
<th>N leaching</th>
</tr>
</thead>
<tbody>
<tr>
<td>Field Capacity</td>
<td>0%</td>
<td>-8%</td>
<td>27%</td>
<td>-25%</td>
<td>0%</td>
<td>-11%</td>
<td>-28%</td>
</tr>
<tr>
<td>Wilting Point</td>
<td>-1%</td>
<td>-1%</td>
<td>0%</td>
<td>2%</td>
<td>0%</td>
<td>0%</td>
<td>0%</td>
</tr>
<tr>
<td>SOC</td>
<td>0%</td>
<td>-76%</td>
<td>73%</td>
<td>0%</td>
<td>99%</td>
<td>-78%</td>
<td>9%</td>
</tr>
</tbody>
</table>

4.3.3.3 Fourth “global” analysis

The last combination of the input parameters for the soil showed some interesting results (Figure 4.6). Hydroconductivity in that combination of selected parameters is not making any contribution to the changes in the outputs. Additionally, pH is the only parameter which is contributing in the changes of N₂, and that may be partly due to the fact that SOC was not
selected in this analysis. Nitrogen oxide is influenced almost equally by the changes in pH and field capacity. As well as the influence of field capacity on N leaching, field capacity also influences the dissolved SOC and N\textsubscript{2}O, which was not shown in the previous analysis. This was because of the presence of more influential input parameters such as clay and SOC. Although from the previous analysis the model seems not to be sensitive to the changes in wilting point, the grazed biomass for this analysis was affected by changes in the wilting point changes.
4.3 Results

![Coloured correlations between the selected input parameters and the results. Table of the contribution of each of three of the main climate input parameters in seven main outputs of the model (4th “global”)](image)

<table>
<thead>
<tr>
<th>Hydroconductivity</th>
<th>Grazed Biomass C</th>
<th>Dissolved SOC</th>
<th>N₂O</th>
<th>NO</th>
<th>N₂</th>
<th>NH₃</th>
<th>N leaching</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grazed Biomass C</td>
<td>1%</td>
<td>0%</td>
<td>0%</td>
<td>0%</td>
<td>0%</td>
<td>-8%</td>
<td>-0%</td>
</tr>
<tr>
<td>Field Capacity</td>
<td>11%</td>
<td>-78%</td>
<td>85%</td>
<td>45%</td>
<td>1%</td>
<td>-50%</td>
<td>-88%</td>
</tr>
<tr>
<td>Wilting Point</td>
<td>-88%</td>
<td>-22%</td>
<td>0%</td>
<td>4%</td>
<td>0%</td>
<td>10%</td>
<td>1%</td>
</tr>
<tr>
<td>pH</td>
<td>0%</td>
<td>0%</td>
<td>14%</td>
<td>-51%</td>
<td>99%</td>
<td>31%</td>
<td>11%</td>
</tr>
</tbody>
</table>

4.3.4 Most influential parameters analysis

The most influential input parameters of the model from the previous 4 analyses were selected for the final analysis. These parameters are atmospheric background CO₂ concentration, clay content and SOC and were selected due to their effects on the outputs of the previous “global” analyses (Figure 4.7). The model still showed high sensitivity to the atmospheric background CO₂ concentration values as grazed biomass C and dissolved
SOC are highly dependent on it. The influence that this parameter has on the rest of the outputs has been reduced compared with the 1st “global” analysis due to the presence of other two input parameters to which the model is sensitive. Soil organic carbon value changes have a large positive influence on the emissions of N₂O and N₂, and large negative effect on NH₃. Dissolved SOC values are determined by the change of SOC in the model by at 30%. In the previous analyses, changes in clay had a large effect on the model outputs but in this specific analysis the correlations are showing less dependence on the changes of clay. Interestingly, clay in this comparison has limited influence on the outputs of the model. The only noteworthy influence was in the NO and in leaching values.
4.3 Results

Figure 4.7: Coloured correlations between the selected input parameters and the results. Table of the contribution of each of four of the main soil input parameters in seven main outputs of the model (5th “global”).

<table>
<thead>
<tr>
<th>Atmospheric background CO₂ concentration</th>
<th>Grazed Biomass C</th>
<th>Dissolved SOC</th>
<th>N₂O</th>
<th>NO</th>
<th>N₂</th>
<th>NH₃</th>
<th>N leaching</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clay</td>
<td>-12%</td>
<td>5%</td>
<td>0%</td>
<td>49%</td>
<td>0%</td>
<td>13%</td>
<td>-78%</td>
</tr>
<tr>
<td>SOC</td>
<td>0%</td>
<td>-31%</td>
<td>98%</td>
<td>0%</td>
<td>96%</td>
<td>-87%</td>
<td>16%</td>
</tr>
</tbody>
</table>
4.3.5 Outputs uncertainty

After the sensitivity analysis, which highlighted the input parameters to which the model is sensitive, an uncertainty test was essential. The uncertainty indicated the range of the values of the results for each sensitivity analysis. The analysis specified and quantified the range of the possible values of the outputs of the model. For the uncertainty test the output data were in a different scale and therefore it was not possible to plot them on the same graph. In order to be able to have a better understanding on the relative uncertainty of the results, the data that were used were normalized against their mean values.

For the first analysis, the dissolved SOC and grazed biomass C showed the greatest uncertainty compared to the other outputs (Figure 4.8). This was due to the sensitivity of these outputs to atmospheric CO₂ concentrations. For the remaining four analyses of the soil characteristics, the uncertainty showed that the N₂ was consistently the most uncertain output. Moreover nitrous oxide emissions were one of the results that showed great uncertainty in all of the analyses. The values of the grazed biomass C and the NO were the least of the uncertain. This analysis highlights that it is important to have the input values for the model as precise as possible, since the uncertainty associated with values can create variability in the outputs.

One of the outputs that showed one of the highest uncertainties in the analyses that were performed was N₂O. The output values of the results in
most of the analyses are showing distributions which are close to normal distribution with an exception of the last analyses. In this analysis is the distribution is closer to uniform (Figure 4.9). The values that were plotted are the 10 years average predicted values of the rotations. The third analysis is the one with the highest variability of the simulated values of the N₂O as the spectrum extends from 48 kg N ha⁻¹ to 135 kg N ha⁻¹ with a standard deviation of 21.2 kg N ha⁻¹ (Table 4.3). The lowest variation in N₂O values occurred in the default atmospheric data analysis (1st global analysis) with a range of only 33 kg N ha⁻¹.

Table 4.3: Characteristics of the distributions of N₂O from all the analyses (kg N₂O – N ha⁻¹ rotation⁻¹)

<table>
<thead>
<tr>
<th></th>
<th>1st “global” analysis</th>
<th>2nd “global” analysis</th>
<th>3rd “global” analysis</th>
<th>4th “global” analysis</th>
<th>5th “global” analysis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Minimum</td>
<td>80.5</td>
<td>54.8</td>
<td>48.9</td>
<td>65.7</td>
<td>55.9</td>
</tr>
<tr>
<td>Maximum</td>
<td>113.4</td>
<td>134.5</td>
<td>135.5</td>
<td>115.4</td>
<td>128.9</td>
</tr>
<tr>
<td>Deviation</td>
<td>8.5</td>
<td>19.8</td>
<td>21.2</td>
<td>12.9</td>
<td>19.8</td>
</tr>
</tbody>
</table>
Figure 4.8: Uncertainty of the seven main outputs of the Monte Carlo simulation for all the five "global" analyses (a=1st "global" analysis, b=2nd "global" analysis, c=3rd "global" analysis, d=4th "global" analysis, e=5th "global" analysis)
Figure 4.9: Nitrous oxide emissions distributions from the five different analyses. Dashed lines represent mean values of the output distribution and dotted
lines represent the standard deviation respectively (a=1st “global” analysis, b=2nd “global” analysis, c=3rd “global” analysis, d=4th “global” analysis, e=5th “global” analysis).

4.4 Discussion and Conclusions

Progress in the development of biogeochemical models in predicting important GHG emissions have been made in recent years. However, the sensitivity of the models and the uncertainty of the outputs are crucial parts for overcoming challenges that the modelling activity can create. This study represents an attempt to perform a sensitivity analysis using UK-DNDC own built-in Monte Carlo test. For a range of input parameters the sensitivity of UK-DNDC was assessed. The analyses focused on seven outputs namely: grazed biomass C, the dissolved SOC, N₂O, NO, N₂, NH₃ and N leaching. Most of the sensitivity studies that have been conducted were one year long (Hutchinson et al., 2007; Li et al., 1992; Li et al., 2004). In this study a long term sensitivity analysis was conducted, which is important for the simulations of SOC and hence is crucial for this type of model (Qin et al., 2013).

The “local” sensitivity that was performed in this project was for only one of the main crop parameters of legume crops, the N fixation index. This parameter is indicating the amount of N which is fixed by the crop in the soil. The outputs that were not affected were the C related outputs as it was expected. For the N related outputs most of them had a positive effect by the
change of the N fixation index by 100%. The NH$_3$ was affected heavily while the N$_2$O was influenced as well by almost 35%.

The three atmospheric input data are seldom measured or difficult to get a precise measurement for them (atmospheric background NH$_3$ concentration, N concentration in rainfall, atmospheric background CO$_2$ concentration). The results from these three input parameters were polarised and the model was only sensitive to the atmospheric background CO$_2$ concentration value. Evidently the variation of the atmospheric background NH$_3$ concentration and N concentration in rainfall did not have any effect or had a small effect on the specific seven outputs of the model assessed. Li et al. (1992), in their study, highlighted the small influence of those parameters on the outputs of the model, especially for N$_2$O production.

As for the soil input parameters, the model shows consistently high sensitivity to the clay fraction of the soil and the initial SOC. Other studies have highlighted the importance of the uncertainty of clay and SOC in the outputs of the model (Li et al., 1992; Qin et al., 2013; Hastings et al., 2010). Outputs like N leaching, NO and grazed biomass C are highly dependent on the clay content of the soil. On the other hand, the changes in the initial SOC value seem to influence more the NH$_3$, N$_2$O, N$_2$ and dissolved SOC. It was highlighted through the sensitivity analyses that the changes in two of the selected parameters, hydroconductivity and atmospheric N deposition, did not show any effect on the output values. The last three input parameters considered were pH, wilting point and field capacity, which did not show great effects on the outputs when the input parameters of clay content and SOC were also varied. For pH in particular, Hastings et al. (2010) indicated
in their research that pH had a small influence on the outputs assessed and especially the N₂O. However in the fourth “global” analysis, when the clay content and the SOC did not change, the relative effect of pH, wilting point and field capacity were highlighted by showing their effects on the outputs.

In the last “global” analysis, the three most influential input parameters were tested in one single sensitivity analysis. Clay, SOC and atmospheric background CO₂ concentration have shown different effect in this analysis while all the rest of the input parameters were unchanged. The results from the model showed that it was highly sensitive to these inputs; however, they affected different outputs. The carbon related outputs are highly dependent on the atmospheric background CO₂ concentration while SOC has a small effect on the dissolved SOC. It is noticeable that N₂O emissions were constantly showing a dependence on the SOC value across the analyses. This is due to the fact that SOC is directly linked with the soil microbial pool size and denitrification will be affected.

The uncertainty analysis allowed an assessment of the effect of the input parameters on the range of each of the outputs considered. Nitrous oxide emissions showed a consistent high range of uncertainty in almost all the analyses as it was highlighted form the graphs in Figure 4.8. This highlights the importance of precise input data for the model in order that the GHG emissions can be simulated precisely and as close to the reality as possible. Alongside N₂O, N₂ showed high variability. However, outputs like NH₃, NO and grazed biomass showed quite small uncertainty. For the four analyses of the soil characteristics, the uncertainty of each output seems to
follow the same pattern in all the uncertainties of each output. However, in
the default atmospheric data this pattern is slightly different as the
uncertainty of the outputs is not following the same trend as in the analyses
of the soil characteristics.

The model has a simplified built-in property for a sensitivity analysis
which can be useful for a quick check of a specific question that the model
user has for the sensitivity of the model. The Monte Carlo test is a 50 step
discrete uniform distribution for the selected range of values instead of a
total random selection of numbers within the given range with a distribution
of values that the user could choose. It would be beneficial for the analysis if
the user was able to repeat the test in order to generate different values as
they would be randomly selected and tailor the test to the needs of the
research question. Due to 50 step discrete uniform distribution for the
selected range of values that was not possible. These features consequently
would give a more sophisticated and smooth analysis of the model’s
sensitivity. In addition, regarding the results it would be interesting, to give
the ability to the user to choose between annual outputs or daily outputs.
That would resulted in testing the model’s sensitivity for really important
input parameters, which their changes are constant during the year like
temperature and rainfall. Even if the effect on the annual emissions exists the
fine details that can determine the trends during the year are missing.
Another aspect that would be useful to assess are the parameters that are
embedded in the code of the model. However, this activity requires a code
that is open to the user with adequate documentation.
Chapter 5

5 Validation and Calibration of the model

Voilà ce que je vois et ce qui me trouble. [...] La nature ne m’offre rien qui ne soit matière de doute et d’inquiétude.³

Blaise Pascal, (1669)

5.1 Introduction

Environmental modelling and especially biogeochemical dynamics has attracted substantial interest over the last decades. These models are usually useful tools applied in decision making and problem solving situations. A common question raised amongst the scientific community,

³This is what I see and what troubles me. [...] Nature presents to me nothing which is not matter of doubt and concern.
regards the level of confidence that users can have in relation to the accuracy of the model outputs. For that reason, validation of the model by the developer before the release of the model is one of the main stages in model development. Validation can be performed by the end user to ensure the appropriateness of the model for the study. Schlesinger et al. (1979) defined model validation as “the substantiation that a computerised model within its domain of applicability possesses a satisfactory range of accuracy consistent with the intended application of the model”. Although the validity of a model is really important, the absolute validation of a model cannot be achieved (National Research Council, 1990).

Validation should not be confused with verification of the model as the meanings of the two words are closely related, however in modelling terms these represent different activities. Verification of the model takes place during the development phase of the model and it refers to the demonstrating that the logic of processes has been implemented correctly. A verified model does not guarantee the validity of the model (Hoover and Perry, 1989). Validation of the model includes the comparison of the simulated numerical outcomes of the model with the observed measurement data from the field (Aral, 2014). If that demonstration shows a good agreement between modelled and measured data, then the model is adequate for use. Nevertheless, according to Oreskes et al. (1994) the success of that assessment does not prove or imply that the model is expressing the real system logically, which can only be tested through the verification process. What it proves is that the model can be declared validated for specific contexts assessed. If the context changes, the model needs to be validated again; nevertheless is still validated for the previous context that
was used (Rykiel and Edward, 1996). In order to perform a successful validation of the model, particular criteria have to be met and can be defined by the user who performs the test. Equivocal situations can evolve when not all the criteria are met so they need to be prioritised. Generally, in order to characterise a model valid, its content (both systematic and theoretical) has to satisfy the scope and objectives for which it was created (Aral, 2014; Hoover and Perry, 1989; Sargent, 1984).

The aim of the study in this chapter is to assess the performance of UK-DNDC (v. 3.0) for yield data, water content and N₂O emissions from both organic and inorganic sites across the European Union. UK-DNDC (v. 3.0) is a model based in the combination of DNDC (v. 9.4) and UK relevant databases. The DNDC model has been widely used and validated for a number of sites and crops across the world (Smith et al., 2010; Wang et al., 2008; Qiu et al., 2009; Frolking et al., 2004).

5.2 Materials and Methods

5.2.1 Sites

The sites that have been modelled using UK-DNDC represent a wide variety of climatic conditions and crops across Europe. There were a number of sites and databases of field data like N₂O, yield and water content varying in characteristics and properties available for this project. For the validation phase, data for crop production and N₂O emissions within crop rotations was provided from the experimental sites involved in the EU funded project Legume Futures (project number 245216, DG Research, Agriculture, EU).
(Table 5.1). As the model is a new development, an additional grassland site was included in the validation process to determine whether the model could simulate N₂O emissions from more conventional agricultural systems.

