Sustainable biomass supply chain optimization-
Bioethanol and bio-electricity production

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Energy Engineering and Management

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Abstract

The transportation sector, with its high consumption of fossil fuels, stands as a good sector for energy improvements through the introduction of alternative and sustainable energy sources, by means of electric cars and bifuel vehicles.

The present work deals with the development of a mathematical model to optimize a biomass supply chain (SC) to produce bioethanol and bio-power. The base of this study is to improve the works of Zamboni et al. [1,2], Giarola et al. [3] and d'Amore and Bezzo [4]. Multi-period and spatially explicit features are embodied in a Mixed Integer Linear Programming (MILP) framework to optimize a multi-echelon SC simultaneously in terms of economic (Net Present Value, NPV) and environmental performance (greenhouse gases emissions), considering biomass cultivation, transport, conversion into bioethanol or bio-power, distribution and final usage in alternative vehicles. Bioethanol and bioelectricity SCs are assessed considering corn, stover, Arundo Donax, Miscanthus, Poplar and wood residues as possible biomass feedstock to multiple first and second generation conversion technologies. The environmental analysis is done not only based on the CO_2 emissions related to all the Life Cycle stages of the operation, but also by measuring the environmental impacts under different Life Cycle Assessment (LCA) methodologies (*ReCiPe, Ecological Scarcity 2013, EDIP 2003, EPS 2000* and *Impact 2002+*), to understand how the SC structure is affected by different impact evaluation methods.

It was possible to see that the sustainable production of energy to feed the transport infrastructure can be done in a profitable way both for the investors and for the final users, and this economic performance was enhanced by the implementation of new biomass types, although in terms of environmental performance it did not bring noticeable improvements. It was verified that the method used to assess the environmental impacts affects not only the economic performance, but also the SC configuration.

Key words: bioenergy supply chain, bio-power, bioethanol, optimization, sustainability

Resumo

O setor dos transportes, com o seu elevado consumo de combustíveis fósseis, destaca-se como um bom sector de melhorias de energia através da introdução de fontes de energia alternativas e sustentáveis, por meio de carros elétricos e veículos de biocombustível.

O presente trabalho lida com o desenvolvimento de um modelo matemático para otimizar a cadeia de abastecimento de biomassa para produzir bioetanol e bio-electricidade. A base deste estudo serão os modelos desenvolvidos por Zamboni et al. [1,2], Giarola et al. [3] e d'Amore e Bezzo [4], para o desenvolvimento de um modelo multi-período e espacialmente explicito para otimizar a cadeia de abastecimento simultaneamente em termos económicos (Valor Líquido Actualizado) e desempenho ambiental (emissões de gases de efeito de estufa), considerando-se o cultivo de biomassa, transporte, transformação em bioetanol e bio-electricidade, distribuição e uso final em veículos alternativos. A produção de bioetanol e bio-eletricidade será avaliada considerando milho, resíduos de milho, Arundo Donax, Miscanthus, Álamo e resíduos de madeira como possíveis matérias-primas para serem utilizadas em várias tecnologias de conversão de primeira e segunda geração. A análise ambiental será feita não só com base nas emissões de CO_2 relacionadas com todas as etapas da Avaliação do Ciclo de Vida da operação, mas também através da medição dos impactos ambientais por diferentes metodologias (*ReCiPe, Ecological Scarcity 2013, EDIP 2003, EPS 2000* and *Impact 2002+*) para compreender como a estrutura da cadeia de abastecimento é afetada pela utilização de diferentes métodos de avaliação de impacto.

Foi possível concluir que a produção sustentável de energia para alimentar o sector dos transportes pode ser feita de uma forma rentável, tanto para os investidores e para os utilizadores finais, e este desempenho económico foi melhorado pela implementação de novos tipos de biomassa, embora em termos do desempenho ambiental não tenham trazido melhorias assinaláveis. Verificou-se ainda que o método utilizado para avaliar os impactos ambientais afeta não só o desempenho económico, mas também a configuração da cadeia.

Palavras chave: Cadeia de abastecimento de bioenergia, bio-electricidade, bioetanol, otimização, sustentabilidade

Table of contents

List of figures

List of Tables

List of Acronyms

AFV – Alternate Fuel Vehicle

BEV – Battery Electric Vehicle

BRICS – Brazil, Russia, India, China and South Africa

C+R – Combustion and Rankine Cycle

CHP – Combined Heat and Power

DGP – Dry Grind Process

DDGS – Distillers Dried Grains with Soluble

EU – European Union

EV – Electric Vehicle

FCEV – Fuel Cell Electric Vehicle

G+MCI – Gasification and Internal Combustion Engine

G+TG – Gasification and Turbo Gas Cycle

GHG – Greenhouse Gases

HEV – Hybrid Electric Vehicle

IEA – International Energy Agency

LCA – Life Cycle Assessment

LCEP – Ligno-Cellulosic Ethanol Process

LCIA – Life Cycle Impact Assessment

MILP – Mixed Integer Linear Program

NPV – Net Present Value

OECD – Organization for Economic Co-operation and Development

PHEV – Plug-in Hybrid Electric Vehicle

SC – Supply Chain

USA – United States of America

1. Introduction

1.1 Context

Energy requirements worldwide have been increasing for the past years due to the exponential growth of the world's population and the development of global economy, mainly in the emergent countries [5]. Nowadays, the energy market is mostly based on fossil fuels, which represent 80% of the primary energy demand [6]. This consumption of fossil fuels can lead to an unsustainable economic and environmental situation, due to the increase in petroleum price, the possible depletion of resources, and the climate changes caused by Greenhouse Gases (GHG) emissions [5].

The transport sector is one of the major consumers of fossil fuels [6], so the transportation sector stands as a leading sector when energy improvements are the target. This problem can be solved by two different approaches: 1) by reducing the overall energy consumption by applying energy savings programs, which are focused on the development of more efficient products and processes; 2) based on the utilization of renewable energy sources as a substitute [7]. When applying the second approach, to the transportation sector, this can be made in two different ways: 1) by replacing the fossil fuels for biofuels (fuels produced from biomass); 2) by the use of electric vehicles, having in mind that the production of such electricity should be from renewable sources as well, namely bio-power which is produced from biomass [8].

Bioethanol is the biofuel which presents the highest consumption worldwide, and can be produced from several different raw materials such as corn, sugarcane, wheat and sugar beet. This biofuel has been commercialized attaining good results in the European Union (EU), the United States of America (USA) and especially in Brazil [9]. The electric vehicles market is also growing, supported mainly by hybrid-electric cars.

Promoting the aforementioned alternatives to the transportation sector, many studies have been presented in the literature in order to optimize the energy SCs structures. In this sense, several models have been developed regarding the production of bio-power and the production of bioethanol individually, aiming to optimize the entire SC.

One of the models has been presented by d'Amore and Bezzo [4]. This mathematical model aims to optimize the bioenergy SCs for ethanol and electricity production, both in terms of economic (NPV) and environmental performances (GHG emissions). The aforementioned model included the whole SC, from the upstream SCs, with raw material extraction to the downstream, where the final consumer needs were taken into account in the optimization.

In this study of d'Amore and Bezzo [4] the SC is optimized considering only corn and stover as biomass feedstocks. For a better comprehension of the subject, further biomass types should be added to the model, so that stronger conclusions regarding bioenergy SCs can be taken. Therefore, this thesis builds on the previous work considering a wider range of possible biomass sources: Arundo Donax, Miscanthus, Poplar and forestry wood residues. The economic performance will be evaluated in terms of the SC NPV and of the end user potential savings in purchasing and driving an alternate fuel vehicle (AFV) instead of a traditional one. The environmental impact will be primarily assessed in terms of GHG emissions, by considering the impact of the GHG emissions of each single life cycle stage of the operation. Other impact assessment methods, that consider different types of indicators other than GHG emissions, will be applied (*ReCiPe, Ecological Scarcity 2013, EDIP 2003, EPS 2000* and *Impact 2002+*) in order to understand how the SC design and economic performance are influenced by the methodology chosen.

1.2 Objectives

This thesis aims to assess if the sustainable production of bioenergy to supply the vehicles market can be competitive. To do so, two objectives should be fulfilled: study the profitability and environmental impact of a bioenergy SC that has bioethanol and bio-power as outputs, considering several different biomass feedstocks and conversion technologies; and to understand the influence of using different environmental impact assessment techniques on the SC design.

These objectives can be characterized as intermediate goals:

- Identifying the problem:
  - Analyze energy and renewable energy supply around the world and its trends
  - Characterize the different types of biofuels, production policies and global market
  - Analyze the bioethanol market, production processes and SC
  - Analyze the bio-power market, production processes and SC
  - Analyze electric vehicles market and trends
- Literature review:
  - SC management
  - SC design
  - Sustainable SCs
  - Bioethanol SCs
  - Bio-power SCs
- Model development and data collection:
  - Creation of an optimization model based on the models developed by Zamboni et al. [1, 2], Giarola et al. [3] and d'Amore and Bezzo [4], implementing new biomass types as possible feedstock and the new environmental methods
  - Collection and analysis of data required to achieve the desired solutions
- Model application
  - Obtain results for the different scenarios
  - Analysis of the results

1.3 Methodology

This section presents the adopted methodology in this thesis. The main steps are presented in Figure 1.

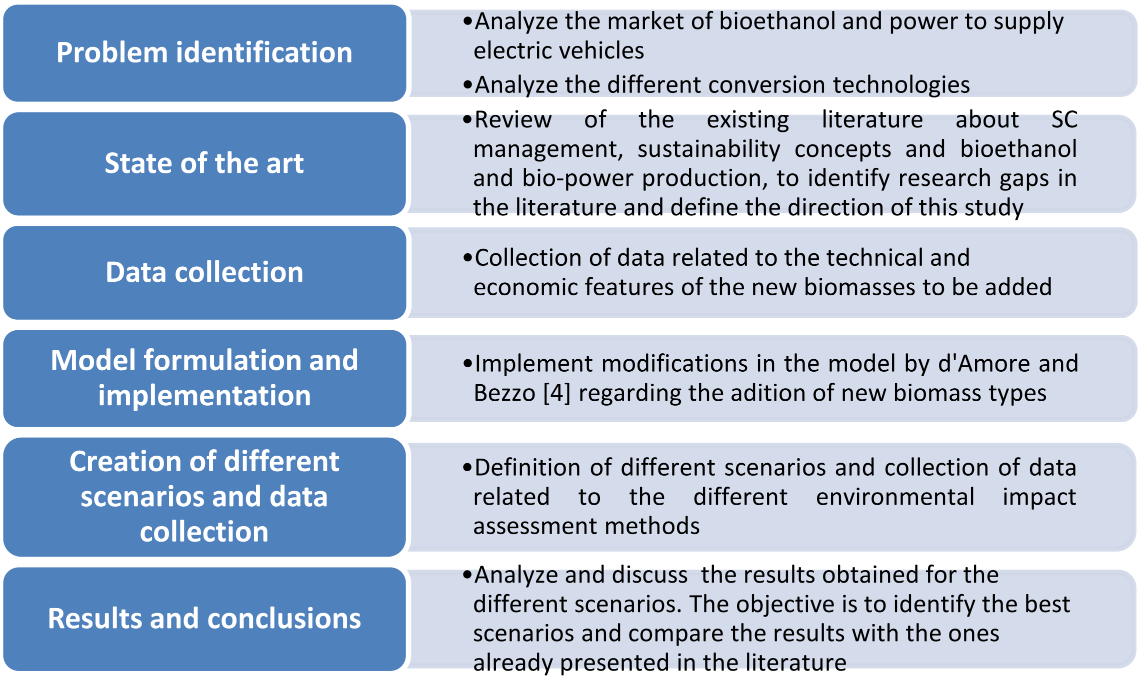


Figure 1 – Methodology to follow in the thesis

1.4 Structure of the thesis

This thesis is presented in seven main chapters:

- The first chapter consists of an approach of the problem studied and the objectives of this project;
- The second chapter comprises a contextualization of the global energy supply and the renewable energy sources as an alternative to fossil fuels. Biomass based sources are presented as a promising alternative. Biofuels classification, production and consumption policies, and global market are analyzed in this chapter. Production processes and global market of bioethanol and bio-power, the main focus of this work, are also presented in this chapter;
- In the third chapter, a review of the literature is presented. Concepts such as SC management and sustainability were analyzed. It also displays a review on the models developed regarding bioethanol and bio-power SCs;
- The fourth chapter contains the model overview and mathematical formulation, as well as the data collected and the assumptions made;
- Fifth chapter presents the resolution of the problem, analysis and interpretation of the results obtained, regarding the economic and environmental optimizations of the SC;
- The sixth chapter presents the results related to the environmental optimization considering several different impact assessment methods, as well as the study of their influence on the final SC structure and economic performance.
- The seventh chapter presents a sensitivity analysis to the prices of power and ethanol;
- The last chapter reveals the main conclusions of this thesis, as well as some ideas for future developments.

2. Bioenergy Market Characterization

In this chapter bioethanol and bio-power are presented as an energy source. A characterization of the renewable energy global market is presented, in order to give the context of the problem to be studied. In section 2.1 a global analysis of the energy market is presented, considering primary energy supply and consumers. An overview of the renewable energy sources and global market is presented in section 2.2. In section 2.3 the different types of biofuels are discussed, regarding their classification and global market. Section 2.4 regards bioethanol, analyzing the global market and describing the production processes. In section 2.5 an analysis about bio-power is made, starting at the global market analysis, presenting the electric vehicles as possible consumer, and describing some of the bio-power production processes. The last section, 2.6, sets the final conclusions of this chapter.

2.1 Energy Market

Energy is present in every activity, playing a huge role in the modern society. It is one of the bases of the economic and social development. Energy needs are increasing worldwide, mostly because of the population growth and economic expansion, mainly in the emergent countries [10, 11]. Due to this economic and demographic growth, it is expected that, from 2009 to 2035, the energy demand worldwide will increases 40%, from 12132 to 16961 Mtoe [12].
From Figure 2 it is possible to conclude that there is an increase in global demand, supported by a huge market of fossil fuels. This growth of fossil fuels consumption can lead to an unsustainable economic and environmental situation, due to the possible depletion of resources, the increase in petroleum price and the GHG emissions produced by the production and use of such fuels [13]. Anticipating this scenario, renewable energy sources have been presented as a sustainable alternate way for energy generation [13].

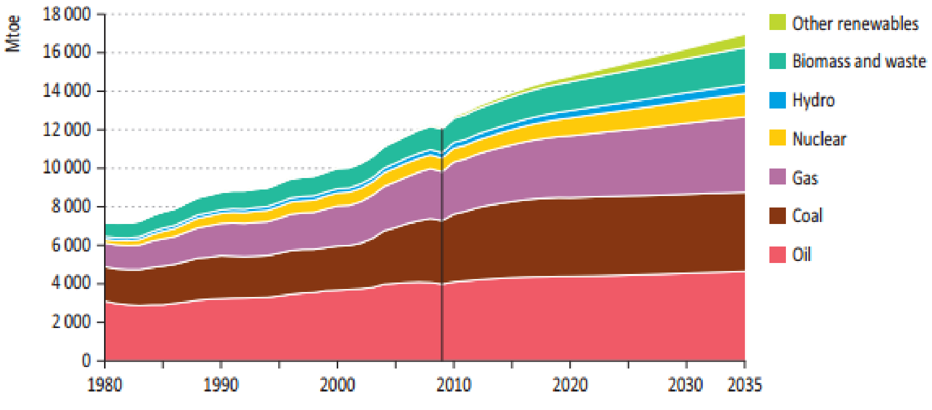


Figure 2 - World primary energy demand by fuel, 1980-2035 [12]

Oil has the biggest share among energy sources, and within oil consumption the transport sector is the most relevant. Today fossil fuels take up to 80% of the primary energy consumed in the world, of which 58% alone is consumed by the transportation sector [14]. Forecasts predict that energy demand in the transportation sector will increase 43% to reach 3260 Mtoe by 2035 [12]. This means that transportation sector has a huge influence in the oil market, as it is possible to verify in Figure 3.

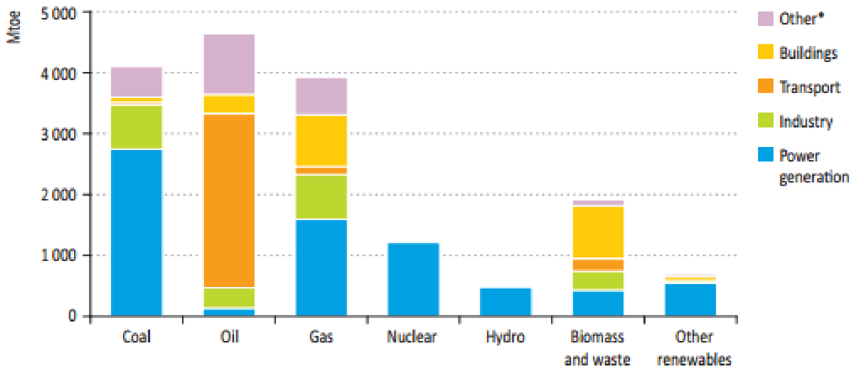


Figure 3 – World primary energy demand by fuel and sector in 2035 [12]

The use of fossil fuels as energy source is creating a huge impact in world's climate, causing the increase of global warming, due to the GHG emissions, which leads to severe negative effects including climate change, receding of glaciers, rise in sea level, loss of biodiversity, etc [14]. Reports state that since 1970, GHG emissions from the energy supply sector have grown by over 145%, while those from the transport sector by over 120% [14]. GHG emissions are strictly related to energy consumption, and as said before the energy consumption will only increase. This situation demands a sustainable development strategy that does not compromise future generations.

Accordingly, transportation is a good sector to attain energy improvements towards a sustainable development.

In this sense there are two different approaches that can be considered. The first one is related to the reduction on the dependency in fossil resources. This strategy consists on the reduction of the energy consumption by applying energy savings programs, which are focused on the development of more efficient products and processes. The second strategy to achieve this goal is based on using renewable energy sources as a source of replacement of fossil fuels [7].

2.2 Renewable energy

Renewable energy sources can be defined as clean sources of energy that minimize environmental impacts and are sustainable, based on current and future economic and social needs [11]. There is a broad variety of renewable sources, like biomass, hydropower, geothermal, solar, wind and marine energies. Renewable energy technologies are known to be less competitive than the traditional energy production mainly due to their high maintenance costs and low conversion levels. Nonetheless, renewable energy sources have several advantages, such as the decrease in dependence on fossil fuel resources and the reduction in GHG emissions to the atmosphere and climate changes [7].

The market of renewable energies is predicted to grow over the future years. Forecasts expect an increase from a share of 18% to 30-80% of the total energy generation in 2100 [11].

This outlook is strongly influenced by the commitment made by BRICS, USA and EU, by implementing several policies regarding climate changes, promoting the growth of renewable energy sources.
Total primary energy demand from biomass in 2015 was approximately 16,666 TWh. The bioenergy share in total global primary energy consumption has remained steady since before the year 2005, at around 10% [8]. Bio-power capacity increased by an estimated 5 GW in 2015, to a total of 106 GW globally. Bio-power generation followed this growth, from 429 TWh in 2014 to about 464 TWh in 2015. Worldwide, the biggest producers were the United States, Germany, China and Brazil [8].
As mentioned before, the transport sector is a major contributor to the climate changes, which makes it a good target to apply policies regarding the growth on the renewable energies market.
Energy generated from biomass stands as the source with most potential to challenge oil in short-term as a substitute to gasoline or diesel in the transportation sector [6]. Biofuels are fuels generated from biomass, and their production has been promoted by several governmental policies, as they appear as a plausible substitute for fossil fuels. Yet, the transport sector can also be improved in environmental terms, by introducing hybrid vehicles that run both on electricity and petroleum products.
The renewables share in transportation sector remains small. Renewable energy represented 3.5% of global energy demand for road transport in 2013, up from 2% in 2007. Liquid biofuels represent the bulk of the renewable share. Biofuels' contribution to the transport sector is significant in some European countries, in the United States, and in Brazil, where renewable energy accounted for an estimated 4% of global road transport fuel in 2015. Advances in new applications and markets for biofuels will continue. In 2014, commercial flights in Norway and Sweden were fueled by aviation biofuel, and airlines in several other countries announced aviation biofuel supply agreements or plans to integrate aviation biofuel into future flights.
Beyond liquid biofuels, other pathways for the integration of alternative energy sources into transportation were developed, and renewables can also be used in the form of electricity for trains, light rail, trams, and road electric vehicles. The electrification of the transport sector broadened, with the number of electric passenger vehicles on the road nearly doubling from 350000 in 2013 to 665000 in 2014 [8].
The use of electric vehicles empowers "the integration of renewable energy into the transport sector, but only to the extent that the associated electricity demand is met with new renewables, as electric vehicles are only as "renewable" as their power source" [8].