Table 5.1: Selected sites with the crops cultivated for each one of them

<table>
<thead>
<tr>
<th>Sites</th>
<th>Bush, UK</th>
<th>Foulum, Denmark</th>
<th>Tulloch, UK</th>
<th>Easterbush, UK</th>
<th>Logården, Sweden</th>
<th>S. Marco Argentano, Cosenza, Italy</th>
</tr>
</thead>
<tbody>
<tr>
<td>Agro climatic Zone</td>
<td>Atlantic North</td>
<td>Atlantic North/ Continental</td>
<td>Atlantic North</td>
<td>Atlantic North</td>
<td>Boreal</td>
<td>Mediterranean North</td>
</tr>
<tr>
<td>Crops</td>
<td>Barley</td>
<td>Beans</td>
<td>Potato</td>
<td>Winter wheat</td>
<td>Grass/ clover</td>
<td>Grass/ clover</td>
</tr>
</tbody>
</table>

Previous management data was available which describes the associated management practises, weather and the initial conditions of the soil from each site. Previous management data gives the opportunity of simulating a rotation closer to reality, as it allows the real management to be
used in the model simulation for the stabilising period. There were some cases where not all of the input data was available for a particular site. Under those circumstances, input values were based upon typical values published for the site or region, or based on values from local experts who were responsible for the monitoring sites. The biogeochemical modelling activity described in this chapter focuses on the analysis of modelled versus measured data for grain yield, N₂O emissions and water-filled pore space. A list of the most important soil data that were used for the model is displayed in Table 5.2.
Table 5.2: Site data for the six sites that were used in UK-DNDC.

<table>
<thead>
<tr>
<th>UK-DNDC Parameters</th>
<th>Site Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bush, UK</td>
<td>Latitude: 55.4</td>
</tr>
<tr>
<td>Foulum, Denmark</td>
<td>Mean temperature in the rotation(°C): 8.85</td>
</tr>
<tr>
<td>Tulloch, UK</td>
<td>Annual mean rainfall in the rotation(mm): 1051</td>
</tr>
<tr>
<td>Easterbush, UK</td>
<td>UK-DNDC soil classification: Sandy Loam</td>
</tr>
<tr>
<td>Logården, Sweden</td>
<td>pH: 6.6</td>
</tr>
<tr>
<td>S. Marco Argentano, Cosenza, Italy</td>
<td>SOC (kg C kg(^{-1}) soil (0-5cm): 0.0312</td>
</tr>
<tr>
<td></td>
<td>Soil bulk density (g/cm(^3)): 1.17</td>
</tr>
<tr>
<td></td>
<td>Hydro conductivity (m/hr): 0.13</td>
</tr>
<tr>
<td></td>
<td>Foulum, Denmark</td>
</tr>
<tr>
<td></td>
<td>Mean temperature in the rotation(°C): 8.45</td>
</tr>
<tr>
<td></td>
<td>Annual mean rainfall in the rotation(mm): 770</td>
</tr>
<tr>
<td></td>
<td>UK-DNDC soil classification: Sandy Loam</td>
</tr>
<tr>
<td></td>
<td>pH: 6.5</td>
</tr>
<tr>
<td></td>
<td>SOC (kg C kg(^{-1}) soil (0-5cm): 0.015</td>
</tr>
<tr>
<td></td>
<td>Soil bulk density (g/cm(^3)): 1.27</td>
</tr>
<tr>
<td></td>
<td>Hydro conductivity (m/hr): 0.015</td>
</tr>
<tr>
<td></td>
<td>Tulloch, UK</td>
</tr>
<tr>
<td></td>
<td>Mean temperature in the rotation(°C): 8.33</td>
</tr>
<tr>
<td></td>
<td>Annual mean rainfall in the rotation(mm): 900</td>
</tr>
<tr>
<td></td>
<td>UK-DNDC soil classification: Sandy Loam</td>
</tr>
<tr>
<td></td>
<td>pH: 5.8</td>
</tr>
<tr>
<td></td>
<td>SOC (kg C kg(^{-1}) soil (0-5cm): 0.01782</td>
</tr>
<tr>
<td></td>
<td>Soil bulk density (g/cm(^3)): 1.17</td>
</tr>
<tr>
<td></td>
<td>Hydro conductivity (m/hr): 0.1248</td>
</tr>
<tr>
<td></td>
<td>Easterbush, UK</td>
</tr>
<tr>
<td></td>
<td>Mean temperature in the rotation(°C): 8.85</td>
</tr>
<tr>
<td></td>
<td>Annual mean rainfall in the rotation(mm): 1051</td>
</tr>
<tr>
<td></td>
<td>UK-DNDC soil classification: Sandy Clay Loam</td>
</tr>
<tr>
<td></td>
<td>pH: 5</td>
</tr>
<tr>
<td></td>
<td>SOC (kg C kg(^{-1}) soil (0-5cm): 0.0516</td>
</tr>
<tr>
<td></td>
<td>Soil bulk density (g/cm(^3)): 1.35</td>
</tr>
<tr>
<td></td>
<td>Hydro conductivity (m/hr): 0.02268</td>
</tr>
<tr>
<td></td>
<td>Logården, Sweden</td>
</tr>
<tr>
<td></td>
<td>Mean temperature in the rotation(°C): 7.75</td>
</tr>
<tr>
<td></td>
<td>Annual mean rainfall in the rotation(mm): 678</td>
</tr>
<tr>
<td></td>
<td>UK-DNDC soil classification: Silty Clay Loam</td>
</tr>
<tr>
<td></td>
<td>pH: 7.1</td>
</tr>
<tr>
<td></td>
<td>SOC (kg C kg(^{-1}) soil (0-5cm): 0.0178</td>
</tr>
<tr>
<td></td>
<td>Soil bulk density (g/cm(^3)): 1.54</td>
</tr>
<tr>
<td></td>
<td>Hydro conductivity (m/hr): 0.076</td>
</tr>
<tr>
<td></td>
<td>S. Marco Argentano, Cosenza, Italy</td>
</tr>
<tr>
<td></td>
<td>Mean temperature in the rotation(°C): 16.8</td>
</tr>
<tr>
<td></td>
<td>Annual mean rainfall in the rotation(mm): 667</td>
</tr>
<tr>
<td></td>
<td>UK-DNDC soil classification: Sandy Clay Loam</td>
</tr>
<tr>
<td></td>
<td>pH: 8.47</td>
</tr>
<tr>
<td></td>
<td>SOC (kg C kg(^{-1}) soil (0-5cm): 0.0084</td>
</tr>
<tr>
<td></td>
<td>Soil bulk density (g/cm(^3)): 1.18</td>
</tr>
<tr>
<td></td>
<td>Hydro conductivity (m/hr): 0.02268</td>
</tr>
</tbody>
</table>
5.2.2 Site Descriptions

5.2.2.1 Bush, Scotland

An intercrop experimental site, was established in the Atlantic agro-climatic zone near Edinburgh (55° 50’ 4” N; 3° 12’ 29.44” W, altitude 190 m above sea level) on a sandy loam soil (Macmerry Series), on twelve hydrologically isolated plots (25m × 9m) (Pappa et al., 2011). The rotational experiment was carried out over a three year period (2006-2008) and it consisted of four treatments (Table 5.3).

Table 5.3: Details of the cropping management at Bush, Edinburgh

<table>
<thead>
<tr>
<th>Year</th>
<th>1st</th>
<th>2nd</th>
<th>3rd</th>
<th>4th</th>
</tr>
</thead>
<tbody>
<tr>
<td>2006</td>
<td>Barley/ Clover</td>
<td>Barley/ Pea cv Zero 4</td>
<td>Barley/ Pea cv Nitouche</td>
<td>Barley</td>
</tr>
<tr>
<td>2007</td>
<td>Oats</td>
<td>Oats</td>
<td>Oats</td>
<td>Oats</td>
</tr>
<tr>
<td>2008</td>
<td>Perennial Grass</td>
<td>Perennial Grass</td>
<td>Perennial Grass</td>
<td>Perennial Grass</td>
</tr>
</tbody>
</table>

Annual precipitation was 927, 1288 and 1132 mm for 2006, 2007 and 2008, respectively. In 2006, the water content at field capacity was 19 ± 0.5% (v/v), the soil bulk density was 1.19 ± 0.01g cm⁻³ (mean ± SE, n = 5). Extractable soil N was 4.8 mg NH₄⁺-N kg⁻¹ and 21.9 mg NO₃⁻-N kg⁻¹ in 0–20 cm soil depth at the start of the experiment.
5.2.2.2 Foulum, Denmark

Foulum is a sandy loam soil located in the south of Denmark (56° 28’ 8.51’’ N; 9° 37’ 3.78’’ W, altitude 38m above sea level), which is in the Atlantic North/ Continental agroclimatic zone. Field experimental site was monitored between 2006 and 2009 with annual precipitation of 551, 718, 665 and 619 mm and the mean annual temperature was 8.1°C, 8.8°C, 8.9°C and 8.6°C for 2005, 2006, 2007 and 2008, respectively.

The experiment consisted of three different treatments, two organic and one conventional (Chirinda et al., 2010) with the cropping rotations for each treatment being described in Table 5.4. The manure / slurry and fertiliser applications applied to the treatments are described in Table 5.5.

Table 5.4: The 4 years crop rotation of the experiment in Foulum

<table>
<thead>
<tr>
<th>Year</th>
<th>Organic (O2)</th>
<th>Organic (O4)</th>
<th>Conventional (C4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2005</td>
<td>Spring barley /Grass /Clover</td>
<td>Spring barley</td>
<td>Spring barley</td>
</tr>
<tr>
<td>2006</td>
<td>Grass /Clover</td>
<td>Faba bean</td>
<td>Faba bean</td>
</tr>
<tr>
<td>2007</td>
<td>Potato / Winter wheat</td>
<td>Potato / Winter wheat</td>
<td>Potato / Winter wheat</td>
</tr>
<tr>
<td>2008</td>
<td>Winter wheat /Grass/ Clover</td>
<td>Grass/Clover</td>
<td></td>
</tr>
</tbody>
</table>
Table 5.5: Manure and fertiliser applications in Foulum site at each treatment

<table>
<thead>
<tr>
<th>Year</th>
<th>Type</th>
<th>Amount (C kg/ha)</th>
<th>C/N Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>O2</td>
<td>1&lt;sup&gt;st&lt;/sup&gt; Cattle/ Pig slurry</td>
<td>245</td>
<td>4.2</td>
</tr>
<tr>
<td></td>
<td>3&lt;sup&gt;rd&lt;/sup&gt; Cattle/ Pig slurry</td>
<td>533</td>
<td>4.8</td>
</tr>
<tr>
<td></td>
<td>4&lt;sup&gt;th&lt;/sup&gt; Cattle/ Pig slurry</td>
<td>428</td>
<td>4</td>
</tr>
<tr>
<td>O4</td>
<td>1&lt;sup&gt;st&lt;/sup&gt; Cattle/ Pig slurry</td>
<td>210</td>
<td>3.56</td>
</tr>
<tr>
<td></td>
<td>3&lt;sup&gt;rd&lt;/sup&gt; Cattle/ Pig slurry</td>
<td>438</td>
<td>3.9</td>
</tr>
<tr>
<td></td>
<td>4&lt;sup&gt;th&lt;/sup&gt; Cattle/ Pig slurry</td>
<td>447</td>
<td>3.7</td>
</tr>
<tr>
<td>C4</td>
<td>1&lt;sup&gt;st&lt;/sup&gt; NH₄NO₃</td>
<td>130</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3&lt;sup&gt;rd&lt;/sup&gt; NH₄NO₃</td>
<td>140</td>
<td></td>
</tr>
<tr>
<td></td>
<td>4&lt;sup&gt;th&lt;/sup&gt; NH₄NO₃</td>
<td>72</td>
<td></td>
</tr>
</tbody>
</table>

5.2.2.3 Tulloch, Scotland

Tulloch is in NE Scotland near Aberdeen (57°10.5’ 22”N 2°15.7’ 15”W, altitude 132 m above sea level) and is located in the Atlantic North agroclimatic zone. The experiment was initiated in the spring of 1991 and involved the conversion of farmland to organic production, which met the requirements of the EU organic regulations and is certified by the Soil Association. The texture of the soil is sandy loam while the pH was measured at 5.8 in 1994.

There are two rotations that were initiated in 1991. The first rotation included three years of grass/white clover which followed by spring oats,
swedes and under sown spring oats (T3). The second rotation was based on four years of grass/white clover which was followed by two years spring oats, with the last year being undersown with grass-clover (T4) (Ball et al., 2014) for further details). In the T3 rotation, the grass in the 1st year was grazed whilst two and one silage cuts were taken in the 2nd and 3rd years respectively. In both the 2nd and 3rd year following the harvest of the oats in the undersown crop, grazing by sheep occurred. In T4, the 1st and 3rd year grass was grazed; two silage cuts were taken from the 2nd year grass, while a single cut was taken from the 4th year grass. Following the silage cuts and the harvest of the oats from the undersown crop, the grass was grazed by sheep. The plots that were used for this project were number 3 and 12.

5.2.2.4 Easter Bush, Scotland

Easter Bush is a long-term grassland experimental site which covers approximately 10 ha of land on the Bush Estate in Penicuik, 10 km south of Edinburgh, Scotland UK (55° 51’ 55.24” N; 3° 12’ 22.37” W, altitude 190 m above sea level) (Jones et al., 2006; Jones et al., 2005). The grassland is intensively managed with Italian perennial ryegrass dominating the vegetation. The grassland was continuously and intensively grazed with sheep and cattle during the 7 years of the simulation (2002-2008). It was assumed that one livestock unit (LSU) is equivalent to one dairy cow weighing 600 kg (SRUC, 2013). Easterbush was grazed mainly by sheep (LSU 0.1), lambs (LSU 0.04) and sporadically by heifer calves (LSU 0.75). The fertiliser applications rates and the grazing days are described in Table 5.6.
The experimental site had a sandy clay loam soil type with bulk density 1.43 g cm\(^{-3}\) and pH 5.1.

Table 5.6: Fertiliser and grazing in Easterbush

<table>
<thead>
<tr>
<th>Year</th>
<th>Fertiliser Application NH(_4)NO(_3) (kg N ha(^{-3}))</th>
<th>Grazing days</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1(^{st}) March</td>
<td>2(^{nd}) May-June</td>
</tr>
<tr>
<td>2002</td>
<td>96</td>
<td>60</td>
</tr>
<tr>
<td>2003</td>
<td>96</td>
<td>60</td>
</tr>
<tr>
<td>2004</td>
<td>60</td>
<td>48</td>
</tr>
<tr>
<td>2005</td>
<td>60</td>
<td>25</td>
</tr>
<tr>
<td>2006</td>
<td>69</td>
<td>52</td>
</tr>
<tr>
<td>2007</td>
<td>69</td>
<td>52</td>
</tr>
<tr>
<td>2008</td>
<td>69</td>
<td>52</td>
</tr>
<tr>
<td>2009</td>
<td>70</td>
<td>52</td>
</tr>
</tbody>
</table>

5.2.2.5 Logården, Sweden

An existing field experiment at the Logården research farm (60 ha) in south-west Sweden (58° 20’ 23’’N; 12°38’ 14’’E, altitude 50 meters above sea level) was also used for validating the model. The site belongs to the Boreal agroclimatic zone in Europe. The mean annual precipitation at the site is 604 mm and mean annual air temperature 6.3 °C (30-year average for 1961–1990).
The experiment consists of two different systems; an organic and a conventional system and took place in 2004-2008. The organic crop rotation was managed according to the Swedish certification system for organic farming and consisted of beans, spring wheat, grass and rye while the conventional one consisted of beans and spring wheat (Stenberg et al., 2012). Tillage in the conventional system primarily consisted of tine cultivation to 10 cm instead of mouldboard ploughing to 20 cm in the organic system (Table 5.7). The legume crops that were incorporated in both the systems was red clover mixed with grass, and faba bean.

Table 5.7: Tillage events in Logården

<table>
<thead>
<tr>
<th>Sites</th>
<th>Year</th>
<th>Date</th>
<th>Depth (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conventional</td>
<td>2007</td>
<td>25/10</td>
<td>10</td>
</tr>
<tr>
<td></td>
<td>2005</td>
<td>10/12</td>
<td>20</td>
</tr>
<tr>
<td>Organic</td>
<td>2006</td>
<td>23/4</td>
<td>20</td>
</tr>
<tr>
<td></td>
<td>2007</td>
<td>20/8</td>
<td>20</td>
</tr>
</tbody>
</table>

5.2.2.6 San Marco Argentano, Cosenza Italy

San Marco Argentano is a sandy clay loam soil located in the southern Italy in the Calabria area. The site (39° 38’ 8.22” N; 16°13’ 41.2”E, altitude 100 m above sea level) belongs to the Mediterranean North agroclimatic zone. The field data was collected from an experiment that took place in 2010 and 2011. Annual precipitation was 729 and 565 mm respectively for the years of
the experiment, while the mean temperature was around 17°C in both 2010 and 2011. The crop rotation studied consists of pea followed by faba bean, then a six-row barley followed by a mixture of pea and barley and for the last year faba bean and barley mixture. The experiment was under rainfed conditions using traditional tillage methods. Tortorella et al (2013) provide further details for the site and for the experiment.

5.2.3 Parameterizing the UK-DNDC model

Model validation was conducted using yield, N₂O and water filled pore space data, depending on availability of data in each site. In terms of soil organic carbon (SOC), the model describes the existence of six different pools. The initial input value used in the model is the measured value from the field expert for the given soil at the site. In all the cases, simulations were created for at least a 10 year period. This period allows the model to ‘spin up’ and thus to reach a steady state for the carbon pools and may minimize some inaccurate situations that are developing in the beginning of the run as there is no reference point for the model (Fumoto et al., 2008; David et al., 2009). The exact period of the simulations, was dependent on the length of the rotations at each site. The main concern was to ensure that all the runs finished in the last year of a full rotation. One of the priorities for this chapter was to create parameters for the crop properties that were uniform for the whole experimental period and for all the sites. Numerous runs were performed in order to achieve parameters that are meaningful, which can be used to simulate crop production for European conditions appropriately. During this process, parameters were selected on the basis that they produced the best approximation to the measured values and hence
obtaining the ‘best case’ parameters set. The Home Grown Cereals Authority (HGCA) literature (HGCA, 2008; SRUC, 2013; HGCA, 2009) as well as local agronomists and experts were consulted in order to incorporate their expertise in the validation phase of the model. This enabled us to have a model that can respond in an acceptable way in most of the European cases with the same EU level parameters. An analysis of the best case parameters set showed that the model performed well, fitting closer with the measured yield than the default values (Table 5.8).

Table 5.8: The crop values that were used in for the validation and calibration of the model

<table>
<thead>
<tr>
<th>Crops</th>
<th>C/N ratio for grain</th>
<th>C/N ratio for leaf and stem</th>
<th>C/N ratio for roots</th>
<th>Maximum grain production, kg dry matter/ha</th>
<th>Thermal degree days</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alfalfa</td>
<td>10</td>
<td>25</td>
<td>35</td>
<td>140</td>
<td>2000</td>
</tr>
<tr>
<td>Barley</td>
<td>45</td>
<td>75</td>
<td>85</td>
<td>5400</td>
<td>1000</td>
</tr>
<tr>
<td>Beans</td>
<td>9.2</td>
<td>45</td>
<td>55</td>
<td>1250</td>
<td>1900</td>
</tr>
<tr>
<td>Clover</td>
<td>20</td>
<td>14.9</td>
<td>43.2</td>
<td>130</td>
<td>2300</td>
</tr>
<tr>
<td>Corn</td>
<td>50</td>
<td>80</td>
<td>80</td>
<td>11000</td>
<td>2550</td>
</tr>
<tr>
<td>Grassland</td>
<td>33</td>
<td>33</td>
<td>50</td>
<td>111</td>
<td>2500</td>
</tr>
<tr>
<td>Oats</td>
<td>35</td>
<td>75</td>
<td>85</td>
<td>6000</td>
<td>1600</td>
</tr>
<tr>
<td>Pea</td>
<td>11.5</td>
<td>13.6</td>
<td>75</td>
<td>7500</td>
<td>1600</td>
</tr>
<tr>
<td>Perennial grassland</td>
<td>35</td>
<td>35</td>
<td>50</td>
<td>466</td>
<td>2000</td>
</tr>
<tr>
<td>Potato</td>
<td>40</td>
<td>40</td>
<td>60</td>
<td>16000</td>
<td>2100</td>
</tr>
<tr>
<td>Rye</td>
<td>20</td>
<td>50</td>
<td>50</td>
<td>2150</td>
<td>2000</td>
</tr>
<tr>
<td>Winter Wheat</td>
<td>40</td>
<td>95</td>
<td>95</td>
<td>9000</td>
<td>1500</td>
</tr>
</tbody>
</table>
5.3 Results

5.3.1 Bush, UK

The measurement data that are presented in that section as well as in the subsequent ones are not complete datasets due to limitations on the actual datasets.

The modelled underestimated barley yield for 1st and 4th treatments; nevertheless, the relative differences between the treatments were replicated in the model (Figure 5.1). The measured grain yield of barley in the first treatment was 3358 kg ha⁻¹ while from the modelled was 3028 kg ha⁻¹. In the fourth treatment, the barley grain yield was 1844 kg ha⁻¹, while the UK-DNDC model predicted 1442 kg ha⁻¹. The predicted grass yield was within the range of that observed for the 2nd treatment. However the grass yield was slightly under estimated in the 1st and 3rd treatments (Figure 5.2). The trend in measured yields between treatments observed is also reflected in the predicted yields.
Figure 5.1: The measured (dots) and the predicted (lines) barley grain yield for the first (a) and the fourth (b) treatment. The measured value is a mean value (n=3) ± SE bars.

Figure 5.2: The measured (dots) and the predicted (lines) for grass yield for the three treatments at Bush. The measured value is a mean value (n=3) ± SE bars.

The fit between measured data and modelled outputs for N\textsubscript{2}O emissions is illustrated in Figures 5.3-5.7 for a range of crops and years.
Generally, the model provided reasonable predictions that are in close agreement with measured N₂O emissions. Nevertheless, there were some peaks that the model failed to match, which may be partly explained by the variability in the measurements. Nitrous oxide emissions are affected by management events and it seems that harvest is triggering the enhancement of the fluxes. The harvest indicates the presence of fallow land with crop residues, situations that may create issues to the model in terms of N₂O production. It is important to note that there is high variability in the measurements as illustrated by the error bars. In addition, the model predicted peaks which were not observed. Some of the measured peaks were observed during periods for which there were no measurements and therefore it is impossible to verify the predictions from the model at these times. In all five graphs a high peak around August was observed at different dates depending on the year. These large peaks were associated with intensive rainfall events during the day of the large peak (~ 50mm). Nevertheless, the model reflected the general trend and the magnitude of the measured data.
5.3 Results

Figure 5.3: Daily fluxes of N₂O from Bush in 2006 from the 1st treatment. The measured value is a mean value (n=3) ± SE bars.

Figure 5.4: Daily fluxes of N₂O from Bush in 2008 from 2nd treatment. The measured value is a mean value (n=3) ± SE bars.
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Figure 5.5: Daily fluxes of N₂O from Bush in 2008 from 3rd treatment. The measured value is a mean value (n=3) ± SE bars.

Figure 5.6: Daily fluxes of N₂O from Bush in 2006 from the 4th treatment. The measured value is a mean value (n=3) ± SE bars.
5.3 Results

Figure 5.7: Daily fluxes of N₂O from Bush in 2006 from the 2nd treatment. The measured value is a mean value (n=3) ± SE bars

The cumulative values from Figures 4.8 to 4.12 show good agreement between measured and simulated values (Figure 5.8). The differences between measured and simulated are considerably low for the first three graphs (a, b, c) with differences of around 5% while for the last two (d, e) the measured cumulative values are higher than the simulated by a third. Although there was a high difference in the cumulative, the coefficient of determination (R²) of the time series of the data is noticeably high with 0.952 and 0.997. In all the cases the coefficient of determination was high, which indicates that the model explains all the variability of the response data around its mean. All the outputs for N₂O cumulative time series of all the sites are presented in Appendix C. Measurement values used to calculate cumulative N₂O emissions originate from the mean of 3 replicates. However there was access only to the mean values of the measurements and not to the
raw data. Therefore as a result, there is an absence of error bars for measurement values, which could assist in the interpretation of the fit between the data.
5.3 Results

Figure 5.8: Cumulative values of N₂O emissions from measured and simulated values from Bush. R squared for the time series of measured against simulated values. (a= Bush in 2006 from 1st treatment, b= Bush in 2008 from 2nd treatment, Bush in 2008 from 3rd treatment, d= Bush in 2006 from the 4th treatment, e= Bush in 2006 from the 2nd treatment)

5.3.2 Foulum, Denmark

For this site data for the WFPS and N₂O concentrations were available. The modelled wfps from the organic site (Figure 5.9) showed good agreement with the measurements. However there are some mismatches, especially with regards to the permanent wilting point, where the model
predicted lower WFPS than that which was observed. In general the modelled values followed the trend of measured data in most cases where measurements were available.

![Diagram showing measured and modelled water filled pore space (wfps) and rainfall for Foulum O2 at a depth of 30 cm in 2008. The measured value is a mean value (n=3) ± SE bars. The bars represent the SE.](image)

Figure 5.9: The measured and modelled water filled pore space (wfps) and rainfall for Foulum O2 at a depth of 30 cm in 2008. The measured value is a mean value (n=3) ± SE bars. The bars represent the SE.

There was limited experimental N₂O concentrations data available for the validation process. Nevertheless, the model was generally able to represent the trend of N₂O emissions observed at Foulum in the C4 treatment, although the magnitude of some of the modelled peaks was greater than the measured values. This was especially evident in the conventional rotation for 2007. A peak in mid-April when deep tillage of 30cm depth and a fertiliser application (140 kg NH₄NO₃) took place during this time. The combination of these two main management events can explain the reason for this peak. The same reason is applied for the organic
sites where the peak was observed couple of days before than the organic rotations but instead of the fertiliser application it was applied manure (Figure 5.10-5.12).

Figure 5.10: Daily fluxes of N\textsubscript{2}O from Foulum C4 for 2007. The measured value is a mean value (n=3) ± SE bars
Chapter 5: Validation and Calibration of the model

Figure 5.11: Daily fluxes of N₂O from Foulum O2 for 2007.

Figure 5.12: Daily fluxes of N₂O from Foulum O4 for 2007. The measured value is a mean value (n=3) ± SE bars
In addition, the good fit of the modelled values to the measured data was shown by the small differences during the cumulative assessment of N₂O fluxes (Figure 5.13). The differences between simulated and measured data for cumulative values were between 11% and 27%. The coefficient of determination (R²) was more than 0.9 for all the three years which shows that the time series of the measured and simulated values were close to each other and had a good agreement.

Figure 5.13: Cumulative values of N₂O emissions from measured and simulated values from Foulum. R squared for the time series of measured against simulated values (a= Foulum C4 in 2007, b= Foulum O2 in 2007, c= Foulum O4 in 2007)

5.3.3 Tulloch Scotland

Validation data for N₂O emissions were limited for this site. Nevertheless historic N₂O emissions data for the T3 rotation in 2006 showed
a good agreement with the modelled data (Figure 5.14). It is important to note that there was a large variability associated with the measurements at this site. The largest SE was 120% of the actual measurement. This value was excluded from the cumulative assessment that was performed as its robustness is questionable. Each large plot within Tulloch has a very dynamic system, which can be influenced by many different factors that are complex and sometimes unknown. The variability of the soil conditions that exist in each soil type can create high unpredictability in the measurements and therefore in the model. The magnitude and the trend of the measured data were simulated in a way that agrees with the measurements.

![Image](image_url)

**Figure 5.14:** Daily fluxes of N₂O from oats at Tulloch T3 in 2006. The measured value is a mean value (n=3) ± SE bars.

The results of the simulation showed a good fit between the measured and modelled data for the silage yields. All the modelled predictions for the
5.3 Results

Annual silage cuts for T3 (Table 5.15) were within the 95% confidence intervals of the measured values. In the T4 plot (Figure 5.16) the model tended to underestimates the yields, although with two exceptions the values were within the 95% confidence intervals.

Figure 5.15: Linear regression for the measurements versus the modelled data for the silage yields from T3 rotation (plot 3). The black line represents the fitted relationship and the dashed red line is the 95% of confidence intervals and the dotted green line is the prediction intervals.
Figure 5.16: Linear regression for the measurements and the modelled data for grass cut amounts from T4 rotation (plot 12). The black line represents the fitted relationship and the dashed red line is the 95% of confidence intervals and the dotted green line is the prediction intervals.

Cumulative assessment of N$_2$O emissions at the Tulloch site showed that the simulated values were very close to measured values. The model under predicted the total N$_2$O emissions by 8% for almost the whole year in 2006. As mentioned before, the value that was associated with high standard error was eliminated from the assessment. The coefficient of determination ($R^2$) is close to 0.9 proving the good agreement, not only in the final cumulative value but for how the values progressed during the year in both the model and in reality (Figure 5.17)
5.3 Results

Figure 5.17: Cumulative values of N₂O emissions from measured and simulated values from Tulloch T3 in 2006. R squared for the time series of measured against simulated values from the same site and period.

5.3.4 Easter Bush, Scotland

The water filled pore space (WFPS) was measured at Easter Bush to a depth of 3.5 cm and 7.5 cm, while the model simulated results at 1cm, 5cm and 10 cm (Figure 5.18). The WFPS measurements of the two depths were plotted against the 5 cm results from the model. The majority of model predictions are close to measurements during the years. However, the model over predicted the WFPS in September. During dry periods the model predicts a rapid decline in WFPS, which were not observed in the measured data. These anomalies are likely to be due to the simulated and measured WFPS representing different soil depths. Due to this mismatch the 5cm WFPS model output was selected for further analysis as it showed the closest
relationship to the measurement depths. In subsequent graphs (Figures 4.2-4.4), the fit between measured and modelled N₂O data for all years between 2006 and 2008 are presented. In general the simulations demonstrate good agreement between data produced from UK-DNDC model and the measured values. However, there is a tendency for the model to predict more peaks than that observed. The majority of steep peaks in Figure 5.19-5.21 are due to the timing of tillage management events, as the model is sensitive to soil disturbance with regards to N₂O fluxes.

Figure 5.18: Water filled pore space (%) and rainfall (mm) from Easter Bush in 2008.
5.3 Results

Figure 5.19: Daily fluxes of N\textsubscript{2}O from Easter Bush for 2006. The measured value is a mean value (n=3) ± SE bars.

Figure 5.20: Daily fluxes of N\textsubscript{2}O from Easter Bush site for 2007. The measured value is a mean value (n=3) ± SE bars.
Figure 5.21: Daily fluxes of N₂O from Easter Bush for 2008. The measured value is a mean value (n=3) ± SE bars.