These two approaches of the use of biofuels and the use of electric vehicles powered by electricity from renewable sources, to change the transportation sector, will be presented in the next sections.

2.3 Biofuels

Biofuels are nothing new, they have been around as long as cars have. Rudolf Diesel, inventor of the diesel engine, originally designed an engine to run on vegetable oil. In the beginning of the 20th century, Henry Ford originally designed a car to run on ethanol. However, petroleum based fuel originally won out the market over biofuel because of cost. During the World War II, the demand for biofuel increased once again as fossil fuels became less abundant. The popularity of this fuel went up during the energy crisis of the nineteen-seventies and finally established its position in the market in the nineteen-nineties in response to tougher emissions standards and increasing demands for enhanced fuel economy [15].

Biofuels are combustible materials directly or indirectly derived from biomass, commonly produced from plants, animals and micro-organisms but also from organic wastes [16]. They can be solid, such as fuelwood, charcoal, and wood pellets; or liquid, such as ethanol, biodiesel and pyrolysis oils; or gaseous, such as biogas (methane) [6].

In order to analyze the different types of technology and feedstock used in biofuels production, next section presents the classification of diverse biofuel types.

2.3.1 Biofuels classification

Biofuels can be produced in different ways depending on their source of raw material or the technology adopted. They can be classified into primary and secondary biofuels. Primary biofuels concern a raw utilization, they are used in an unprocessed form, primarily for heating, cooking or electricity production such as fuelwood, wood chips and pellets. Secondary biofuels require the transformation of the biomass into bioethanol, biodiesel or others. Secondary biofuels can be classified in first, second and third-generation, depending on the raw material and technology used for their production [6], as it is possible to see in Figure 4.

First-generation biofuels are made from sugar, starch, vegetable oil or animal fats and requires a relatively simple process to produce the final fuel product. The basic feedstock is often seeds or grains. First-generation biofuels were first acknowledged as the most appropriate solution for a short-term gasoline substitution and rapidly assumed a leader position within the biofuels market. However recent concerns on environmental degradation and economic sustainability are bringing these practices to a debate. On one hand, the economic feasibility of the first-generation technologies depends deeply on feedstock supply costs, on the incomes coming from by-products as well as governmental incentives. On the other hand, there is the competition for the land and water with the food sector [3].

Second-generation technologies appear as the answer to the concerns raised about first-generation biofuels. Second-generation biofuels are generally produced from lignocellulosic biomass, which are non-edible feedstocks. The main advantage of using this generation of biofuels is that it limits the competition between food versus fuel, associated with the first-generation ones. The feedstock involved in the process can be bred specifically for energy purposes, increasing production per unit land area, which will further increase land use efficiency compared to first-generation biofuels [6]. Nonetheless, several problems relate to these technologies: the high conversion costs and complex logistics, the soil quality exhaustion and the competition with other agricultural uses or industries such as electricity generation [3].

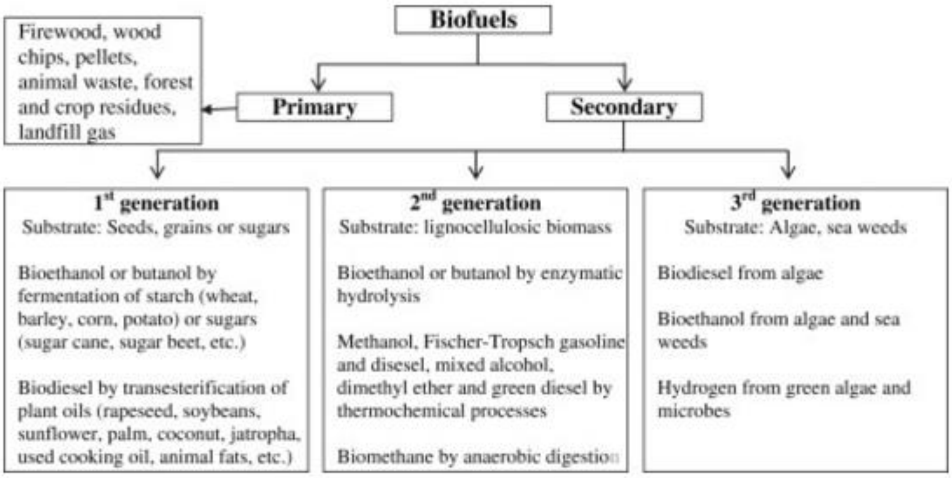


Figure 4 – Biofuels classification scheme [6]

Third-generation biofuels, derived from microbes and microalgae, are considered to be a viable alternative energy resource that avoids the major drawbacks associated with first and second-generation biofuels. As with everything, algae have a down side. Algae, even when grown in waste water, require large amounts of water, nitrogen and phosphorus to grow. So much that the production of fertilizer to meet the needs of algae used to produce biofuel would produce GHG emissions that were saved by using algae based biofuel to begin with. It also means the cost of algae-base biofuel is much higher than fuel from other sources [6, 17].

2.3.2 Biofuels global market

Governments around the globe have supported the growth of the biofuels production as substitute of fossil fuels in the transport sector, by implementing policies that influence different steps of the biofuel SC.

In USA significant financial incentives have been offered for biofuel manufacturers, which have led this country to be the largest bioethanol producer. There is a law that imposes that at least 136 billion liters of fuel have to be produced per year by this sector until 2022. From this volume, 57 billion liters have to be produced by conventional biofuels (>20% GHG savings, compared to gasoline) and the other 79 from advanced biofuels (>50% GHG savings, compared to gasoline). Besides this law there are many incentives implemented by this country such as tax credits and import tariffs [18, 19, 20].
Brazil has the most developed and integrated biofuels program in the world. Its initiation dates back to the oil crisis of the 1970s. Brazil's ethanol is recognized as the most price-competitive biofuel in the world. In 2006, 83% of the automobiles sold were flex-fuel. This situation was helped by the implementation of a regulation that imposes a minimum 25% of bioethanol blended in gasoline by 2003. Nowadays, there are no direct subsidies for ethanol production. The government maintains preferential treatment of the ethanol industry compared to gasoline producers. Since 2004 ethanol does not face any excise tax and federal duties are much higher for gasoline [9].

France and Germany are the major biodiesel producers and their biofuel consumption is mainly driven by blending mandates established by the EU. Several policies have been applied to guarantee a minimum market share to biofuels, the goal was 5.75% by 2010 and 10% by 2020. These goals were not met, so the EU revised the policies, declaring an overall 10% share of renewable energies in final energy demand within the transport sector for all member states by 2020. The policies also outline mandatory sustainability criteria, considering minimum savings of GHG emissions, aiming at a 6% reduction of GHG emissions from fuels consumed in the EU by 2020 [18].

In October 2012, the European Commission published a proposal to minimize the climate impact of biofuels, considering:

- To increase the minimum GHG saving threshold for new installations to 60%
- To limit the amount of food crop-based biofuels and bioliquids that can be counted towards the EU's 10% target for renewable energy in the transport sector by 2020, to the current consumption level, 5% up to 2020, while keeping the overall renewable energy and carbon intensity reduction targets;
- To provide market incentives for biofuels with none or low indirect land use change emissions, and in particular the 2nd and 3rd generation biofuels produced from feedstock that do not create an additional demand for land [21].

In 2014, there was an agreement to cap at 7% the contribution of biofuels and bioliquids produced from cereals and other starch-rich crops, sugars, and oil crops to the EU-wide renewable transport fuel target (10% of total transport fuel); this compares with the European Commission's 2013 recommendation of a 5% cap [8].

These incentives have led to a huge growth in the biofuels market, as it can be seen in Figure 5. Bioethanol is the largest biofuel produced. Global production of fuel ethanol grew from 30.8 billion liters in 2004 to 76 billion liters in 2009 at an average annual growth rate of 20%. The two leading producers, the US and Brazil, accounted for about 88% of the total in 2009 [22].

The production of bioethanol increased from around 17 to 86 billion liters since the beginning of the century while the biodiesel increased from 0.8 to around 21 billion liters [23].

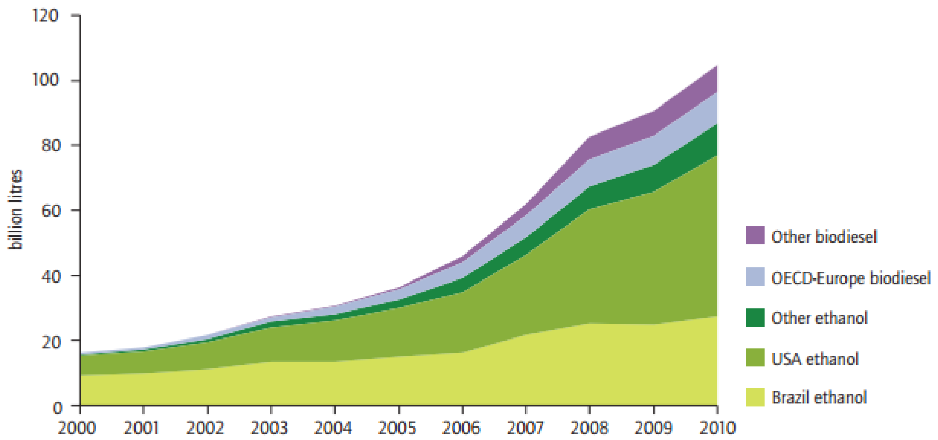


Figure 5 – World biofuel production evolution [24]

Global production of fuel ethanol had an average annual growth rate of 20% between 2004 and 2009, going from 30.8 billion liters in 2004 to 76 billion liters in 2009. In 2006, the US surpassed Brazil, the longtime leader, to become the leading fuel ethanol producer in the world by producing over 18 billion liters (20% more than the previous year). Although total production of biodiesel around the world remains small in comparison to ethanol, with an increase from 2.3 billion liters in 2004 to 17 billion liters in 2009, it reached an average annual growth rate of approximately 50% [22].