The cumulative N₂O flux values (annual) confirmed the satisfactory agreement between the measurements and the simulated data of N₂O (Figure 5.22) that was noted on the previous graphs. The differences between modelled and measured cumulative N₂O fluxes were low for all the three cases (a, b and c) where the model under predicted the N₂O emissions with 3%, 8% and 13% respectively. The good fit between model and measured values was verified by the coefficient of determination. In all cases the coefficient of determination was close to 1 (88%-95%) indicating how close the data are to the fitted regression line.
5.3 Results

Figure 5.22: Cumulative values of N\textsubscript{2}O emissions from measured and simulated values from Easter Bush. R squared for the time series of measured against simulated values (a= Easter Bush in 2006, b= Easter Bush in 2007, c= Easter Bush in 2008)

5.3.5 Logarden Sweden

Measured data from Logarden were limited only to crop yields (Figure 5.23). In general, the model yields showed good agreement with the measured values and were within the correct magnitude. In most of the graphs it can be noted that the model is overestimating the C content of the yield by up to 15% more than the upper limit of the standard error of the measured values.
Chapter 5: Validation and Calibration of the model

5.3.6 San Marco Argentano, Cosenza Italy

Measured N₂O fluxes from the San Marco Argentano site were consistently low; however the model was generally able to capture the trend of values observed (Figures 5.24 and 5.25). In May 2011, the model did not successfully predict the peak that occurred, although the modelled values

Figure 5.23: Carbon yield from the conventional rotation a) Faba bean in 2007, b) Spring wheat in 2008, c) Faba bean in 2005, d) Spring wheat in 2006
were close to the measured data during the rest of the measurement period. In Figure 5.24 there was a peak during the first half of October which can be explained by the very large rainfall event on that day (31.4 mm) and the tillage event (50cm) that took place just before the large peak. The same large peak was noticed again in Figure 5.25, which is also associated with an intensive rainfall event (29.2mm)

![Daily fluxes of N₂O from San Marco Argentano with faba bean and barley for 2011. The measured value is a mean value (n=3) ± SE bars.](image)

Figure 5.24: Daily fluxes of N₂O from San Marco Argentano with faba bean and barley for 2011. The measured value is a mean value (n=3) ± SE bars.
Figure 5.25: Daily fluxes of N₂O from San Marco Argentano planted with peas for 2010. The measured value is a mean value (n=3) ± SE bars.

For the San Marco Argentano site, the cumulative assessment showed a small difference between measured and simulated values. It is interesting to note that for the cumulative assessment in 2010 the difference was only 3% in the final cumulative value but the coefficient of determination (R²) was low at 0.287 (Figure 5.26). This shows that the measured and simulated values were not progressed in the same way during the assessment period. That was caused by the large peak of the model in October (Figure 5.25) which was not depicted in the measurements.
5.4 Conclusions

The results of the simulations undertaken have provided the UK-DNDC user community with a better understanding of the model and its outputs as well as contributing to the validation and improvement of the model. Measurement data from six European experimental fields were used to assess the performance and to validate the UK-DNDC model. UK-DNDC was used instead of DNDC (v. 9.5), because this model provides the potential to link to the UK databases so is more applicable for the UK. Considerable development has been involved in modifying the crop parameters in order to have more realistic simulations and make them suitable for European agriculture. The improvement of the model is an on-going process that is
taking time and involves an iterative process of problem identification, resolution and testing. This has involved extensive collaboration with Professor Chang-Sheng Li (University of New Hampshire USA), who is the developer of the model.

In conclusion, the validation and calibration of UK-DNDC showed that the model can represent and simulate gaseous N emissions effectively. The model responds to the key management drivers that result in gaseous emissions and in most cases, had a good fit with measurements of N\textsubscript{2}O emissions, cumulative N\textsubscript{2}O emissions, yields and WFPS. However the model tends to overestimate the daily N\textsubscript{2}O in some cases and that has been also seen in other studies (Beheydt et al., 2007). Some of the peaks that were produced from the model were not possible to be tested as there was lack of measurements during or around these periods.

Where legume crops were present in the rotations, the model showed a good response in both yields and N\textsubscript{2}O emission simulations. The N\textsubscript{2}O data from legumes were limited only in one site which makes difficult to draw firm conclusions but gives us a good indication of the simulations. The response of the model in legume crops was equally well with other arable crops. The handling of the crop residues rich in N in terms of N\textsubscript{2}O production from the model perspective may be an issue, a situation that is expected after the harvest of the legume crops.

In general, the model had a good agreement with the measured crop yield and in most cases the predictions were within the bounds of measurement uncertainty. Nitrous oxide emissions are highly sensitive to
soil disturbance. After tillage events, it is expected that there is a high possibility of increased emissions. It has been noted that deeper disturbances increase the likelihood of higher emissions, although this is also dependent on the availability of soil N. Management events such as harvest can stimulate the N₂O emissions. Fallow systems are complicated for the model to simulate, as the model has been developed to simulate productive agricultural systems. For this reason, it is also recognised that the simulation of crop growth and emissions from fields receiving no nitrogen fertiliser also shows a level of complexity. The handling of crop residues from the model also seems to contribute to the complexity and therefore to the enhancement of emissions. The above issues needs more investigation from the model developing team and information to be provided to the model users of how exactly the model is working with the crops residues and fallow fields. On the other hand when the field is cultivated and there is a crop growing, the model was sometimes overestimating N₂O fluxes. This might be happening due to the fact that the soil is rich in organic matter and the N₂O emissions are highly sensitive to SOC (Li et al., 1996; Li et al., 2001). The cumulative values of all the sites that N₂O were available indicate that the model could express the measurements really closely. The differences in the final cumulative values varied from 3% to around 30% but with most of the differences being around 10% while the coefficient of determination in most of the cases was around 0.9 which highlights that the model explains nearly all the variability of the measured cumulative data. The coefficient of determination of all the cumulative N₂O values for data shown in Figures 5.8, 5.17, 5.22 and 5.26 for all the sites was 0.88 which indicates good fit between the measured values and the simulated.
The results from the WFPS, where data was available also showed the good response of the model in relation with the measurements. As the model is driven heavily by the precipitation (Li et al., 1992), it is essential that the sub-model which describes the soil moisture is adequately representing reality.

Another reason for discrepancies might be the use of different cultivars of crops across all these European countries. Due to the nature of the model, simulations may have been improved if site specific parameterisation of the crops had been used; however, the objective of this testing was to generate crop parameters that were universal for that specific crop for Europe.

The model performed well for both arable lands and grasslands. In both Tulloch and Easter Bush where temporary leys were included in the rotation the response of the model was close to the measurements in all the categories of data (N\textsubscript{2}O, WFPS and yields). Similar good fits have been noted in grasslands in New Zealand with the use NZ-DNDC, a model which is based in the same model as UK-DNDC (Saggar et al., 2007). The fit at Easter Bush showed that the model can predict the magnitude or the trend of N\textsubscript{2}O fluxes, although there were some mismatches in the timing of the peaks. Moreover the limited amount of measurement data created issues in performing relative tests that could lead to drawing useful conclusions. However the cumulative values of N\textsubscript{2}O emissions showed that the model was performing in an acceptable way for the grasslands. For Tulloch, the measured amounts of grass cuts against the model are showing a good agreement as they are most of them were within the 95% of confidence level.
5.4 Conclusions

Fine details and some trends failed to match measured data which may be partly explained by the spatial variability within the field and the complex dynamics of the N system within the soil. Many of the input data are referring to a single value (e.g. pH, SOC and bulk density) so it is challenging to have a value that can be representative across of the whole study field. Except the field input, weather is one of the main drivers of the model. The weather data that were used for the simulations in all the cases were reliable as they were coming from a weather station close to the field and often only few meters away.

The challenges on this research are to have simulations that can be trusted with no changes in the crop parameters across the sites and to have a model that can prove its ability to simulate cropping systems and rotation for a spectrum of agro climatic conditions. Biophysical modelling cannot substitute field measurements. The robust validation and calibration of the model that was performed was only possible because of the valuable information that is contained with the measurement data which can aid our understanding of the limitations of the system (Tonitto et al., 2007). A way forward would be a better measurement programme, which has been followed in other projects (e.g. DEFRA Science and Research Project: Minimising nitrous oxide intensities of arable crop products (MIN NO) - LK09128, Project number: RD-2008-3474), where the design of the experiment would actually help to provide data that would be used for modelling. The experimental data that this study used were more designed to monitor emissions. However a better experimental design, in order to fit on the modelling needs, would include a measurement programme that focus on
frequent measurements when major management activities are taking place in the field (e.g. fertiliser/manure application and tillage).

UK-DNDC can be a useful tool in identifying where and when high emissions can occur and in highlighting the effect of the management practices on emissions and exploring the impact of alternative managements on emissions.
6 Options assessment for five European regions by incorporating legume crops

Modelling is not only about simulating our data but rather stimulating our thinking

Unknown

6.1 Introduction

For the period 2000-2004, three quarters of the global protein rich crops were imported into Europe with the greatest share coming from South and North America (Crépon, 2004). Due to a high deficit in the production of crops rich in protein like legumes in Europe, there are great pressures on the environment (Eriksson et al., 2005; van der Werf et al., 2005) with extensive
cultivation of these crops in South American countries having adverse implications on the local natural ecosystem (Achard et al., 2002). Increasing legume production in European agriculture has the potential for identifying ways to decrease the negative effects in Europe and Southern American countries, which are affected by deforestation, due to European demand for protein crops.

Nitrous oxide (N\textsubscript{2}O) emissions are one of the main contributors of climate change (Ravishankara et al., 2009). In agriculture, N\textsubscript{2}O is produced as part of soil denitrification and nitrification processes in soils in both anaerobic and aerobic conditions (Ball et al., 1999) (See more information in Chapter 2). The ability of legumes to fix atmospheric N in the soil makes them an important addition to crop rotations as their incorporation in the ecosystem can alter the nitrogen dynamics, improving soil fertility (Diaz-Ambrona and Minguez, 2001; Lupwayi and Kennedy, 2007). Legumes reduce the N\textsubscript{2}O emitted from a crop rotation due to the reduction in fertiliser applications required and there is some evidence to suggest that biologically fixed N does not result in N\textsubscript{2}O emissions (Nemecek et al., 2008). Hence, incorporating legumes into the crop rotations, either as a whole or in an intercropping context, has the potential to benefit the environment (Pappa et al., 2011; Gomes et al., 2009). However, there is also evidence that shows Rhizobium may be a source of N\textsubscript{2}O or contributes in several ways to the N\textsubscript{2}O emissions in the ecosystem (Zhong et al., 2009).

Options appraisal provides an opportunity to simulate conditions that would be challenging to be tested in real life, for example long term
experiments (>100 years), combination of crops and soil conditions. The options assessment as a scientific tool has strong advantages in somewhat relieving issues mentioned above due to allowing the user freedom in changing the setup of experiments. The outcome of appraising experimental options can demonstrate an effective way to reach optimum results at a field level (Aral, 2014). A thorough analysis of results generated from this process can create substantial information, which has the potential to assist in the identification of system limitations. In addition the evaluation of proposed mitigation strategies can be conducted in order to contribute to alleviating environmental issues.

The main objective of this chapter is to assess environmental sustainability according to the N₂O production of different crop rotations for five case studies across the European Union. These rotations are divided in two groups of legume based rotations and non-legume based rotations.

6.2 Materials and Methods

6.2.1 Case study regions

In order to represent the variability in soils, climate and the biological productivity of European agriculture, five NUTS 2 agro-climatic regions were selected: namely one site in each of the following countries; Germany, Italy, Sweden, Scotland and Romania (Figures 6.1 and 6.2). These regions represent a range of soil types and agro climatic zones (Table 6.1).
Table 6.1: The selected case study countries and regions with the associated agroclimatic zones across Europe.

<table>
<thead>
<tr>
<th>Agro-climatic zone</th>
<th>Country</th>
<th>NUTS2 code</th>
<th>Region</th>
<th>Area covered by site classes in the countries</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nemoral</td>
<td>Sweden</td>
<td>SE23</td>
<td>Vastra Gotaland</td>
<td>50%</td>
</tr>
<tr>
<td>Mediterranean</td>
<td>Italy</td>
<td>ITF6</td>
<td>Calabria</td>
<td>58%</td>
</tr>
<tr>
<td>Continental North</td>
<td>Germany</td>
<td>DE41, DE42</td>
<td>Brandenburg</td>
<td>99%</td>
</tr>
<tr>
<td>Atlantic</td>
<td>Scotland</td>
<td>UKM2</td>
<td>Eastern</td>
<td>66%</td>
</tr>
<tr>
<td>Continental South</td>
<td>Romania</td>
<td>RO31</td>
<td>Sud Muntenia</td>
<td>42%</td>
</tr>
</tbody>
</table>

Figure 6.1: Selected case study regions across Europe (Source Eurostat, M. Reckling (2014))
Figure 6.2: Environmental stratification of Europe according to Metzger et al. (2005).

Weather data for the five European regions highlights the variability of the different weather conditions that prevail in Europe. The weather data used in this study does not correspond with continuous calendar years due to limitations in weather data coverage available for each site. Mean annual daily temperature and mean rainfall is described in Figure 6.3. It is noticeable that Italy is the warmest country with an average daily
temperature of almost 17°C, while Scotland is the wettest with a mean annual rainfall of 1050 mm for the period of this study.

Figure 6.3: Average daily temperature and annual rainfall for the period of rotation for each case study.

6.2.2 Options selection

The creation of the legume based rotations for arable and forage systems was carried out by colleagues, from The Leibniz Centre for Agricultural Landscape Research (ZALF) in Germany (Reckling et al., 2014), in consultation with local experts from each region. The rotations that were used for this chapter were based on surveys with local experts of each area. Expert opinion suggested what is growing currently in each region and recommended what should be the minor changes to them in order to change them in a legume based rotation. Moreover the data used in this study were
derived from previous assessments, support discussions with stakeholders and experts on the sustainability and possible restrictions in the implementation of the different rotations. An evaluation of the crop rotations as a whole was performed as well. The evaluation takes into account the long term effects of rotations with respect to the whole system. The long term effects refer to N balances and efficiency as well as gross margins for the rotation and a pest, disease and weeds infestation risk. For more detailed information on the data collected and the development of options can be found in Legume Futures Report by Reckling et al. (2014).

6.2.3 Selected rotations

The baseline rotation (Cr) did not contain any legume crops, representing a typical and current rotation of each area. Novel crop rotations (Lr) consisted of legume incorporation to the existing baseline rotation or in other cases the non-legume crop was replaced by a legume crop. These changes were agreed between local agronomists at each site and scientists from the agricultural sector. For more detailed information on the data collected and the development of options can be found in Legume Futures Report by Reckling et al. (2014).