The International Energy Agency (IEA) predicts that the biofuels demand will rise exponentially until 2050, as shown in Figure 6.

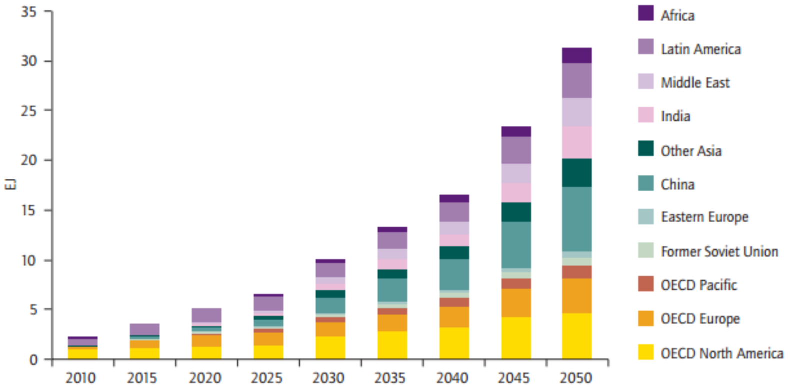


Figure 6 – Global biofuel demand by region 2010-50 [24]

Forecasts show that demand for biofuels will increase worldwide and that North America will always have high share in the global market. It is expected that in 2050, China will be the largest consumer and that other regions follow towards the same direction due to the continuous incentive policies and the need to change.

Summarizing, bioethanol is the largest and the most influent biofuel produced around the world. Taking this into account, in the next section an analysis on its global market and on the elements of its SC will be done.

2.4 Bioethanol

Bioethanol is a product derived from the fermentation of biomass, and it can be used directly in cars or blended with petroleum products [6]. Its use is a way to reduce both consumption of crude oil and the environmental impacts caused by the GHG emissions [25].

Bioethanol is the most used biofuel in the transport sector. A liter of ethanol contains 66% of the energy provided by the same volume of petrol. However, it has a higher octane level, and when mixed with petrol for transportation the bioethanol improves its performance. Ethanol also improves the fuel combustion in vehicles, by that reducing the emission of carbon monoxide, unburned hydrocarbons and carcinogens [6].

Being bioethanol the major type of biofuel it is interesting to understand how its market is distributed.

2.4.1 Bioethanol global market

Global bioethanol production has been increasing in the past years, as it is possible to see in Figure 7. Brazil and the USA are the two major ethanol producers, accounting for 26.72% and 56.72% of the world production, respectively. The production of bioethanol is mainly depended on sucrose from sugarcane in Brazil or starch, mainly from corn, in USA [26].

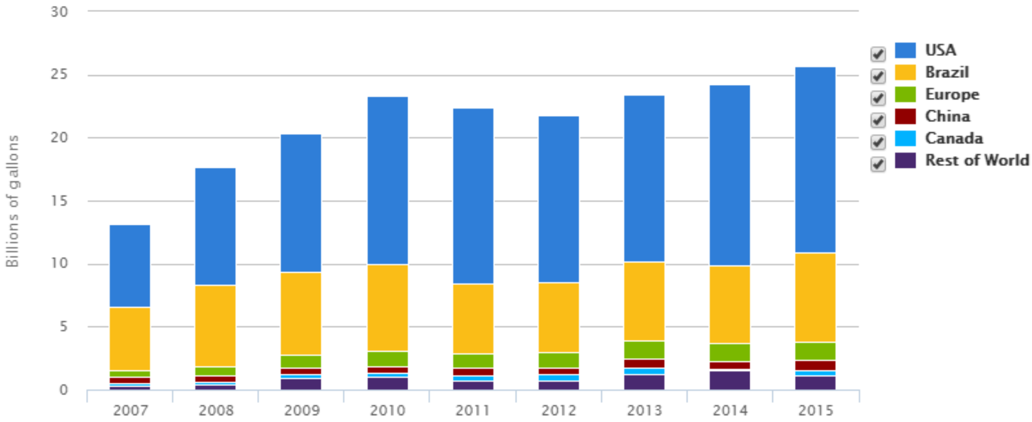


Figure 7 – Global ethanol production 2007-15 [27]

One of the goals of bioethanol production is to reduce the dependency on fossil fuels, as stated before. This can be made by blending the bioethanol with petrol. This mixture can have various levels, in the EU, if the car does not suffer any modification, the amount of bioethanol blended is typically 5% but can actually go up to 10%, or even 85% (E85) if the engine is modified to a flex-fuel type. This situation also occurs in the USA where 10% (E10) is usually the level of mix between bioethanol and gasoline. Brazil is the country that presents more developments in this area since about 83% of all cars sold are flex-fuel which allows drivers to run on gasoline or on ethanol [20, 28].

2.4.2 Production processes

As previously mentioned, bioethanol can be classified in first, second and third-generation, depending on raw materials which lead to different processes applying different technologies in its production. The production processes will be described in the following points.

First-generation

First-generation bioethanol has two main feedstock types: sugarcane in tropical areas such as India, Brazil and Colombia, while it is dominantly corn in other areas such as the United States, European Union, and China. Ethanol production from sugar crops accounts for about 40% of the total bioethanol produced and about 60% corresponds to starch crops. The availability and feasibility of using corn as a feedstock is in stake, due to its increase in demand as a food source and its rising price, which can limit the use of first-generation feedstock for ethanol production.

Ethanol production can be summed into the major three steps: (1) to obtain the solution containing fermentable sugars, (2) conversion of sugars into ethanol by fermentation and (3) ethanol separation and purification [29].

The most common bioethanol production process used with conventional corn-based is known as dry grind process (DGP), which is commonly used as a reference. In this process the raw material is transformed in ethanol and a co-product, Distillers Dried Grains with Soluble (DDGS), which is a valuable animal feeder. A diagram of this process is presented in Figure 8.

In the first plant section, the corn is milled down to the proper particle size in order to facilitate the water penetration. The mixture reacts in a slurry tank where sterilization is achieved. During this process starch hydrogen bonds are broken so that water can be absorbed. The next step is liquefaction where the viscosity of the mixture is reduced by the action of enzymes. This mixture is cooled down and then conducted to a fermentation reactor where a simultaneous saccharification and fermentation occurs: starch oligosaccharides are almost completely hydrolyzed into glucose molecules.

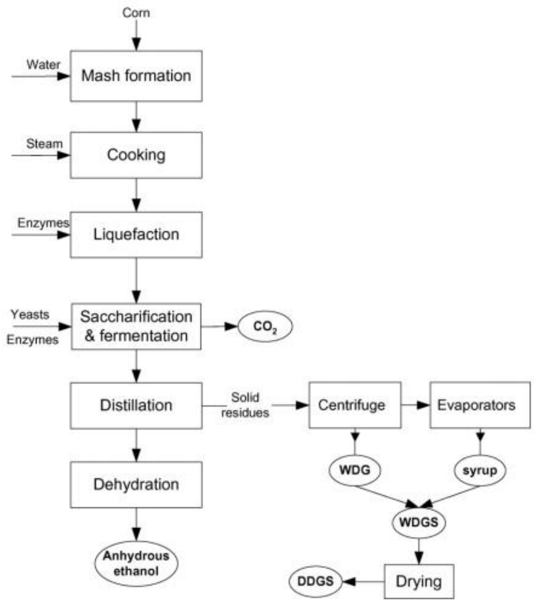


Figure 8 – Flowsheet of the dry grind process [30]

Then a distillation section is presented, which involves three distillation columns: the fermentation broth is split into two stripping columns at different pressure. The distillate products of these columns are sent to a final rectifying column where bioethanol is produced with high purity.

The non-fermentable products of the feedstock, consisting of grain solids, dissolved material and water, are sent to a centrifuge where a wet cake and a *thin stillage* are obtained. This *thin stillage* is sent to an evaporator where it is concentrated into final solid, *syrup*. The wet cake and the *syrup* are mixed and dried up in order to produce DDGS [30].

Second-generation

Second-generation fuels use, frequently, non-edible lignocellulosic biomass, which includes agricultural residues, grasses, and forestry and wood residues. Cellulosic feedstock is composed of cellulose, hemi-cellulose, lignin, and solvent extractives [29].
The overall conversion of lignocellulosic biomass to ethanol production process includes five main steps: biomass pre-treatment, cellulose hydrolysis, fermentation, separation and effluent treatment, as shown in Figure 9.

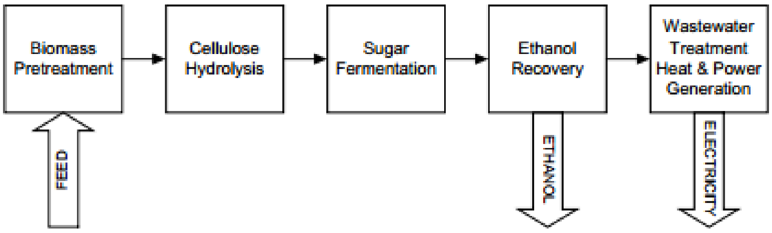


Figure 9 - Conversion of lignocellulosic biomass to ethanol [31]

During biomass pre-treatment, the structure of cellulosic biomass is altered, lignin seal is broken, hemicellulose is reduced to sugar monomers and cellulose is made more accessible to the enzymes.
The next step is the cellulose enzymatic hydrolysis, i.e. the cellulose conversion into fermentable glucose by means of cellulose, a complex mix of enzymes. The broth is then ready for sugar fermentation, where the simultaneous saccharification and fermentation process is usually preferred as it allows higher ethanol yields with lower amounts of enzyme required.
Ethanol is then obtained by conventional distillation, residual solid is collected in the distillation bottoms and can be burned as fuel to power the process [31, 32].