The legume crop included in crop rotations was either peas or faba beans, which are the main species grown in Europe. In the grass/arable based rotations for forage systems (For), the grass was replaced by a grass-clover crop, which was cut for silage.
Chapter 6: Options assessment for five European regions by incorporating legume crops

The assessments used existing weather data from each country from the last 10 years. For the Swedish options was performed an option assessment using 2 completely controversial weather patterns a wet and a dry scenario in addition to the existing weather scenario. Thirty years’ worth of data was examined and 7 years (as the length of the longest option) of wet and dry years was selected. The average rainfall for the wet and dry weather dataset was 760 and 532 mm respectively. The modelled crop rotations for the sites in Sweden, Germany, Italy, Scotland and Romania are described in Tables 6.2-6.6 respectively.
Table 6.2: Current and legume based rotations for both arable and forage systems in Sweden

<table>
<thead>
<tr>
<th>Rotation type</th>
<th>Arable</th>
<th>Forage</th>
</tr>
</thead>
<tbody>
<tr>
<td>System</td>
<td>Current</td>
<td>Legume</td>
</tr>
<tr>
<td>Rotation code$^1$</td>
<td>Arable</td>
<td>LR1a</td>
</tr>
<tr>
<td>1st yr</td>
<td>W wheat</td>
<td>W wheat</td>
</tr>
<tr>
<td>2nd yr</td>
<td>Spring Oats</td>
<td>Spring Oats</td>
</tr>
<tr>
<td>3rd yr</td>
<td>W wheat</td>
<td>W wheat</td>
</tr>
<tr>
<td>4th yr</td>
<td>Faba bean</td>
<td>W wheat</td>
</tr>
<tr>
<td>5th yr</td>
<td>Spring Oats</td>
<td>W wheat</td>
</tr>
<tr>
<td>6th yr</td>
<td>W wheat</td>
<td></td>
</tr>
<tr>
<td>7th yr</td>
<td>Pea</td>
<td></td>
</tr>
</tbody>
</table>

$^1$(Cr= Current, Leg=Legume, Ara=Arable, Liv=Forage, u/s=undersown)
$^2$(W= Winter)
Table 6.3: Current and legume based rotations for both arable and forage systems in Italy

<table>
<thead>
<tr>
<th>Rotations type</th>
<th>Forage 1</th>
<th>Forage 2</th>
<th>Arable</th>
</tr>
</thead>
<tbody>
<tr>
<td>System</td>
<td>For</td>
<td>For</td>
<td>Ara</td>
</tr>
<tr>
<td>Rotation code</td>
<td>CR1</td>
<td>LR1</td>
<td>CR3</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Crop year</th>
<th>Cr</th>
<th>Leg</th>
<th>Cr</th>
<th>Leg</th>
<th>Leg</th>
<th>Cr</th>
<th>Leg</th>
<th>Leg</th>
</tr>
</thead>
<tbody>
<tr>
<td>1st yr</td>
<td>W</td>
<td>W</td>
<td>Cr</td>
<td>Leg</td>
<td>Leg</td>
<td>Cr</td>
<td>Leg</td>
<td>Leg</td>
</tr>
<tr>
<td>2nd yr</td>
<td>W</td>
<td>W</td>
<td>Maize</td>
<td>Maize</td>
<td>Maize</td>
<td>Oat</td>
<td>Oat</td>
<td>Oat</td>
</tr>
<tr>
<td></td>
<td>W</td>
<td>W</td>
<td>W</td>
<td>W</td>
<td>W</td>
<td>W</td>
<td>W</td>
<td>W</td>
</tr>
<tr>
<td>3rd yr</td>
<td>Clover</td>
<td>Faba bean</td>
<td>Pea</td>
<td>Clover</td>
<td>Faba bean</td>
<td>Pea</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

1(Cr= Current, Leg=Legume, Ara=Arable, For=Forage)
2(W= Winter)
Table 6.4: Current and legume based rotations for both arable and forage systems in Germany

<table>
<thead>
<tr>
<th>Rotation type</th>
<th>Arable 1</th>
<th>Arable 2</th>
<th>Arable 3</th>
<th>Forage</th>
</tr>
</thead>
<tbody>
<tr>
<td>System</td>
<td>Ara</td>
<td>Ara</td>
<td>Ara</td>
<td>For</td>
</tr>
<tr>
<td>Rotation code</td>
<td>1(Cr=Current, Leg=Legume, Ara=Arable, For=Forage)</td>
<td>2(W=Winter)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1st yr</td>
<td>W rape seed</td>
<td>W rape seed</td>
<td>W rape seed</td>
<td>W rape seed</td>
</tr>
<tr>
<td>2nd yr</td>
<td>W wheat</td>
<td>W wheat</td>
<td>W wheat</td>
<td>W wheat</td>
</tr>
<tr>
<td>3rd yr</td>
<td>W barley</td>
<td>Pea</td>
<td>Faba bean</td>
<td>W rye</td>
</tr>
<tr>
<td>4th yr</td>
<td>W rye</td>
<td>W barley</td>
<td>W wheat</td>
<td>W rye</td>
</tr>
<tr>
<td>5th yr</td>
<td></td>
<td></td>
<td>W barley</td>
<td>W rye</td>
</tr>
</tbody>
</table>

Maize Maize

Maize Maize

Maize W rye

W rye Clover /Grass
Table 6.5: Current and legume based rotations for both arable and forage systems in Scotland

<table>
<thead>
<tr>
<th>Rotation type</th>
<th>Arable 1</th>
<th>Arable 2</th>
<th>Forage</th>
</tr>
</thead>
<tbody>
<tr>
<td>System</td>
<td>Ara</td>
<td>Ara</td>
<td>For</td>
</tr>
<tr>
<td>CR1, LR1a, LR1b</td>
<td>Cr  Leg  Leg</td>
<td>Cr  Leg  Leg</td>
<td>CR  Leg</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Rotation code¹</th>
<th>1st yr</th>
<th>2nd yr</th>
<th>3rd yr</th>
<th>4th yr</th>
<th>5th yr</th>
<th>6th yr</th>
<th>7th yr</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cr</td>
<td>W barley</td>
<td>W barley</td>
<td>W barley</td>
<td>W wheat</td>
<td>W wheat</td>
<td>W wheat</td>
<td></td>
</tr>
<tr>
<td>Leg</td>
<td>W oilseed rape</td>
<td>W oilseed rape</td>
<td>W oilseed rape</td>
<td>W oats</td>
<td>W oats</td>
<td>W oats</td>
<td></td>
</tr>
<tr>
<td>Leg</td>
<td>W</td>
<td>W</td>
<td>W</td>
<td>Grass</td>
<td>Grass</td>
<td>Grass</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Grass/ clover</td>
<td>Grass/ clover</td>
<td>Grass/ clover</td>
<td></td>
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<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>R</td>
<td>W wheat</td>
<td>Winter wheat</td>
<td>W wheat</td>
<td>W barley</td>
<td>W barley</td>
<td>W barley</td>
<td></td>
</tr>
<tr>
<td>O</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>P</td>
<td>W wheat</td>
<td>Faba bean</td>
<td>Pea</td>
<td>W rape seed</td>
<td>Peas</td>
<td>Faba bean</td>
<td></td>
</tr>
<tr>
<td>S</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>²</td>
<td></td>
<td></td>
<td></td>
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<td></td>
<td></td>
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<td></td>
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<tr>
<td>³</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

¹(Cr = Current, Leg = Legume, Ara = Arable, For = Forage)
²(W = Winter)
Table 6.6: Current and legume based rotations for both arable and forage systems in Romania

<table>
<thead>
<tr>
<th>Rotation type</th>
<th>Arable 1</th>
<th>Arable 2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Current</td>
<td>Legume</td>
</tr>
<tr>
<td>System</td>
<td>Ara</td>
<td>Ara</td>
</tr>
<tr>
<td>Rotation code¹</td>
<td>CR1</td>
<td>LR1a</td>
</tr>
<tr>
<td>1st yr CROP</td>
<td>W wheat</td>
<td>W wheat</td>
</tr>
<tr>
<td>2nd yr CROP</td>
<td>Sunflower</td>
<td>Sunflower</td>
</tr>
<tr>
<td>3rd yr CROP</td>
<td>Maize</td>
<td>Maize</td>
</tr>
<tr>
<td>4th yr CROP</td>
<td>Pea</td>
<td>Soybean</td>
</tr>
</tbody>
</table>

¹(Cr= Current, Leg=Legume, Ara =Arable, For=Forage)
²(W= Winter)

Following Reckling et al. (2014), the modelled options assume that N fertiliser application rates for individual crops were the same in the current rotation as those within a legume based rotations. This was based on the assumption that a reduced amount of applied N to the succeeding crop of the legume crop leads to reduced yields (Park et al., 2010; Goverment of Saskatchewan, 2013). It was also assumed that no N fertiliser was applied to legume crops.

Soils were selected according to the site classes of each NUTS 2 region (Table 6.7) as well as discussions with the local experts. For Sweden, there were two soils types. In Italy, the soil was classified as silty loam divided in
two systems with small soil differences to each other. For Germany, LGB 2 and LGB 4 were chosen as these were the most representative of the area. In Scotland, there were four site classes with two soils for each; a heavy (high clay content) and a light (low clay content) soil. For Romania, only one soil type was specified.

Table 6.7: Site classes and soil type per country

<table>
<thead>
<tr>
<th>Country case study</th>
<th>Soil type/ Site Class</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sweden</td>
<td>Lana</td>
</tr>
<tr>
<td></td>
<td>Logården</td>
</tr>
<tr>
<td>Italy</td>
<td>1st system</td>
</tr>
<tr>
<td></td>
<td>2nd system</td>
</tr>
<tr>
<td>Germany</td>
<td>LGB2</td>
</tr>
<tr>
<td></td>
<td>LGB4</td>
</tr>
<tr>
<td>Scotland</td>
<td>LCA*2 (Light and heavy)</td>
</tr>
<tr>
<td></td>
<td>Darleith (Light)</td>
</tr>
<tr>
<td></td>
<td>LCA*3 (Light and heavy)</td>
</tr>
<tr>
<td></td>
<td>Darvel (Light)</td>
</tr>
<tr>
<td>Romania</td>
<td>Loam</td>
</tr>
</tbody>
</table>

* Land Capability for Agriculture

The model was run for all case studies and associated soil types. In all cases, the model run period was a minimum of ten years. The results used for the assessment were taken from the last complete cycle of each rotations. A period of at least 10 years was used as a spin-up period to stabilise the C and N pools (Fumoto et al., 2008; David et al., 2009). For all the rotations UK-
DNDC default values have been used for crop parameters, as it was not possible to validate them with existing historic data from each country. This allowed for comparisons to be made between the crops and the sites with uniform values across all of the options assessment.
<table>
<thead>
<tr>
<th>Country case study</th>
<th>Soil type/site class</th>
<th>Logården</th>
<th>LGB2</th>
<th>LGB4</th>
<th>LCA2</th>
<th>LCA3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sweden</td>
<td>1st</td>
<td>46.5</td>
<td>10.0</td>
<td>10.0</td>
<td>10.0</td>
<td>10.0</td>
</tr>
<tr>
<td></td>
<td>2nd</td>
<td>37.6</td>
<td>14.0</td>
<td>25.0</td>
<td>25.0</td>
<td>25.0</td>
</tr>
<tr>
<td>Italy</td>
<td>Lana</td>
<td>14.0</td>
<td>1.23</td>
<td>1.54</td>
<td>1.24</td>
<td>1.24</td>
</tr>
<tr>
<td></td>
<td>Logården</td>
<td>1.34</td>
<td>1.50</td>
<td>1.50</td>
<td>1.50</td>
<td>1.50</td>
</tr>
<tr>
<td>Germany</td>
<td>LCA2</td>
<td>7.80</td>
<td>6.20</td>
<td>6.20</td>
<td>6.20</td>
<td>6.20</td>
</tr>
<tr>
<td></td>
<td>LCA3</td>
<td>7.42</td>
<td>5.63</td>
<td>5.63</td>
<td>5.63</td>
<td>5.63</td>
</tr>
<tr>
<td>Scotland</td>
<td>LGB2</td>
<td>7.10</td>
<td>5.30</td>
<td>5.30</td>
<td>5.30</td>
<td>5.30</td>
</tr>
<tr>
<td>Romania</td>
<td>LGB4</td>
<td>7.42</td>
<td>5.26</td>
<td>5.26</td>
<td>5.26</td>
<td>5.26</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Soil characteristics for all the classes in all countries/case studies</th>
<th>Lana</th>
<th>Logården</th>
<th>LGB2</th>
<th>LGB4</th>
<th>LCA2</th>
<th>LCA3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clay content (%)</td>
<td>46.5</td>
<td>37.6</td>
<td>14.0</td>
<td>25.0</td>
<td>25.0</td>
<td>25.0</td>
</tr>
<tr>
<td>Bulk Density (g cm(^{-3}))</td>
<td>1.24</td>
<td>1.54</td>
<td>1.34</td>
<td>1.23</td>
<td>1.50</td>
<td>1.50</td>
</tr>
<tr>
<td>Density (g cm(^{-3}))</td>
<td>7.20</td>
<td>7.42</td>
<td>7.10</td>
<td>7.80</td>
<td>6.20</td>
<td>6.20</td>
</tr>
<tr>
<td>Field capacity (wtr%, %)</td>
<td>77</td>
<td>40</td>
<td>24</td>
<td>24</td>
<td>24</td>
<td>24</td>
</tr>
<tr>
<td>Willing point (wtr%, %)</td>
<td>37</td>
<td>24</td>
<td>37</td>
<td>24</td>
<td>24</td>
<td>24</td>
</tr>
<tr>
<td>Porosity (0-1)</td>
<td>0.52</td>
<td>0.411</td>
<td>0.42</td>
<td>0.42</td>
<td>0.42</td>
<td>0.42</td>
</tr>
<tr>
<td>SOC (0-5 cm) (kg C kg(^{-1}) soil)</td>
<td>0.012</td>
<td>0.007</td>
<td>0.016</td>
<td>0.019</td>
<td>0.044</td>
<td>0.044</td>
</tr>
</tbody>
</table>
6.3 Results

6.3.1 Sweden

For Sweden, the model was run for the two predominant soils located in Lana and Logården, for an arable and forage system. In the arable set rotations, LR1a showed considerable reductions in the production of N₂O emissions with 53% and 62% for Lana and Logården respectively compared with the baseline non-legume rotation (CR1). In contrast, LR1b did not show the same trend. Depending on the soil type, the N₂O emissions, from the second alternative of the arable rotation (LR1b), were either unaffected by the change of the rotation or slightly increased when legumes were incorporated. For the Lana forage rotation, the legume based rotation (LR2) showed that there was a slight increase in N₂O emission compared with the baseline rotation (CR2). On the other hand, at Logården with the same set of rotations, there was a large reduction (40%) in the emissions for the change between a baseline (CR2) and a legume based rotation (LR2) (Figure 6.4).
Chapter 6: Options assessment for five European regions by incorporating legume crops

Figure 6.4: Annual average percentage of difference of N₂O emissions from the baseline (CR) (black dashed line) and the alternatives rotations (columns) from the Swedish case study from both soil types (top graphs refers to Lana soil type, bottom graph refers to Logården soil type) and type of rotations (a and c refer to the arable rotation, b and d refer to the forage).

Nitrogen budgets were determined for the Lana arable options to assess the differences between inputs and outputs of N (Figure 6.5). Results show that the LR1b rotation has the lowest N inputs in the system compared with the rest of the rotations. Both of the legume based rotations have lower N inputs from the baseline rotation (CR1) due to no additional N fertiliser being applied in years with legume crops incorporated. The CR1 option
shows the highest system outputs in total but LR1b has the highest emissions of N₂O amongst the three rotations. Highest emissions were seen around periods of pea planting and harvesting and when the field was fallow. This highlights that rich N residues are more likely to be causing the increased emissions seen in the results.

The values that are presented for N budgets refer to average values of the total rotation period, which they are highly depended on. The LR1b rotation period was for seven years while the LR1a was four years long. The N budget showed that the fertiliser inputs were higher on average in the CR1 but the total actual amount of N fertiliser increased by 30% in LR1b compared to the baseline. Moreover the unavoidable difference in rotation length creates some variability in weather data used as inputs for each rotation. Due to the fact that the model is sensitive to weather data, as well as N₂O, some differences seen in the emissions may be a function of this variability on the weather data.
Figure 6.5: N budget for the arable rotations from Lana soil type from the Swedish case study

The N budgets for Lana forage rotations were also calculated (Figure 6.6). In this case, the three consecutive years of grass clover mixture led to a high level of N fixation. The amount of fertiliser is the same in both rotations (non-legume and legume based) as the grass in the non-legume based rotation did not receive any N input. The increase of N due to N fixation resulted in higher emissions from the legume based rotation and higher crop uptake. In the last year of the rotation when the grass clover was cut, 43.5% of emissions were emitted and 55% in the consecutive year (the 1st year of the next rotation) indicating that the N rich residues are creating the high N₂O emissions. However that was not the case for Logården, were the legume based rotation showed lower N₂O production. The Lana soil has higher organic carbon and clay contents than that at Logården and this is associated with higher emissions.
Figure 6.6: N budget for the forage rotations from Lana soil type from the Swedish case study.

6.3.1.1 Scenario of controversial weather patterns

In order to demonstrate variability to the weather changes, two options with controversial weather patterns were selected. The two options assessment of a wet and a dry period was performed in the Swedish site for the Lana soil type. Interestingly the results showed similar patterns as the results from the existing weather dataset with a rainfall of an average of 677.7mm. In both the wet and the dry conditions the first alternative legume based rotation of the arable system is giving lower N\textsubscript{2}O emissions while the second one is giving higher. Regarding the forage system here we have a slight increase of 10% for the wet conditions. Both of them are following the trend that was observed in the forage system of the existing weather dataset.
Chapter 6: Options assessment for five European regions by incorporating legume crops

Figure 6.7: Annual average percentage of difference of N₂O emissions from the baseline (CR) (black dashed line) and the alternatives rotations (columns) from the Swedish case study under wet conditions from both systems (arable and forage).