In the end user's perspective, the blending of bioethanol with gasoline is not the only solution considered in this thesis. Another way to surpass the problem exposed is by means of utilizing electric cars, which should be powered by renewable sources. To do so, there is the possibility to produce electricity from biomass. The details about bio-power market and production processes are presented in the next section.

2.5 Bio-power

Bio-power is the generation of electricity using biomass as a source and it can be produced by several different processes [33]. In the next sections these production processes will be presented, as well as bio-power's global market.

2.5.1 Bio-power global market

Electricity can be generated from many sources, which can be renewable or not. The share of electricity sources in 2015 can be seen in Figure 10:

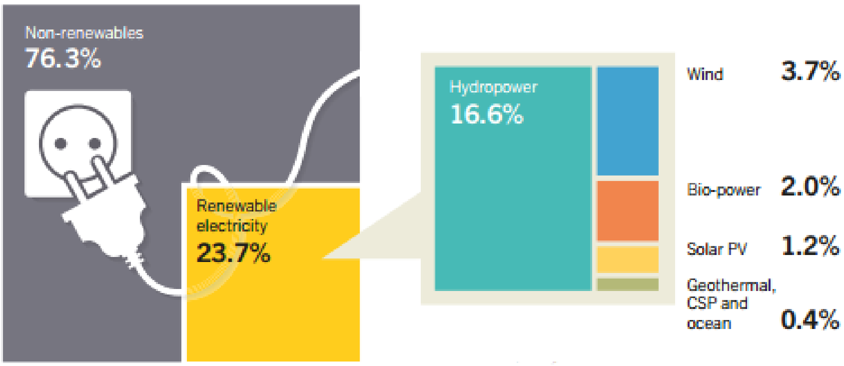


Figure 10 - Estimated Renewable Energy Share of Global Electricity Production in 2015 [8]

The most significant renewables growth in 2015 occurred in the power sector, with global renewable power capacity reaching an estimated 1,849 GW at year's end, an increase of 9% over 2014.
As Figure 10 shows, 2% of global electricity produced in 2015 had biomass as a source. Bio-power capacity increased by 5 GW in 2015, bringing the global total to approximately 106 GW. Bio-power generation also increased, from an estimated 429 TWh in 2014 to about 464 TWh in 2015.
This growth can be strongly associated with the role of the bio-power generation leader countries: United States, Germany, China, Brazil, and Japan [8].

	Global	EU-28	BRICS[1]	China	United States	Germany	Japan	India	Italy	Spain
TECHNOLOGY	GW			GW						
Bio-power	106	36	31	10.3	16.7	7.1	4.8	5.6	4.1	1

Figure 11 - Renewable electric power global capacity, top regions and countries in 2015 [8]

As shown in Figure 11, USA was the country with the highest installed capacity of 16.7 GW, which resulted in a production of 69.3 TWh. Although the United States continued to lead global bio-power generation and capacity, only 0.6 GW was added in 2015. Germany installed capacity adds up to 7.1 GW total capacity, most of which relies on biogas, lead them to produce 50 TWh of electricity with biomass as source. In 2015, China's bio-power capacity increased by 0.8 GW to 10.3 GW, to produce 48.3 TWh. Most of the total (about 53%) was from agricultural and forestry products, and from municipal solid waste (about 45%). Brazil's bio-power sector has seen continuous market growth. An estimated 250 MW of new capacity brought Brazil's total to 9.7 GW in 2015, leading Brazil to produce 32.9 TWh in that year. Japan's capacity reached 4.8 GW, producing 36 TWh.

As it can be seen in Figure 11, about 39% of all bio-power installed capacity held by the EU, and the BRICS countries have a share of 31%. The USA by itself represents an installed capacity of about 17% [8].

The European Commission has issued non-binding recommendations on sustainability criteria for biomass, applied to energy installations of at least 1MW electrical power [34]:

- the use of biomass from land converted from forest, other high carbon stock areas, as well as highly biodiverse areas is forbidden
- biofuels should emit at least 35% less GHG over their life cycle, when compared to fossil fuels. For new installations this amount rises to 50% in 2017 and 60% in 2018
- favor national biofuels support schemes for highly efficient installations
- encourage the monitoring of the origin of all biomass consumed in the EU to ensure their sustainability.

Consumers

The bio-power can be applied in several areas. Considering the purpose of this work, the bio-power produced is supposed to supply an increasing demand in electric vehicles (EVs) market. There are three main types of electric cars, depending on the degree of electrification: hybrid electric vehicles (HEV), that are already on the roads, they add an electric traction motor and battery bank to a smaller version of the existing internal combustion engine to provide two sources of motive power; plug-in hybrid electric vehicle (PHEV) that has batteries that can be charged from the grid while parked, so some gasoline use is replaced with electricity; the final step in this electrification evolution is an all-electric vehicle that has the purpose to eliminate the internal combustion engine, there are two all-electric vehicles types, the fuel cell electric vehicle (FCEV) powered by hydrogen and the battery electric vehicle (BEV) that would depend exclusively on the electrical grid for all its energy [35]. Forecasts predict a growth in the electric vehicles market, as Figure 12 shows.

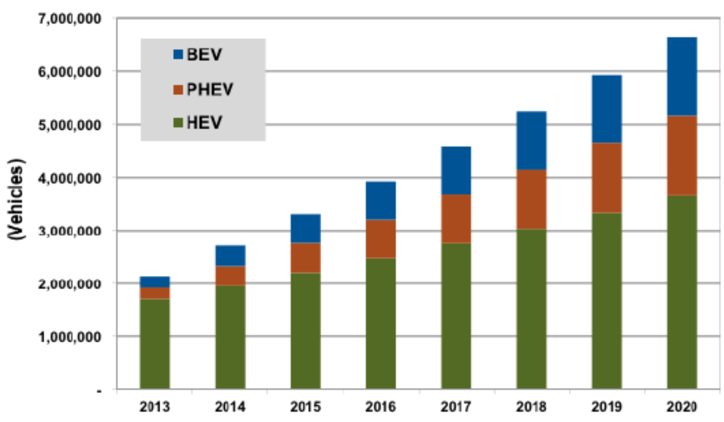


Figure 12 - Annual electric vehicle sales by vehicle type, 2013-20 [36]

HEV will have the biggest share among electric vehicle sales in the next years. However, BEV and PHEV will see their importance in the market increasing.

This growth in the electric vehicles market is a consequence of the several measures and policies made by the government to stimulate the market. This stimulation comes through incentives such as: tax deduction or tax credit for the purchase of the vehicle, sales tax exemption, vehicle emissions test exemption, registration tax exemption and parking fee reduction or exemptions [37].

2.5.2 Production processes

There are three primary processes with different technologies used to produce bio-power from biomass [33, 38]:

1) Pyrolysis - the thermal destruction of biomass in the absence of oxygen, without the addition of steam or air, to produce gases and condensable vapors. Combustion of these gases occurs in a gas turbine, typically combined cycle.

2) Gasification - biomass is partly oxidized to produce combustible gases, which have a high calorific value. Product gases are fed into a combined cycle gas turbine power plant, or internal combustion engines.

3) Direct combustion - the complete oxidation of biomass to produce hot flue gases that are used to heat process water to steam, which drives a turbine, typically via a Rankine cycle.

Direct combustion is the oldest and simplest, but most inefficient technology. Gasification and pyrolysis have higher efficiencies, however they require more process control and investment [33].

Technically, gasification is a pyrolysis process [38], and it is not as commonly used as combustion or gasification [33]. Given this and the maturity of the technologies, this thesis will focus on gasification and direct combustion.

Combustion

As stated before, combustion is a process that presents a low efficiency, of about 30% [33]. Biomass firstly undergoes pretreatment steps, such as drying, grinding or the removal of metal constituents. It is then fed into a boiler, where direct fire combustion of biomass happens, producing hot flue gases, which then produce steam in the heat exchange section of the boiler. The steam is then expanded to a low temperature and pressure through to a steam turbine where electric power is generated [39], as it is shown in Figure 13.

The high-pressure steam is produced in a boiler, the core of the system.

Stokers are designed to feed fuel onto a grate where it burns with air passing up through it. The stoker is located within the furnace section of the boiler and is designed to remove the ash residue after combustion. Stoker units use mechanical means to shift and add fuel to the fire that burns on and above the grate located near the base of the boiler.

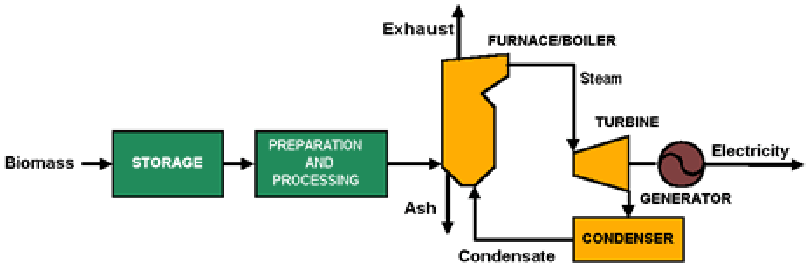


Figure 13 – Direct combustion of biomass diagram [40]

In fluidized bed, fuel is burned in a bed of hot inert, or incombustible, particles suspended by an upward flow of combustion air that is injected from the bottom of the combustor to keep the bed in a floating or "fluidized" state. The scrubbing action of the bed material on the fuel enhances the combustion process by stripping away the CO_2 and solids residue (char) that normally forms around the fuel particles. This process allows oxygen to reach the combustible material more readily and increases the rate and efficiency of the combustion process.

The fluidized bed boiler has several advantages, comparing with the stoker. Fluidized bed has a bigger area of combustion, a faster mass transfer rate and the excess air is easier to control, which translates into a higher efficiency. The emissions on the fluidized bed are also lower than the ones of the stoker. As a downside, the fluidized bed is much more expensive than the stoker boiler [39].

Gasification

The gasification process converts biomass into a gaseous mixture called syngas, that consists mainly of H_2, CO, CO_2, N_2, small particles of char, ashes, tars and oils.

The gasification process starts by drying the biomass. The feedstock is then fed to a gasifier, where the different stages of gasification happen, using steam as an oxidant agent. The stages are: heating and drying of solids, pyrolysis, oxidation or partial combustion of some gases and finally reduction or gasification of the char. The result of this process is a gas made up mainly of CO, H_2, N_2, CO_2, H_2O and hydrocarbons. After treatment, this gas can be used cleanly in gas engines or turbines to produce mechanical or electrical energy with no waste products [41]. Figure 14 presents a flowsheet of bio-power production through a gas turbine in integrated biomass gasification facility.

There are two types of gasifiers, fluidized and fixed bed.

Fixed bed gasifiers typically have a fixed grate inside a refractory-lined shaft. The fresh biomass fuel is placed on top of the pile of fuel, char, and ash inside the gasifier. Air can flow up or down the grate, to be collected as biogas.

Fluidized bed gasifiers utilize the same gasification processes and offer higher performance than fixed bed systems, but with greater complexity and cost. Similar to fluidized bed boilers, the primary gasification process takes place in a bed of hot inert materials suspended by an upward motion of oxygen deprived gas. As the amount of gas increases to achieve greater throughput, the bed will begin to levitate and become "fluidized". Notable benefits of fluidized bed devices are their high productivity (per area of bed) and flexibility [39, 41].

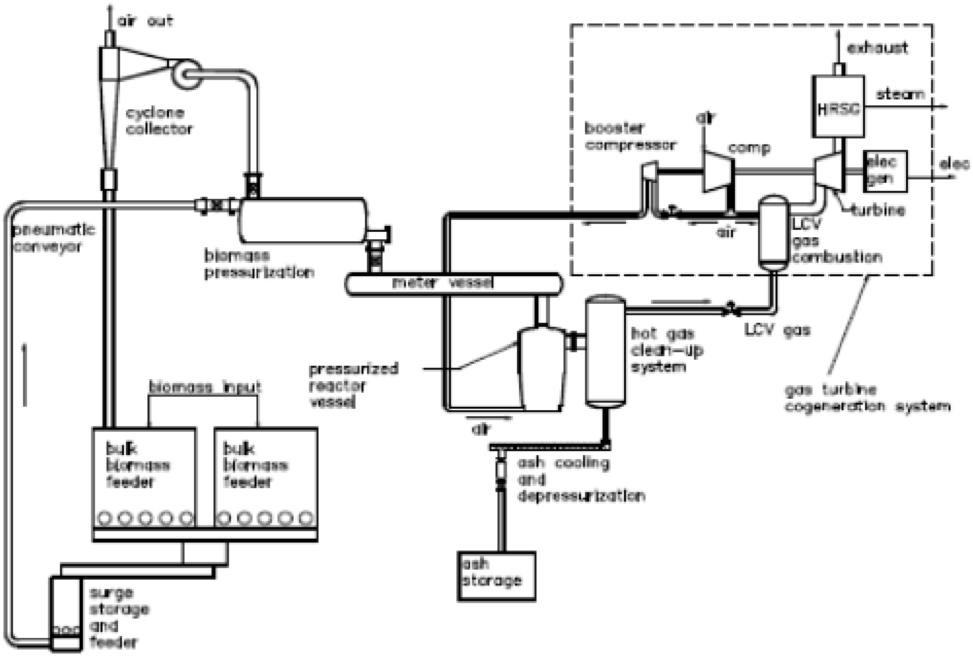


Figure 14 – flowsheet of bio-power production through a gas turbine in integrated biomass gasification facility [39]

2.6 Chapter conclusions

The dependency on fossil fuels in the world energy demand is a problem, not only because of resource scarcity, but also because of the climate changes provoked by their production and use. Efforts have been made to supply the energy demand using alternative sources. Policies are being applied by several governments in order to promote these alternatives, and the transport sector is one of the principal targets.

There are two main ways to modify the transport sector: changing the vehicles from internal combustion engines to electric cars; or changing their type of fuel, where biofuels come as a good alternative.

Biofuels can be classified in primary and secondary, and secondary biofuels can be categorized in first, second or third generation, depending on the raw material and production technology.

Considered as a promising substitute of petroleum products, bioethanol is the largest biofuel produced worldwide, and its market is expected to keep growing in future years.

Following this idea, it is possible to produce electricity from biomass, bio-power that can feed the needs of electric cars growing market.

In this work the two referred approaches are combined in one, since the objective is to develop a model to optimize the design of a bioenergy SC that has biomass as input and bioethanol and bio-power as output, having in consideration not only the economic aspects, but also environmental.

3. State of the art

This chapter presents a literature review about the scientific background required to develop this dissertation.

In section 3.1 the SC concept is presented, along with the three different types of SCs. Subchapter 3.2 presents a review of the models developed in the literature about SC design. In section 3.3 the concept of sustainability is shown, as well as the importance of its connection with SC management. A literature review of existing models related to sustainable SCs is presented. Section 3.4 offers a literature review of the papers developed regarding the design of bioethanol SCs. Lastly, section 3.5 exposes an analysis of the works done in the field of bio-power SCs and section 3.6 presents the chapter conclusions.

3.1 Supply chain

A SC is a network of suppliers, manufacturing plants, warehouses, and distribution channels organized to acquire raw materials, convert these raw materials to finished products, and distribute these products to customers [42].

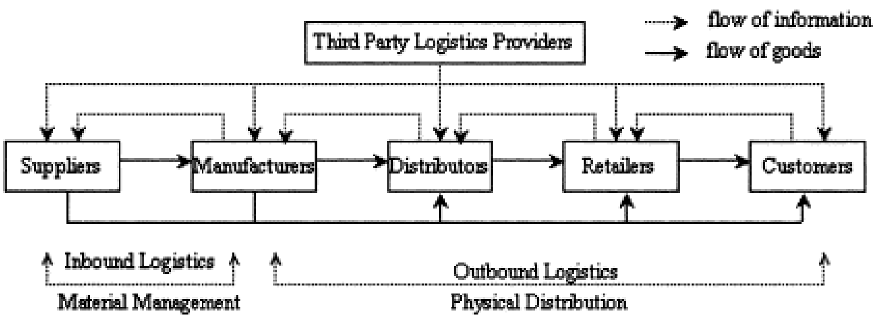


Figure 15 – Supply chain process [43]

As it is possible to see in Figure 15, a SC is comprised of two main business processes: material management, which is concerned with the acquisition and storage of raw materials, parts, and supplies; and physical distribution, which contains all outbound logistics activities related to providing customer service [43].

A SC design problem comprises the decisions regarding the number and location of production facilities, the amount of capacity at each facility, the assignment of each market region to one or more locations, and supplier selection for sub-assemblies, components and materials [41].

In today's global marketplace, individual firms no longer compete as independent entities, but as integral part of SC links. Therefore, the success of a firm will depend on its ability to integrate and coordinate the network of business relationships among SC members [43].

SCs can be classified in three different types, according to the modelled flow: forward flow, which ends at the final customer; reverse flow, which starts at customers and ends in factory/recovery plants; and finally, closed loop SCs, which considers simultaneously forward and reverse flows [44].

A SC can be described as an integrated system which synchronizes a series of inter-related business processes in order to: acquire raw materials and parts; transform these raw materials and parts into finished products; add value to these products; distribute and promote these products to either retailers or customers; facilitate information exchange among various business entities, such as suppliers, manufacturers, distributors, third-party logistics providers, and retailers [43].

This type of SC is characterized by a forward flow of goods and a backward flow of information.

Forward SC's objective is to improve efficiency, profitability and competitiveness of all the partners [43].

A reverse SC retrieves the used product from its final destination, in order to remanufacture, recycle or proceed with proper disposal. It includes flows for disposal, reprocessing or repacking [45].

The concern with environmental issues has been growing, particularly about energy consumption and resource limitation that may lead to consequences such as global warming and climate changes as well as resources scarcity. Therefore, companies are being forced to consider environmental aspects in different levels of their activity and SC activities are not an exception [45]. Not only an efficient forward SC is required, but also the design and management of a reverse SC should be in place. In this way, and waste prevention, material recycling, energy recovery, and disposal options should be considered in the SC design [46].

The establishment of reverse networks independently of the forward chains may result in higher infrastructure costs. In this way, it is necessary a network design and planning that contemplates simultaneously the forward and reverse flows, in order to maximize efficiency and profits [45].

Closed loop SCs are planned and designed considering reverse logistics activities simultaneously with forward SC activities. This type of SC is considered to have a huge potential in economic, social and environmental terms [45].

The main goal of SC design is to define a network that efficiently integrates suppliers, manufacturers, warehouses, and stores, so that merchandise is produced and distributed at the right quantities, to the right locations, and at the right time, in order to minimize system wide costs while satisfying service level requirements [44].

3.2 Supply chain design

Management of SCs is a complex task mainly due to large size of the physical supply network and inherent uncertainties. To achieve a successful management of a SC several decisions need to be made [44]:

- Number, size and location of manufacturing sites, warehouses and distribution centers, and the resources inside them.
- Production decisions related to plant production planning and scheduling.
- Network connectivity (allocation of suppliers to plants, warehouses to markets etc.).
- Management of inventory levels and replenishment policies.
- Transportation decisions concerning mode of transportation and also sizes of material shipments.