Figure 6.8: Annual average percentage of difference of N₂O emissions from the baseline (CR) (black dashed line) and the alternatives rotations (columns) from the Swedish case study under dry conditions from both systems (arable and forage).
6.3.2 Italy

Three different options, an arable and two forage, were chosen for the Italian case study. For legume based forage rotation options there was a substantial reduction in N\textsubscript{2}O emissions compared to baseline rotations (CR1 and CR2) shown in Figure 6.9. In the second forage 2 option, the change between rotations from the baseline (CR2) to the second alternative legume based (LR2a) rotation, resulted in a reduction of N\textsubscript{2}O emissions of up to 75% (Figure 6.9b). In the arable rotation, the legume based (LR3a and LR3b) options resulted in there being no change or higher losses of N as N\textsubscript{2}O compared to the baseline.
Figure 6.9: Annual average percentage of difference of N\textsubscript{2}O emissions from the baseline (black dashed line) and the alternatives rotations (columns) from the Italian case study from the 1\textsuperscript{st} system (a and b refer to the forage 1 and forage2, c refer to the arable).

The N budget for the arable dataset, showed that the total outputs of N are higher in the second legume based rotation (LR3b) in comparison with other rotations for both NO\textsubscript{3} leaching and N\textsubscript{2}O (Figure 6.10). The highest emissions of N\textsubscript{2}O occurred during the year of harvest of the legume crop and the year that the rotation received the highest amount of N fertiliser. For
LR2b there was enhanced NO₃ leaching, which was not observed in other rotations.

![Graph showing N budget for the arable rotations from the irrigation system from the Italian case study.](image)

**Figure 6.10:** N budget for the arable rotations from the irrigation system from the Italian case study

In the 2nd system of the Italian case study, the inclusion of legumes into crop rotations resulted in a reduction of N₂O emissions (Figure 6.11) and followed a similar pattern as in the 1st system for the forage rotation but not for the arable rotation. In this system (2nd) the arable alternative rotations showed reductions in comparison with the baseline rotation. The differences between the two systems were in the soil characteristics, which focused more in small changes in bulk density, soil pH and SOC. In the 2nd system, SOC is slightly lower and this effects N₂O production (see Chapter 6 for further details).
Figure 6.11: Annual average percentage of difference of N₂O emissions from the baseline (black dashed line) and the alternatives rotations (columns) from the Italian case study from the 2nd system (a and b refer to the forage 1 and forage2, c refer to the arable)

6.3.3 Germany

For the German case study, there were three arable and one forage rotations for two soil types (LGB2 and LGB4). The results for LGB2 soil class showed that the legume based rotations emitted less N₂O than the current rotations. Nitrous oxide emissions were reduced by up to 82% for the forage based rotations shown in Figure 6.12.
The results of LGB4 soil class showed similar trends (Figure 6.13). The reduction in N₂O emissions, were lower by approximately 5% than LGB2 due to the differences in soil characteristics. The second arable rotation in this soil class did not follow the trend of the previous soil class. Legume based rotations LR2a and LR2b showed an increase in N₂O production in comparison with the baseline rotation (CR2). More specifically, in the first alternative legume rotation (LR2a) there is an increase of almost 4 kg ha⁻¹ yr⁻¹ Figure 6.13b.
Figure 6.13: Annual average percentage of difference of N₂O emissions from the baseline (black dashed line) and the alternatives rotations (columns) from the German case study from the LGB4 (a to c refer to the arable 1 to arable 3, d refer to the forage)

In the LGB4 soils of Germany, only LR2a and LR2b legume based rotations did not show a reduction in N₂O emissions. The N budget in the second arable rotations showed that N fixation was higher for the first alternative legume based rotation (LR2a) than for the second alternative (LR2b) due to the presence of peas instead of faba bean (Figure 6.14). Total N outputs were also higher in the first alternative (LR2a) compared to the
baseline (CR2) and the second alternative (LR2b). For this set of options the alternative legume based rotations were two years longer than the baseline rotation. In the additional two years it was one non legume crop and one legume crop were included. This resulted in higher total actual N fertiliser amount applied by 25% in both of the legume based rotations. The highest N$_2$O emissions were produced in the year of legume crop harvest, which highlights the important role of N rich residues that have on the N$_2$O emissions.

Figure 6.14: N-budget for the second arable rotations from the fourth site class from the German case study

### 6.3.4 Scotland

For the Scottish case study, both high/heavy (LCA2) and low/light (LCA3) clay contents were used for options appraisal (Figure 6.15). The model was run for 20 to 28 years depending on the length of the rotations. Two arable and a forage rotations were assessed.
Results showed the general trend of light soils producing lower emissions than heavy soils. The high rainfall of the Scottish case study created some challenges, as the inclusion of legumes did not reduce the N$_2$O emissions in all cases. It was noticeable that there were increased losses of N in the form of NO$_3^-$ leaching (Figure 6.16). The high N leaching can be explained by high rainfall encountered in the Scottish options during the period of the study. Scotland is the wettest of the five case studies and almost 40% more than the second wettest location, Sweden. The N budget showed that legume presence in the first alternative rotation of the second arable set (LR2a) was beneficial for the crops, as the average crop uptake increased by approximately 20%. This was also the case for the forage rotation. For the second alternative rotation of the second arable rotation, the crop uptake was not increased. This indicates that the N fixed from the crops is possible, leading to higher crop uptake when it is abundant. Leaching of NO$_3^-$ was affected by the presence of legumes, as it was reduced by 40% and 55% for the two alternative rotations of the second arable set. The forage rotation, which contained clover, received the same amount of N fertiliser, in both the baseline and alternative legume based rotations. However, N$_2$O emissions from legume based rotations were higher in comparison with the baseline. The same trend was observed for the case study in Sweden, but not in Germany or Italy. This might be a function of the combination of increased N inputs due to biological N fixation and the high rainfall of the two countries, Scotland and Sweden.
6.3 Results

Figure 6.15: Average N\textsubscript{2}O emissions from all four soils in Scotland (a refer to the first arable rotations with soil characteristics from LCA2 light soil type, b refer to the second arable rotations with soil characteristics from LCA2 heavy soil type, c refer to the forage options with soil characteristics from LCA3 light soil type and from LCA3 heavy soil type.
The Romanian case study comprises two sets of arable rotations, with one soil type. The model was run for a period of 21 years. The second alternative legume based rotation (LR1b) resulted in a slight reduction of N\textsubscript{2}O emissions whereas the first option (LR1a) showed the same emissions as the baseline (Figure 6.17). Both the alternative legume based rotations (LR2a and LR2b) of the second arable, resulted in increased emissions. All three rotations of the second arable set received the same amount of fertiliser. However, the baseline rotation received the highest amount per year (baseline rotation was 3 years while legume based were 4 so the same amount of fertiliser was distributed in 3 years and 4 years). The N budget for the second arable rotations suggests that legume rotations (LR2b and LR2c)
show a decreased N budget with lower crop uptake but higher losses of N in NO₃ leaching and N₂O (Figure 6.18).

Figure 6.17: Annual average percentage of difference of N₂O emissions from the baseline (black dashed line) and the alternatives rotations (columns) from the Romanian case study (a and b refer to the arable 1 and arable 2 respectively)
6.4 Discussion and Conclusions

The present study of five European case study countries evaluates the inclusion of legumes into existing local traditional rotations. N₂O emissions were assessed through the use of modelling options with UK-DNDC. One advantage, from an environmental perspective, is that legume crops can offer a pre-crop effect that can influence the management of the succeeding crop and in particular the fertiliser application (Kopke, 1987; Charles and Vullioud, 2001). At the same time, reducing nitrogen fertiliser applications in the succeeding crop may create pressures for maintaining yields by creating small N deficiencies. Nitrogen fertiliser application rates can be reduced by up to 100% in the succeeding crops, depending on the legume crop type and field conditions (Park et al., 2010). On the other hand, if the N fertiliser
applied is not reduced then the succeeding crop may have a higher yield potential. This study assumed that the fertiliser applied to the non-legume crops was not affected by the inclusion of legumes into the rotation. There was no N applied to legume crops. One of the main targets for this research was to contribute to the knowledge for the farmers’ decision making by identifying potential environmental benefits resulting from the inclusion of legumes into agricultural systems.

The changes between baseline and legume based rotations were simple changes consisting of rotations with the inclusion of a legume crop, resulting in minimum changes that could possibly be easily adopted. If the only focus is environmental implications of the new rotations, they could be applied in a different manner with more sophisticated changes in these rotations. This study focused on the assessment of options that would provide a more realistic and practical application for both farmers and the European market. As the cultivation of legumes in the European Union has dramatically declined and is not supported heavily, it is suggested that the changes that can be adopted by the European agriculture should be modest and subtle. The assessment of 24 legume rotation options, over five European countries clearly shows that the inclusion of legumes into European agricultural systems has the potential to reduce N₂O emissions. In most of the countries / case studies that were assessed in this study there were cases with significant environmental gains in the amount of N₂O that was emitted by the use of legumes.
In contrast, there were cases in which the combination of selected crops, weather and soil characteristics of the region did not show that legumes contributed to reducing N₂O emissions. This is potentially due to the handling of the residues and fallow fields. Residue incorporation is a crucial part of the agronomic system as they can play an important role in the soil nutrient status during the fallow periods of the field. With the inclusion of legume crops into the system, the succeeding crop following legumes receives the preceding crop effect, thus it is rich in N as legume crop residues (Kopke, 1987; Charles and Vullioud, 2001). Due to this effect, the residues are rich in N and this may create N₂O hotspots during residue decomposition stages (Baggs et al., 2000; Huang et al., 2004).

The results of the cases studies show an effect of N₂O production due to the change to a more legume based rotation. In Sweden there was an average annual reduction in emissions of 62% while in Italy N₂O reduction was up to 75%. In three of the four case studies in Germany, there was a reduction in N emitted as N₂O. The second combination of arable systems did not show a positive effect on the legume crop inclusion, in terms of N₂O emissions. In Romania, the gains of reduced emitted N₂O were either lower, or there were slight increases of N₂O from the legume based rotations. In Scotland, the inclusion legumes resulted in variable results with some cases showing increases.

More specifically in Sweden, the second legume based rotation (LR1b) from the arable rotations (Winter wheat/ Spring Oats/ Winter wheat/ Winter wheat/ Spring Oats/ Winter Wheat/ Pea) in both soil types showed higher
emissions than the traditional and the first legume based rotation. The main
difference between this rotation and the baseline rotation (CR1) was the two-
fold increase in rotation length. This difference in rotation length can create
inconsistencies in the comparison of the results, due to the effect of
additional years and therefore weather conditions included into the
simulation. For the Swedish forage rotation, N inputs to the system
according to the N budgets were almost 45% more in the legume based
rotation due to the presence of clover. In this case it was noticed that in only
one of the two soils, the emissions were higher from the legume based
rotation in comparison with the traditional one. The Lana soil had higher
emissions and this was associated with higher soil organic carbon and clay
content than the Logården soil.

The inclusion of peas to the German rotations had both positive and
negative effects in terms of the N\textsubscript{2}O production. Jensen (1997) has reported
that peas are not using inorganic N sufficiently in deeper soils and that after
the harvest there are higher amounts of mineral N left in the field in
comparison with a cereal crop. It is therefore important to understand
factors such as how the amount of N that is applied before or after the
legume crop, the N requirements of the succeeding crop, how the field is
managed following harvest and the quantity of residues left in the field. The
modelling activity in the options appraisal study provides an opportunity to
research and test a range of rotations and nitrogen balances before they will
be applied in the field and therefore test the potential sustainability of each
crop rotation system.
In both Italy and Romania, the results suggest that the inclusion of a pea crop leads to an increase in N\textsubscript{2}O emissions. However it is worth noting the huge reductions in N\textsubscript{2}O emissions in some of the sets of the rotations especially in Italy (LR2a, LR2b, LR3a, and LR3b).

In the Scottish case study, there was also the presence of high fixing N crops. A heavy and a light soil were simulated for both the LCA2 and LCA4. It is useful to note that as a general trend the light soils produced more N\textsubscript{2}O emissions than the heavy soils. Scotland was the wettest out of the five case studies by almost 40% rainfall more than the second country Sweden. This is an important factor to consider in biogeochemical modelling as the UK-DNDC model used in this study is heavily driven by the rainfall events (Li et al., 1992). The N budgets also showed a great loss of N as NO\textsubscript{3} leaching. Carrouée et al. (2002) and Fuhrer (2006) reported that the inclusion of legume crops into the crop rotation system can lead to higher rates of NO\textsubscript{3} leaching and especially the presence of peas in comparison with cereals (Jensen, 1997). Scotland as a case study is a more extreme example due to the fact that receives large amounts of water and needs further consideration of how the changes and the inclusion of legumes have to be incorporated.

In general, across the five regions simulated, there were substantial reductions in N\textsubscript{2}O emissions in most of the options that were simulated. This is largely explained by the fact that legume crops do not require additional N fertiliser application and even if they can create some N hotspots the balance in most cases is positive producing an overall N\textsubscript{2}O reduction. Charles and Gosse (2002) highlighted the large reduction in the nitrogenous emissions
from a legume crop in comparison with a cereal crop. Knudsen (2014) showed the overall impact of legume inclusion can lead to a reduction in N₂O emissions to the magnitude of 175-280 kg of CO₂eq per hectare that is cultivated with peas or faba bean instead of wheat.

The following table (Table 6.9) highlights the effects of the legume crops in each country, for both arable and forage systems. As a general trend it can be observed the positive effect of legumes across all the European sites. The 71% of the novel proposed legume based rotations worked in favour of reduction of the N₂O emissions. For Germany and Scotland, the variability on the results is noteworthy as there are positives changes that enhance the N₂O production by 300% and negative changes that reduced the N₂O emissions up to 82% compared with the current rotations. The average values are indicating an average effect in percentages for each country and each soil type for the entire proposed legume based rotations.
Table 6.9: Summary table of the results from different options in different countries around Europe. The numbers refer to the change of \( \text{N}_2\text{O} \) emissions between the new novel sequences of crop options and are expressed in percentage of change from the “current” rotations.

<table>
<thead>
<tr>
<th>Rotations</th>
<th>ARABLE</th>
<th>FORAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td><strong>Country</strong></td>
<td><strong>LCA2</strong></td>
</tr>
<tr>
<td></td>
<td><strong>Sweden</strong></td>
<td><strong>Italy</strong></td>
</tr>
<tr>
<td></td>
<td><strong>Lana</strong></td>
<td><strong>Log</strong></td>
</tr>
<tr>
<td>LR1a</td>
<td>-53</td>
<td>-62</td>
</tr>
<tr>
<td>LR1b</td>
<td>+25</td>
<td>-2</td>
</tr>
<tr>
<td>LR2a</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>LR2b</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>LR3a</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>LR3b</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td><strong>Average</strong></td>
<td>-23%</td>
<td>-15%</td>
</tr>
<tr>
<td>LR1a</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>LR2a</td>
<td>+22</td>
<td>-50</td>
</tr>
<tr>
<td>LR2b</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>LR2c</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>LR3</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td><strong>Average</strong></td>
<td>-14%</td>
<td>-32%</td>
</tr>
</tbody>
</table>

*Rom*= Romania
It is important to use site specific data for the case studies so that the modelling provides a more tailored site specific approach. In addition, for estimations of N₂O emissions, IPCC guidelines can be used (IPCC, 2006). However the IPCC approach to estimating N₂O emissions, does not taking into account differences in weather conditions between countries and site-specific data. According to Knudsen (2014) the following table (Table 6.10) indicates that UK-DNDC predictions were close to the IPCC approach in most of the cases.
Table 6.10: UK-DNDC and IPCC guidelines estimations on carbon footprint for both faba bean and pea across the five European regions. Values are in kg CO₂ eq per t grain DM.

<table>
<thead>
<tr>
<th>Country</th>
<th>UK-DNDC</th>
<th>IPCC</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Total</td>
<td>Contribution from N₂O emissions</td>
</tr>
<tr>
<td>Pea</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Scotland</td>
<td>65</td>
<td>59</td>
</tr>
<tr>
<td>Sweden</td>
<td>106</td>
<td>106</td>
</tr>
<tr>
<td>Romania</td>
<td>102</td>
<td>100</td>
</tr>
<tr>
<td>Italy</td>
<td>152</td>
<td>133</td>
</tr>
<tr>
<td>Germany</td>
<td>127</td>
<td>124</td>
</tr>
<tr>
<td>Faba bean</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Scotland</td>
<td>57</td>
<td>54</td>
</tr>
<tr>
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<td>2</td>
<td>2</td>
</tr>
<tr>
<td>Italy</td>
<td>170</td>
<td>156</td>
</tr>
<tr>
<td>Germany</td>
<td>9</td>
<td>6</td>
</tr>
</tbody>
</table>

The inclusion of legumes into the traditional rotations within European agriculture can offer advantages in agriculture. The transition to a more legume based European agriculture is neither simple nor straightforward. It has been reported in many studies that the presence of many rhizobial species may contribute in the production of the N₂O gas (Galloway, 1998; Daniel et al., 1982). According to Galloway (1998) the N that is fixed from legumes through *Rhizobium spp* can undergo the same process...
of denitrification and nitrification (depending on the condition of the soil) as the soil N hence, if the conditions are in favour, can be emitted as N₂O. The IPCC (2000) refers to increased N₂O emissions globally in the ecosystem and one of the reasons suggested for the increase is the biological N fixation amongst other reasons. Nevertheless, in the next IPCC report (2007), biological N fixation was not included in the calculations for the N₂O emissions due to the fact that there was not convincing evidence to support inclusion (Zhong et al., 2009). It is important to note that UK-DNDC has not incorporated a process to simulate possible rhizobial denitrification.

Novel rotations should be adopted in order to accommodate all different aspects of legume properties. Modelling can help in the understanding of crop systems better and attempt to adjust the existing knowledge, in order to have a more sustainable environment in terms of N₂O production.
7 General Discussion and Conclusions

7.1 Project overview

The purpose of this thesis was to model new legume-supported cropping systems and to assess their nitrous oxide production in comparison with traditional cropping systems in order to reduce the environmental impact of European agricultural systems within a range of agro-climatic zones with the use of UK-DNDC model. The current thesis offered an in-depth analysis of the model’s predictions and the model’s sensitivity to various input parameters.

While this thesis does not claim to offer a sophisticated review of the role of legumes in European agriculture, it does provide a more holistic view of the environmental implications of legumes inclusion, in terms of N₂O production, through modelling that in turn not only provides simulation
results of the effects of the legumes inclusion but could also lead to contributions in a more sustainable European agriculture.

More analytically, Chapter 2 presented a review of the family of legumes and their main attributes as well as the current state of them in the European Union. It presented some of the main critical pressures in the environment (climate change, human growth population and N cycle) and the challenges that these pressures pose for the future.

In Chapter 3, a review of environmental modelling was presented along with brief reviews of other models and a detailed review of the model that was used in the simulations (UK-DNDC).

Through the sensitivity analysis carried out in Chapter 4, it was possible to highlight the importance of some of the input parameters of the model. The multiple global analyses that were performed underscored that three out of the nine input parameters which were tested, have a really significant effect on the model outcomes. These parameters are atmospheric background CO₂ concentration, clay content and SOC while there are other parameters that hardly had any effect on the model’s results (e.g. hydroconductivity).

Chapter 5 presented an extensive validation of the modelling of European sites for a range of crops and agro climatic zones. The UK-DNDC model showed that it is capable of simulating different systems, demonstrating the value of the model; in terms of understanding the dynamics of N within crop rotations, the model has the ability to simulate
them in different agricultural soils in different regions. It can be a useful tool in identifying where and when high emissions can occur and in highlighting the effect of the management practices on emissions and exploring the impact of alternative managements on emissions.

Finally the options assessment was part of Chapter 6. In this chapter the differences in N₂O production between current/ traditional rotations (baseline) and legume based rotations in five European countries were tested. The results showed the direct effect that legume crops have in the N₂O emissions. In most of the proposed options the incorporation of legumes had a reductive effect on the production of the gaseous emissions of N₂O. There were cases in which the inclusion of legumes had as a result the increase of these emissions. This assessment highlighted that the transition to a more legume based European agriculture is not simple and straightforward. Great attention should be paid in the different soil conditions of each country and weather conditions. Through modelling it became clear that in countries that receive substantial amounts of precipitation, like Scotland, the incorporation of legumes in the system has to be done in a more careful manner.

7.2 Overall Discussion and Conclusion

Over the last decades modern agriculture has faced substantial challenges. Climate change, growth of population and the disturbed N cycle are unarguably the most considerable pressures that the planet is facing (Rockström et al., 2009). In the future, humanity will come up against a situation with massive challenges to feed earth’s constantly increasing
population (FAO, 2011). The increased demand of food globally and the high amount of protein that is required for the global food production systems have to be met in the near future. Modern agriculture has to find ways that will put it in a position to accommodate all these needs and at the same time preserve the balances within the ecosystem and minimise adverse consequences for the environment.

As mentioned before (Section 2.3.1) one of the main pressures is on the N cycle. Over the last decades the N losses from the agro ecosystems have increased due to the low efficiency of N use in the soils (Sutton, 2011). One of the main forms that these losses occur is through N₂O emissions (Smith, 2010). Nitrous oxide is one of the most important greenhouse gases that EU has set targets for 2020 and 2050 in order to minimise its production (European Commission, 2014). Legumes can play an important role in the European agriculture towards these targets as they can fix atmospheric N in the soil and they are crops rich in protein and are nutritionally important (Jensen and Hauggaard-Nielsen, 2003; Nemecek et al., 2008). The incorporation of legume crops can assist the ecosystem in various ways by minimising the use of N based fertilisers and the consumption of fossil fuels (Rispail et al., 2010). However, the representation of legume crops in Europe is poor and has been reduced by almost half over the last five decades (FAO, 2014b). These figures and trends have to change and EU will need to rely on its own legume production for food and animal feed while it is minimising negative effects of agriculture in the environment.
The work in this thesis has underlined some of the environmental implications regarding the incorporation of legume crops through modelling in European agriculture; however, it has also highlighted some of the strengths and the shortcomings of modelling with the UK-DNDC.

The model that was used for the needs of this project was UK-DNDC. UK-DNDC was developed in order to estimate greenhouse gas emissions from the UK (Brown et al., 2002) and was based in the DNDC model (Li et al., 1992). One of the main objectives of the project was to validate the model against measured data from six experiments across three different countries in Europe. One of the big challenges of this activity was to have a model which can simulate rotations from different sites from different agroclimatic zones with different crops successfully without changing the crop parameters across the sites. Moreover the available data that were used in some cases were limited and that created some difficulties on the testing and validation of the model. In general, the validation of the model showed that UK-DNDC can successfully simulate N₂O emissions from both grasslands and arable rotations. In all the sites the model predictions had a good agreement with the measured data however there were cases that the model failed to match some fine details of the measurements or some of the measured peaks. Management events like harvest or tillage showed that can enhance the gaseous N emissions.

The cumulative values of the N₂O emissions highlight the fact that the model simulations could represent the reality as expressed through measurements, in an accurate way. The average differences in the final annual values between the simulated and the measured data was around
10%. The average coefficient of determination of all the cumulative values from all the sites was around 0.88. Although the model performed well, some issues were identified regarding the model processes. Fallow fields create some challenges for the model as currently developed, to simulate productive agricultural systems. Handling of the crop residues especially from legumes was another complex situation in which the model simulations did not show a good agreement with the measurements.

The UK-DNDC model is a process based model and overall the validation testing showed that the model is useful in terms of understanding the dynamics of N within crop rotations and has the ability to simulate them in different agricultural soils in different regions.

More than the half of the protein that is consumed within Europe is imported (Crépon, 2004). The incorporation of legumes into European agriculture can be beneficial in multiple ways. The primary assumption made in this study was that legumes can offer a mitigation potential and the main objective was to examine and assess their contribution to the reduction of gaseous N emissions. In Chapter 6 the environmental implications in terms of N₂O production, of the incorporation of novel rotations which include protein rich crops (legumes) was tested. The option appraisal that was performed for five different European case studies showed interesting results.

The incorporation of legumes can have advantages in a crop rotation especially for the succeeding crop due to the fact that they are rich in N (Charles and Vullioud, 2001). The changes that were proposed in order to
move from the traditional rotations to a more legume based rotations were modest and subtle. Even with these changes the differences in N₂O production that were shown were noteworthy. In most of the case studies the legume based rotations showed that there were significant reductions in emitted N₂O in comparison with the traditional rotations that legumes were not included. Regarding the amount of fertiliser that the succeeding crop will receive the decision that was taken was that this would be unchanged aiming in higher yields. For the options appraisal site specific data were used in order to simulate accurately the options. More specifically in Sweden the reduction in N₂O emissions reached the 62% while in Italy the reduction reached up to 75%. In Germany in most of the options assessment there was a significant reduction while in Romania the gains of reduced emitted N₂O were either lower, or there were slight increases of N₂O from the legume based rotations.

The last case study in the options assessment was Scotland. The inclusion of legumes in this case showed variable results and in some cases the emissions were enhanced by the presence of legumes. The high amounts of rainfall that Scotland receives possibly created issues in the model and in handling the balance between soil processes and the emissions. In the Scottish case, NO₃ leaching was high due to the high rainfall especially with the presence of peas (Fuhrer, 2006; Carrouée et al., 2002). Due to the distinct weather conditions in Scotland further consideration of the changes should be taken in order to move in a legume based agriculture.

In general the inclusion of legumes showed some positive signs of reduced N₂O emissions. Legumes do not receive any N based fertiliser and
that highlighted the gains in reduced N\textsubscript{2}O emissions a rotation can have. UK-DNDC showed that it was performing in an acceptable way as its predictions were in close agreement in most of the cases with the IPCC approach (Knudsen \textit{et al.}, 2014). It is important to mention that UK-DNDC has not incorporated a process to simulate possible rhizobial denitrification. This study emphasized the importance of legumes inclusion in the European agriculture. It highlighted the positive potential that can have on the reduction of the gaseous N emissions; however, these changes have to be carefully chosen and applied as they can result in adverse consequences. The options appraisal shows the advantages that environmental modelling can offer as these experiments can be thoroughly tested before they applied in the field.

One of the objectives of this study was to perform a sensitivity analysis of the model using its own built –in function. It is essential the model’s sensitivity of the outputs in relation to the uncertainty of the input parameters of the model (Refsgaard \textit{et al.}, 2007b; Warmink \textit{et al.}, 2010; Pogson \textit{et al.}, 2012). Five “global” sensitivity analyses were performed, one of the default weather atmospheric data and four for the six soil characteristics. These analyses examined the influence of the input data on seven main outputs of the model namely grazed biomass, dissolved SOC, N\textsubscript{2}O, NO, N\textsubscript{2}, NH\textsubscript{3} and N leaching.

The default atmospheric data analysis showed that the atmospheric background CO\textsubscript{2} concentration is the most influential of the three tested input parameters (atmospheric background NH\textsubscript{3} concentration and N
7.2 Overall Discussion and Conclusion

concentration in rainfall) for all the outputs of the model. The outcome from the soil characteristics analyses showed that clay content and SOC were consistently the influential amongst the soil characteristics. Soil characteristics like hydroconductivity and atmospheric N deposition do not show any effect on the output values. The last analysis of the most influential input data showed that the influence of the input parameters is balanced. It is worth mentioning here that the N₂O emissions are highly dependent on the SOC value which can explained as SOC is directly linked with the soil microbial pool size. In the uncertainty analysis was clear that N₂O emissions showed a high uncertainty in all the analyses highlighting the importance of good and accurate input data.

7.2.1 Conclusion

The main question arising in this study was whether the incorporation of legumes can offer a mitigation potential for the European agriculture and the high concentrations of N₂O.

The results presented here highlighted the importance of the presence of legumes in the arable and forage rotations in five different agroclimatic regions. This thesis presents the novel approach of legume based rotations in the European agriculture while testing their sustainability in terms of N₂O production. Concurrently these changes have to be thoroughly tested for their suitability depending on the region and the climate of the area. Legumes can offer a mitigation potential without extra cost for the environment and the farmer. Structural changes have to be made in the markets and in policy making level of European Union in order to facilitate localised production and consumption of rich protein crops.
This research project has shown that the UK-DNDC is a dynamic and deterministic simulation model of carbon and nitrogen biogeochemistry in agro-ecosystems that can successfully be used for simulations for the European agriculture. It is a useful tool as it can help to predict the N hotspots as well as the possible periods of high emissions. Having this knowledge can result in more environmental sustainable experimental designs. With constant improvements and adjustments, the model can be a reliable tool in order to attempt to find solution in environmental problems in relation with greenhouse gases.

Results gathered in this study did not lead to identifying the best novel rotations that can be claimed as being the most environmentally sustainable rotations. However, the results obtained can help provide a more holistic view on the potential of such rotations. We have to move away from a situation that we are pushing ourselves and the system that we live in into an uncertain future and thoroughly question what are the boundaries that we can safely operate in. Identifying these boundaries will give us the opportunity to reconsider our actions and innovations.

7.3 Recommended Future Work and Challenges

The end of this project shows that there are certainly a lot of avenues that require further exploration. One of the most interesting directions for this research is the creation of more sophisticated and well-designed novel
7.3 Recommended Future Work and Challenges

legume based rotations. As was mentioned before in Chapter 6 the rotations that were selected for this project were based on the current/ traditional rotations of the area and these rotations underwent a minor change. In general these changes refer to either the substitution of an existing crop with a legume crop or the extension of the rotation and the addition of the legume crop in the end of the rotation. The idea behind the minor changes of the current/ traditional rotations was that these changes are more possible to be susceptible from the group of people who are directly interested the farmers and stakeholders. Novel rotations should be re-designed from the beginning, giving emphasis in 3 main directions namely, environmental sustainability of the rotation (primarily in terms of GHGs production, and maintenance or promotion of biodiversity); the gross margin for the farmers; and finally the protein needs of the population. This thesis offers a good base for understanding what should be the directions that the research should focus on in order to create novel legume-based rotations that can have a positive effect on the European agriculture.

Another potential future direction that follows directly from the discussion in chapter 4 is the further development of the built-in sensitivity analysis of the existing UK-DNDC model. The fact that the model comes with a built-in property of the sensitivity analysis is one of the advantages of the model. However, there are many aspects of this built-in property that could be upgraded and developed more in order to to tailor to specific research questions. One of the main things that can be changed is the Monte Carlo simulation of the analysis. The 50 step discrete uniform distribution for the selection of the values can change to a true Monte Carlo simulation of a total random selection of numbers within the given range with a
distribution of values that the user could choose. It would also be useful to include in the analysis, the option for the user to choose the desired distribution of the random values (normal, lognormal, uniform, logarithmic etc.). Additional aspects that could be considered for further improvements are the number of the selected parameters, the type of selected parameters and the format of the results. The number of the selected input parameters that can be included in the test has been limited to five and that is probably because the test has been set up in a certain way and more parameters would create extremely high number of runs. If the model could run the sensitivity analysis in a Monte Carlo formation that could make possible the increase on the number of parameters allowed to be changed. The type of parameters that can be changed in the analysis are the input parameters. It would be useful for the user to be able to extend the sensitivity analysis even to parameters of the code of the model in order to be able to perform a further analysis of the model. As for the results the annual values that are produced can limit the assessment of the sensitivity of the model. It would be useful to have the daily values of the outcomes of the model for more detailed analyses.