These decisions can be classified into three levels, strategic, tactical and operational, according to their importance and the length of the planning horizon considered. Strategic choices, with a long term planning horizon, regard the location, capacity and technology of plants and warehouses. Supplier selection, product range assignment, distribution channel and transportation mode selection belong to the tactical level and can be revised every few months. Operational level regards decisions related to flows of raw material, semi-finished and finished product in the network and are easily modified in the short term [42].

In the past, many companies based their strategic planning exercises on managerial judgments about future directions of the firm and the markets in which they compete, often ignoring SC options. However, important SC decisions have gained importance and been incorporated in these exercises, given their influence in the competiveness of the companies. This requires the development and application of: descriptive models, which are used to forecast demands, calculate manufacturing and distribution costs or project the future costs of raw materials; and prescriptive models, which are optimization models, developed from the descriptive ones, that support SC managers in taking better decisions. The most effective prescriptive models are based on linear and mixed integer programming. Companies in the chemical and oil industries have highly developed and used linear and mixed integer programming models to assist decision-making at all planning levels, due to the increasing complexity of the strategic planning problems they face, consequence of complications in crude oil markets, changes in multinational demand markets, and several other factors. Companies in other areas of business, such as in the pharmaceutical industry, turned to the use of optimization models seeking long term use of their capital equipment [47].

Many models were developed in the past years and their evolution will be presented in the next section.

3.2.1 Supply chain design modeling

The SC network design problem consists of taking the decisions previously stated to satisfy customer demands while minimizing the sum of the costs [42].

SC models can be mathematical programming or simulation-based and their application depends on problem to be solved. Mathematical programming models are used to optimize high-level decisions involving unknown configurations, taking an aggregate view of the dynamics and detail of operation [44].

A number of mathematical models have been presented in the recent literature with various features: steady-state or multi period, deterministic or stochastic [44].

Early research in this field was mainly focused on location–allocation, static models. Geoffrion and Graves [48] presented a model to solve the problem of multi-commodity distribution network design, formulated as a mixed integer linear program, applying a technique based on Benders Decomposition [49], which is a classical solution approach for combinatorial optimization problems, based on the ideas of partition and delayed constraint generation [42].

Several years later, in 1987, Brown et al. [50] presented an optimization decision algorithm used to manage complex problems contemplating facility selection, equipment location and utilization, and manufacture and distribution of products. The focus is on operational issues such as production site, production rates of each product in those sites, and from which plant product should be shipped to customer, contemplating variable costs from producing and shipping, and fixed costs of equipment and operation [44].

In 1997 Camm et al. [51] presented a methodology developed by merging integer programming, network optimization and geographical information systems. The overall problem is decomposed into a production problem and a distribution network design problem, in order to reexamine and reengineer Procter & Gamble's North American product supply, helping the company reduce the number of plants and save over 200 million dollars.

Aiming to increase the flexibility of the models, Sabri and Beamon [52] presented in 2000 a research where a multi-objective function is used to optimize simultaneously the strategic and operational planning in the SCs design problem, studying the tradeoffs among cost, customer service level and flexibility in terms of volume produced and delivery dates, so that it is possible to respond to the customer requirements under various sources of uncertainty.

In the next year, Tsiakis, et al. [53] also dealt with uncertainty, describing a MILP optimization problem considering the design of multi product, multi-echelon SC networks with fixed manufacturing sites and costumer zones. The model determines the number, location and capacity of warehouses and distribution centers, the transportation links and the flows and production rates of materials, dealing with demand uncertainty through a scenario tree where each scenario represents a different future outcome, allowing dealing with several future events. In 2008, Tsiakis and Papageorgiou [54] considered production and distribution networks, under operation and financial constraints, with special emphasis on allocation of the production and the work-load balance, duties for material flowing, production and transportation costs and considering outsourcing production when demand cannot be satisfied [44].

A year later, You et al. [55], developed a model using a two-stage stochastic linear programming approach, within a multi-period planning model that takes into account the production and inventory levels, transportation modes, times of shipments, and customer service levels. They introduced risk management models by incorporating risk measures into the model, and the tradeoffs between cost and risk are established by the implementation of multi-objective optimization [56].

In 2011, Georgiadis et al. [57] studied a model under transient demand variations. They developed a MILP problem, comprising multiproduct production facilities with shared production resources, warehouses, distribution centers and customer zones and operating under time varying demand uncertainty. This demand uncertainty was considered in terms of a number of likely possible scenarios during the lifetime of the operation, and helped to understand the effect of inventory levels in the design and operation [56]. Two years later Liu et al. [58], aiming to measure a SC performance by multiple criteria, developed a multi-objective model that considered total cost, total flow time and total lost sales as key objectives, using the ε-constraint method to tackle the multi-objective problem by generating a set of Pareto-optimal solutions [59].

The above mentioned models were designed mainly to improve the economic profit or the customer service. Nowadays there has been an increase concern with environmental issues, here is where the concept of sustainability arrives.

3.3 Sustainable supply chains

Nowadays, considering the possible depletion of non-renewable resources, companies are forced to rethink their strategies to ensure the sustainability of their operations. There are several definitions of sustainability, however there is one central concept that characterizes it, the triple bottom line approach. This concept recognizes the interdependence between three dimensions: the economic, the environmental, and the social performances of an organization [60, 61].

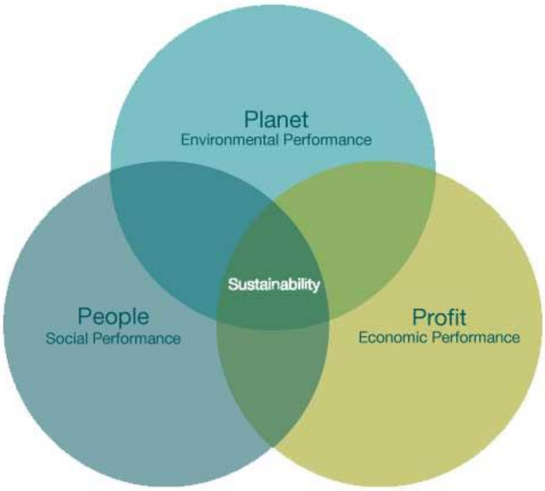


Figure 16 – Triple bottom line [62]

Considering economic sustainability, the aim of SC optimization and scheduling is to maximize the profits, by maximizing products values with minimum raw materials, inventory and production costs.

For social sustainability, products should ensure that the needs of population are met. Social sustainability focuses on both internal (employees) and external communities. It means that organizations provide equitable opportunities, encourage diversity, promote connectedness within and outside the community and ensure the quality of life.

Environmental sustainability is often related to waste and pollution reduction, minimizing the use of non-renewable resources, energy efficiency, a decrease in the consumption of hazardous materials and in the frequency of environmental accidents [63, 64].

Closed-loop SCs are one of the options considered to achieve sustainability. Other approaches include different actions related to one or more phases of the product life cycle such as product design, production planning and control for remanufacturing, inventory management, product recovery, reverse logistics and carbon emissions reduction.

Nonetheless, these actions possibly are not enough to assure long-term sustainability. In fact, recovery and re-processing of used products might not only increase operating costs but also contribute to growth in the GHG emissions [60, 61].

The triple bottom line approach is a way of connecting SCs management with sustainability, coming to the concept of sustainable SC management, which can be defined as the “management of material, information and capital flows as well as cooperation among companies along the SC while integrating goals from all three dimensions of sustainable development, i.e., economic, environmental and social, which are derived from customer and stakeholder requirements. In sustainable SCs, environmental and social criteria need to be fulfilled by the members to remain within the SC, while it is expected that competitiveness would be maintained through meeting customer needs and related economic criteria” [61].

Sustainable SCs modeling can be defined as the integration of sustainability concerns to the decisions of the SC, in order to improve and balance the economic, environmental, and social performances [65].

Most of the optimization models used in strategic network design have the goal to maximize the economic performance of the SCs. However, the concern with environmental issues has been growing and the first models tried to apply such factors at the plant level. The main drawback of these approaches was that although the negative environmental impacts will reduce somewhere in the SC, they might increase in other processes [60].

As a solution to this problem, the Life Cycle Assessment methodology was proposed. LCA is a course for evaluating the environmental impacts linked to a product, process or activity. It identifies and quantifies the energy and materials used and the waste released to the environment, and evaluates and implements opportunities for environmental improvements. The judgment considers the entire life cycle of the product, process or activity, including extracting and processing raw materials, manufacturing, transportation and distribution, maintenance, recycling and disposal [60].

Investigation and application of sustainability concepts in SCs design has been growing, in order to help companies ensure the sustainability in their operations, and a more efficient use of their resources. In this sence, several models have been developed in the past years.

In 2005, Hugo and Pistikopoulos [66] developed a mathematical programming-based methodology with the inclusion of LCA criteria, considering the multiple environmental concerns together with the traditional economic criteria, as part of the decisions related to the design and planning of SC networks. In the next year, Nagurney et al. [67] developed a model that allows for the determination of optimal carbon taxes applied to electric power plants in the context of electric power SC networks.

In 2009, Guillen-Gosalbez and Grossmann [68] presented model concerning the design of sustainable chemical SCs in the presence of uncertainty in the inventory. The model simultaneously accounts for the maximization of the net present value and the minimization of the environmental impact.

Most frequently the studies combine the economic performance with the environmental performance in order to find the trade-off between both. The economic dimension represents the cost or the profit in net present value. Several performance metrics have been developed to evaluate quantitatively the environmental impact, such as the emissions of GHG, waste generation, energy use, and material recovery. Several relevant methods were developed to quantify the environmental impacts based on the Life Cycle Impact Assessment (LCIA), based on different impact categories and weighting techniques. The methods applied in this thesis are *ReCiPe*, *Ecological Scarcity 2013*, *EDIP 2003*, *EPS 2000* e *Impact 2002+*.

EPS 2000 [69] was the first method where uncertainties were fully specified and included, and its indicator unit includes characterization, normalization and weighting. *Impact 2002+* [70] was developed aiming to enable the comparative assessment, avoiding the use of safety factors and conservative assumptions. *EDIP 2003* [71] provides spatially differentiated characterization factors for local impact categories. *Ecological Scarcity 2013* [72] weights environmental impacts, such as pollutant emissions and resource consumption, based on public policy targets. *ReCiPe* [73] integrates the problem oriented approach, which produces results with low uncertainty but high number of impact categories, with the damage oriented approach, which results in only three categories but the uncertainty in the results is higher [74].