This study has highlighted many important aspects of the inclusion of legume crops in the European agriculture. However, further research could also be conducted in order to address the large gaps in measurements and create a better data profile for comparisons. Model is producing daily results while in the same time the measurements that were available for that project were not and in many cases there were large gaps between the measurements. Therefore there were situations produced from the model
that were not able to be either verified or be investigated further. It is essential that projects which include modelling activity have to be carefully designed from the beginning as that could help both agronomists and modellers. Consistent measurements on more N gaseous types could give the opportunity of further validation of the model. The sensitivity analysis of the model showed the most important input parameters of the model and the least important ones. This could also help on better allocation of resources in the project needs in order to focus on the data that matters for the modelling activity.

Finally, it would be interesting to examine the possibility of upscaling the options assessment and their N$_2$O emissions for the whole area of European Union. The current work that was presented in Chapter 6 was focused on the options assessment from NUTS2 regions in five countries in Europe. That showed us in a small scale what can be the influence of incorporation of legumes in current rotations. It would be useful to extrapolate these results and test the difference of N$_2$O emissions in a wider scale. UK-DNDC is capable of performing simulations in a regional scale and especially the UK version which is linked to UK relevant databases and making more relevant for the European agriculture. Upscaling for a wide area as Europe will definitely create some challenges. The difficulty of the challenges is depended on the nature of the research question and how detailed the upscaling of the N$_2$O production is aimed to be. Typical (baseline) rotations have to be created for all the NUTS2 regions and weather data to be collected for these areas.


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Uncertainty in the environmental modelling process: A framework and


School of GeoSciences has issued the guidance for ethical research and review and it is essential to assess the ethical concerns of the project. According to the “Guidance for Ethical Research and Review” of School of GeoSciences:

Researchers are obliged to:

1. Conduct research as capably as their knowledge permits.

2. Protect the dignity and preserve the well-being of human research participants.

3. Protect the environments in which research is conducted.

Meeting these obligations requires:
1. Respect for free and informed consent from research participants. This includes people who might be interviewed or whose property is used in research.

2. Respect for privacy and confidentiality of research participants. This respect begins with the identification of research subjects (and potentially property) and continues through analysis of data and dissemination of results.

3. Minimising the impact and possible risks of research. This applies whether the impact is on individuals, communities, or environments. It is a strong obligation when research subjects are vulnerable or when environments are particularly sensitive or of special scientific interest.

4. Protection of data to comply with agreed procedures regarding storage, archiving, and in some cases, destruction of data.

5. Operating with honesty and integrity in all our work.

From the above obligations and research requirements there are some that are not applicable in terms of ethical consideration to this project. Obligation No. 1 and requirements No. 1 and No. 2 are not applicable to the project as this research is not related to any human being and any human research. In addition obligation No. 3 and requirement No. 3 are not applicable to the specific project as the data that are used have been already collected from other projects all over Europe. There was not any laboratory work or collection of samples in that project so it was not necessary to assess further the environmental impact.
Obligation No.1 and requirement No.5 are compliances that outline protection of individuals. These compliances will be adhered to at all the times in association with good research practices. All safety precautions and risk assessment procedures have followed. With the absence of the field or laboratory work the risks that posed are limited and there are no other relevant parties associated.

As for the research regulation No. 4 all the data will be stored in an electronic form in SRUC’s servers. SRUC’s information system department follow a strategy of keeping a back-up every night of the data that are stored in the servers. That gave us a big advantage in terms of storing data and prevents the loss of the data in the event of computer systems failure. Good data storage practises will be adhered to at all the times. In that project there were no data collected or managed regarding individuals (Data Protection Act 2003).
B.1. Input file UK-DNDC

The following text shows how the dnd file (the file that is produced as an input file from UK-DNDC) is presented. The site that is associated with this input file is Foulum O2

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Appendix B: Model Input and Output

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CO2_increase_rate 0.00000

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  Clay_fraction 0.07700
  BypassFlow 0.00000
  Litter_SOC 0.01000
  Humads_SOC 0.03750
  Humus_SOC 0.95250
  Soil_NO3(-)(mgN/kg) 0.50000
  Soil_NH4(+)(mgN/kg) 0.05000
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  Lateral_influx_index 0.00000
  Field_capacity 0.480000
  Wilting_point 0.075000
  Hydro_conductivity 0.015000
  Soil_porosity 0.480000
  SOC_profile_A 0.200000
  SOC_profile_B 2.000000
  DC_litter_factor 1.500000
  DC_humads_factor 1.500000
Appendix B: Model Input and Output

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Salinity         0.000000
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Appendix B: Model Input and Output

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Appendix B: Model Input and Output

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<td>Manure_ID=</td>
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<tr>
<td>Amount/C\N_ratio=</td>
<td>533.000000 4.800000</td>
</tr>
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Appendix B: Model Input and Output

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Method= 0
Plastic_applications= 0
Ventilation= 0
Flood_number= 0
Leak_type= 1
Water_control= 0
Leak_rate= 0.000000
  Water_gather= 1.000000
  WT_file= None
  Empirical_parameters= 0.000000 0.000000 0.000000 0.000000 0.000000 -107374176.000000
Irrigation_number= 0
Irrigation_type= 0
Irrigation_Index= 0.000000
Grazing_number= 0
Cut_number= 0
YearID_of_a_cycle= 4
Crop_total_Number= 1
Crop_ID= 1
  Crop_Type= 11
  Plant_time= 5 8
  Harvest_time= 12 31
  Year_of_harvest= 1
  Ground_Residue= 0.000000
  Yield= 44.439999
  Rate_reproductive= 0.000000
  Rate_vegetative= 0.000000
  Psn_efficiency= 0.000000
  Psn_maximum= 0.000000
  Initial_biomass= 12.500000
  Cover_crop= 0
  Perennial_crop= 0
  Grain_fraction= 0.010000
  Shoot_fraction= 0.450000
  Root_fraction= 0.540000
  Grain_CN= 33.000000
  Shoot_CN= 33.000000
  Root_CN= 50.000000
  TDD= 2500.000000
  Water_requirement= 300.000000
  Max_root_depth= 1.000000
  N_fixation= 4.000000
  Vascularity= 0.000000
Tillage_number= 3
Tillage_ID= 1
  Month/Day/method= 4 15 2
Tillage_ID= 2
  Month/Day/method= 4 24 2
Tillage_ID= 3
  Month/Day/method= 5 7 2
Fertil_number= 0
FertilizationOption= 0
Manure_number= 1
```

245
Appendix B: Model Input and Output

Manure_ID= 1
Month/Day= 4 15
Amount/C\N_ratio= 428.000000 4.000000
Type= 4
Method= 0
Plastic_applications= 0
Ventilation= 0
Flood_number= 0
Leak_type= 1
Water_control= 0
Leak_rate= 0.000000
Water_gather= 1.000000
WT_file= None
Empirical_parameters= 0.000000 0.000000 0.000000 0.000000 0.000000 -107374176.000000
Irrigation_number= 0
Irrigation_type= 0
Irrigation_Index= 0.000000
Grazing_number= 0
Cut_number= 0
Crop_model_approach 0

0

B. 2. Output file UK-DNDC

B.2.1. Annual Report Output

The following text shows how the .txt file of the annual report of the site in the outputs looks like. The site that is associated with this annual report file is Foulum O2.

ANNUAL REPORT: Site Foulum_O2_28yrs Year 1 Thu May 17 14:36:44 2012

-----------------------------------------------

SOIL SECTION: Unit kg C or N/ha
-----------------------------------------------

SOM pools  ----Litter----  ----Humads----  ----Humus----  ----Total----
C  N  C  N  C  N  C  N
Day 1  608  6  2279  207  57885  5262  60772  5476
Day 365  863  11  2274  207  57807  5255  60944  5473

-----------------------------------------------

Inorganic N pools in kg N/ha
Appendix B: Model Input and Output

<table>
<thead>
<tr>
<th></th>
<th>NO3-</th>
<th>NH4+</th>
<th>NH3(w)</th>
<th>Urea</th>
<th>NO(w)</th>
<th>clay-NH4</th>
<th>N-gases</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Day 1</td>
<td>2.03</td>
<td>0.14</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.09</td>
<td>0.00</td>
<td>2.26</td>
</tr>
<tr>
<td>Day 365</td>
<td>46.92</td>
<td>0.79</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>1.92</td>
<td>0.00</td>
<td>49.64</td>
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</tbody>
</table>

Fluxes

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<tr>
<th>Fluxes</th>
<th>C (kg C/ha/yr)</th>
<th>N (kg N/ha/yr)</th>
</tr>
</thead>
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<tr>
<td>Inputs</td>
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<td></td>
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<tr>
<td>Manure</td>
<td>220.50</td>
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<tr>
<td>Shoot litter</td>
<td>325.97</td>
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<tr>
<td>Root litter</td>
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<tr>
<td>Rain-N deposit</td>
<td>2.90</td>
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<tr>
<td>Irrigation N input</td>
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</tr>
<tr>
<td>Fertilizer-N</td>
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</tr>
<tr>
<td>Soil N fixation</td>
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<td>NH3 deposition</td>
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<td></td>
</tr>
<tr>
<td>Outputs</td>
<td></td>
<td></td>
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<td>Soil-CO2 emission</td>
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<td>CH4 emission</td>
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<td>DOC leached</td>
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<td>0.09</td>
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<tr>
<td>Crop N uptake from soil</td>
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<td></td>
</tr>
<tr>
<td>NO3- runoff</td>
<td>0.06</td>
<td></td>
</tr>
<tr>
<td>NO3- leaching</td>
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<td>NH3 volatilization</td>
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<td>0.40</td>
<td></td>
</tr>
<tr>
<td>NO</td>
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<td></td>
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<tr>
<td>N2</td>
<td>0.09</td>
<td></td>
</tr>
</tbody>
</table>

Mineralization: 507.4 kg C/ha and 34.8 kg N/ha; Soil C/N ratio: 11.1

<table>
<thead>
<tr>
<th>Depth (cm)</th>
<th>kg C/kg</th>
<th>kg C/ha</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 - 10</td>
<td>0.0153</td>
<td>20382</td>
</tr>
<tr>
<td>10 - 20</td>
<td>0.0150</td>
<td>19705</td>
</tr>
<tr>
<td>20 - 30</td>
<td>0.0131</td>
<td>12516</td>
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<tr>
<td>30 - 40</td>
<td>0.0110</td>
<td>6049</td>
</tr>
<tr>
<td>40 - 50</td>
<td>0.0091</td>
<td>2292</td>
</tr>
</tbody>
</table>

CROP SECTION: Unit kg C or N/ha

<table>
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<tr>
<th>Cropping season</th>
<th>1</th>
<th>2</th>
</tr>
</thead>
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<tr>
<td>Crop name</td>
<td>Barley</td>
<td>Grass</td>
</tr>
<tr>
<td>Planting date</td>
<td>112</td>
<td>1</td>
</tr>
<tr>
<td>Growing days</td>
<td>119</td>
<td>365</td>
</tr>
<tr>
<td>Growing season TDD</td>
<td>1003</td>
<td>2508</td>
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<td>Water demand (mm)</td>
<td>336.40</td>
<td>328.58</td>
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<tr>
<td>Water stress</td>
<td>0.36</td>
<td>0.74</td>
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<tr>
<td>Crop N demand</td>
<td>101.64</td>
<td>109.94</td>
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<tr>
<td>Crop N from soil</td>
<td>20.75</td>
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<tr>
<td>Crop N from air NH3</td>
<td>1.01</td>
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<tr>
<td>Crop N fixation</td>
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<tr>
<td>Nitrogen stress</td>
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</table>

Annual crop biomass production:
### Appendix B: Model Input and Output

<table>
<thead>
<tr>
<th>Crop N (kg N/ha)</th>
<th>21.76</th>
<th>5.13</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crop C (kg C/ha)</td>
<td>1152.77</td>
<td>207.48</td>
</tr>
<tr>
<td>-- Grain C</td>
<td>749.30</td>
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</tr>
<tr>
<td>-- Leaf+stem C</td>
<td>230.55</td>
<td>95.44</td>
</tr>
<tr>
<td>-- Root C</td>
<td>172.92</td>
<td>112.04</td>
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<tr>
<td>Photosynthesis (kg C/ha)</td>
<td>5990</td>
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<tr>
<td>Shoot respiration</td>
<td>945</td>
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<tr>
<td>Root respiration</td>
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<td>Crop NPP</td>
<td>1360</td>
<td></td>
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<tr>
<td>NEE</td>
<td>-735</td>
<td></td>
</tr>
<tr>
<td>Stubble (kg C/ha)</td>
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</tr>
<tr>
<td>Fruit cut (kg C/ha)</td>
<td>0</td>
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</tr>
<tr>
<td>Leaf cut (kg C/ha)</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Stem cut (kg C/ha)</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Root cut (kg C/ha)</td>
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<td>0</td>
</tr>
<tr>
<td>Grazed biomass (kg C/ha)</td>
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</tr>
<tr>
<td>Livestock demand for grass biomass (kg C/ha)</td>
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</tr>
</tbody>
</table>

---

**WATER SECTION: Unit mm water/year**

| Precipitation | 556.00 |
| Irrigation    | 0.00   |
| PET           | 624.12 |
| Transpiration | 226.8968 |
| Soil evaporation | 229.7013 |
| Run off       | 2.59   |
| Leaching      | 20.27  |
| Change in soil water | 76.55 |
| Deep water pool | 35.94 |
| Mean wind speed (m/s) | 2.00 |

---

### B.2.2. Soil N output

The following tables show how the excel file of the outputs looks like.

The site that is associated with this input file is Foulum O2
Table B.1: UK-DNDC results in an excel file for the soil N in the first year (continues in the next page).

<table>
<thead>
<tr>
<th>Day</th>
<th>Crop</th>
<th>Urea</th>
<th>N uptake kg N/ha/day</th>
<th>N pools (kg N/ha)</th>
<th>NH4+ exchange</th>
<th>NO3- exchange</th>
<th>NH4+ exchange</th>
<th>NO3- exchange</th>
<th>NH4+ exchange</th>
<th>NO3- exchange</th>
<th>NH4+ exchange</th>
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<th>NH4+ exchange</th>
<th>NO3- exchange</th>
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<td>0.06</td>
<td>0.66</td>
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<td>0.08</td>
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Appendix C

Cumulative Graphs

Cumulative Time Series Graphs

The following graphs are the cumulative time series representation between measured and modeled values of the validation process (Chapter 4)
Figure C.1: Cumulative N₂O emissions time series between modeled and measured from Bush in 2006 from the 1st treatment

Figure C.2: Cumulative N₂O emissions time series between modeled and measured from Bush in 2008 from the 2nd treatment
Appendix C: Cumulative Graphs

Figure C.3: Cumulative N₂O emissions time series between modeled and measured from Bush in 2008 from the 3rd treatment

Figure C.4: Cumulative N₂O emissions time series between modeled and measured from Bush from 2006 from the 4th treatment
Figure C.5: Cumulative N$_2$O emissions time series between modeled and measured from Bush from 2006 from the 2$^{nd}$ treatment.

Figure C.6: Cumulative N$_2$O emissions time series between modeled and measured from Easter Bush in 2006.
Appendix C: Cumulative Graphs

Figure C.7: Cumulative N₂O emissions time series between modeled and measured from Easter Bush in 2007.

Figure C.8: Cumulative N₂O emissions time series between modeled and measured from Easter Bush in 2008.
Appendix C: Cumulative Graphs

Figure C.9: Cumulative N₂O emissions time series between modeled and measured from Foulum C4 in 2007

Figure C.10: Cumulative N₂O emissions time series between modeled and measured from Foulum O2 in 2007
Appendix C: Cumulative Graphs

Figure C.11: Cumulative N₂O emissions time series between modeled and measured from Foulum O4 in 2007

Figure C.12: Cumulative N₂O emissions time series between modeled and measured from Tulloch T3 in 2006
Appendix C: Cumulative Graphs

Figure C.13: Cumulative N₂O emissions time series between modeled and measured from San Marco Argentano for 2011

Figure C.14: Cumulative N₂O emissions time series between modeled and measured from San Marco Argentano for 2010