The social criteria if often left out in the studies and mostly only potential long-term damages to human health are taken into account. However, there are some models that consider other social criteria. In 2011, You et al. [75] designed a biofuel SC considering the maximization of local employment by using a tool that allows estimating the number of direct and indirect local jobs created. Pérez-Fortes et al. [76] created a model for a biomass SC that maximizes the distribution of jobs to be created, by dispersing as wide as possible the location of the production technologies. In 2014, Mota et al. [77] presented a multi-objective mathematical programming model for the design and planning of SCs, integrating the three dimensions of sustainability. Where the economic side is considered as the SC costs, the environmental hand is assessed by applying *ReCiPe* for the first time in SC design management, and finally the social point of view at strategic level, that considers the job creation in less developed regions.

Not only industrial SCs have been the target of studies aiming to achieve economic optimization while considering sustainable principles. Regarding sustainability, as stated before, bioethanol comes as a good substitute for petrol products, and a mean to reduce the dependency on fossil fuels. In order to be a sustainable and economically competitive alternative, all the activities related to its production must be taken into account and organized in a cost effective and sustainable SC optimization model.

3.4 Bioethanol supply chain

The optimal design of the biofuels SC is crucial to ensure long term viability of such a project. In this sense, several mathematical models have been developed to optimize the bioethanol SCs, and some of them are presented in this section.

In 2008, Dunnett et al. [78] proposed a MILP based model to optimize the cost of a lignocellulosic bioethanol SC, considering a wide range of technological, system scale, biomass supply and ethanol demand distribution scenarios. A year later Zamboni et al. [1, 2] presented two papers consisting of a MILP model, designed to help the decision making process for the strategic design of biofuel SCs, that accounts for the minimization of the costs (part a) and the environmental impact in terms of GHG emissions (part b) simultaneously.

In 2010, Huang et al. [79] developed a spatial and temporal mathematical model for the strategic planning of the bioethanol SC, aiming to minimize the costs of the entire SC, from the feedstock to end users over the entire planning horizon.

In 2011, Dal-Mas et al. [80] developed a dynamic, spatially explicit and multi-echelon MILP modeling framework with the aim to help decision-makers and potential investors assessing economic performances and risk on investment of the entire ethanol SC, over the period of ten years, and under uncertainty of feedstock cost and ethanol selling price. During the same year Giarola et al. [3] presented a MILP framework to optimize the financial (net present value) and environmental (GHG emissions) performances for a hybrid first and second generation ethanol SCs. Zamboni et al. [81] proposed a multi-objective optimization model combining LCA and SC optimization in order to show how a crop management strategy can contribute to mitigate global warming in first generation ethanol.

In 2012, Akgul et al. [82] proposed a multi-objective, static modelling framework for the optimization of hybrid biofuel SCs, including the GHG savings and the impact of carbon tax in both economic and environmental performances.

In 2013, Bernardi et al. [83] proposed a multi-objective MILP modeling framework to optimize the economic and environmental performances, considering for the latter not only the carbon footprint (GHG emissions), but also the water footprint (water consumption), which was recognized as a key issue in renewable fuels production. Osmani and Zhang [84] developed a two-stage stochastic mathematical model to maximize profit, in a multi-feedstock lignocellulosic-based bioethanol SC, under uncertainty in each feedstock yield and in feedstock and selling prices. In the next year, Huang and Chen [85] developed a deterministic model to design an economically sustainable 2nd generation bioethanol SC under imperfect market competition. Santibañez-Aguilar et al. [86] presented a multi-objective, multi-period, MILP model that aims to maximize the profit of the SC, minimize its environmental impact and maximize the number of jobs generated by its implementation, considering numerous relevant issues. Lucas et al. [87] studied the influence of including different LCA methods in an optimization model for a bioethanol SC, how each one influences the final network structure and the economic results.

Not only bioethanol can be used to promote the independence of petrol, another way to do so is by the use of EVs supplied by renewable sources, as stated before. The production of power from biomass stands as a good option in this direction. In order for it to be a valid option, it should be economically viable and environmentally sustainable. Again, to achieve these two objectives all the stages must be taken into account and organized in a cost effective and sustainable SC optimization model.

3.5 Bio-power supply chain

Bio-power is also a very important output from biomass, and several models have been developed regarding its SC.

In 2004, Freppaz et al. [88] developed a decision support system to evaluate the possibility of forest biomass exploitation for thermal and electric energy production, aiming for an efficient and sustainable management of the forests. The system helps decide the plants location and size and the type of energy produced, applying a case study to a small Italian mountain area. In 2008 Reche López et al. [89] presented an optimization method to find optimal location of biomass fueled systems for distributed power generation, considering constraints such as the impact on the voltage profile. The objective was to maximize the profit as a function of the net present value of benefits from the sale of electrical energy minus the initial investment, collection, transportation, maintenance and operating costs. In the same year, Bruglieri and Liberti [90] proposed a model for planning an energy production process considering several types of biomasses as feedstock options.

In 2010, Vera et al. [91] developed a calculation tool to find the optimal size, location and supply area of an electricity plant, that offer the best profitability for the investor. After two years, Pérez-Fortes et al. [92] developed a multi objective MILP model, which takes into account economic, social and environmental objectives to solve the problem of designing and planning biomass SCs that use locally available biomass near to the point of use. The model supports decision-making about location and capacity of technologies, connectivity between the supply entities, biomass storage periods, matter transportation and biomass utilization.

In 2013, Shabani and Sowlati [93] presented a nonlinear mixed integer programming dynamic optimization model to maximize the overall value of a typical forest biomass power plant SC. The model considers biomass procurement, storage, energy production and ash management in an integrated framework at the tactical level. A year later, Pantaleo et al. [94] proposed a MILP approach to optimize multi-biomass and natural gas SC strategic design for heat and power generation in urban areas. The model focus was on spatial and temporal allocation of biomass supply, storage, processing, transport and energy conversion (heat and combined heat and power production, CHP) to match the heat demand of residential end users. In the same year, in order to examine the potential for existing power plants to act as a carbon sink as opposed to a carbon source, Akgul et al. [95] developed a mixed integer nonlinear programming model of carbon negative energy generation, considering aspects such as geographical locations of the existing power plants, electricity demand, transport logistics characteristics, supply and different types of raw materials. In 2015, Bazmi et al. [96] developed a general decentralized energy generation optimization model for developing countries, based on a mixed integer nonlinear programming model that minimizes the overall electricity generation cost, presenting decisions regarding the optimal number, locations, and sizes of various types of processing plants, the amounts of biomass transported, and electricity to be transmitted between the selected locations over a selected period. A year later, d'Amore and Bezzo [4] developed a model for optimizing the SCs for ethanol and electricity production from corn and stover, both in terms of economic and environmental performances. In that study not only the upstream SCs for the production were considered, but also the final consumer needs were taken into account in the optimization in terms of alternative vehicles market.

3.6 Chapter conclusions

This chapter presents literature review about SCs and its modeling, starting on a wide approach on SC management and design, which are the base to the chapter. There are three types of SCs, depending on the flow of material, they can be forward flow, reverse flow or closed loop SCs. SC design includes making decisions regarding the structure of the SC in order to minimize its costs and therefore increase the profits, and it can be divided in three levels according to their importance and the length if the planning horizon considered: strategic, tactical and operational.

SCs are usually planned taking into account only the economic performance. Nevertheless with the increasing concern regarding environmental issues, the concept of sustainability gained importance. Sustainability is known as the use of resources to meet the needs of the present without compromising the ability of future generations to meet their own. According to the triple bottom line approach, sustainability lies in the interdependence between three dimensions: economic, environmental, and social.

Biomass has been receiving increasing attention as a renewable resource, as a possible solution to the dependency on fossil fuels. To stand as a good solution, it must be not only economically competitive, but it must also bring environmental advantages, when compared to fossil fuels.

The study of bioenergy SCs has been the target of several studies for the years past. The majority of these studies are focused solely on one product as output. For the literature review for this work, many studies regarding bioethanol SCs and bio-power SCs separately were found, but papers regarding SCs that consider the both products as output are in reduced number. Besides that, the majority of these studies are focused only in the economic performance of the SC, disregarding the other pillars of sustainability. Moreover, the inclusion of new second generation production processes and several biomass types is also very limited. From this, it is possible to infer that there is a gap in the literature relative to the assessment of both economic and environmental performances of biomass SCs with two end products, having in consideration second generation production technologies and several different biomass types as feedstock options.

The problem addressed in this thesis is to understand the profitability and the environmental impact of the energy supply to vehicles as a final market, being the energy produced from biomass. For this bioenergy SC two end products were considered: bioethanol to be integrated in the traditional fossil fuels; and bio-power to supply electric cars. The aim is to understand how the energy SC can be the most profitable, in a sustainable way, regarding the biomass feedstock and the quantity of each product to be produced to supply the transports sector. Nevertheless, this is not the only goal of this thesis, once that most of the works developed in this field evaluate the environmental performance of the SC based on simple environmental assessment methods such as carbon emissions. In this sense, this thesis presents the application of five different methods to assess the environmental impacts of the SC, that consider other impact categories, in order to study how the SC design and economic performance is influenced by the environmental performance assessment technique chosen.

4. Energy supply chain model

Aiming to solve the problem addressed in this thesis, i.e. to study the profitability and environmental performance of a bioenergy SC that has bio-power and bioethanol as outputs that can be produced from several different biomass types in several different technologies in Northern Italy, a MILP model was developed and implemented in GAMS®.

The model developed is based on the model by d'Amore and Bezzo [4] and on the modeling approaches adopted by Zamboni et al. [1, 2] and Giarola et al. [3].

Two main approaches were developed in this work: the first one aiming to optimize the SC on economic and environmental performance adding further biomass types to the model for a better comprehension of the subject; the second part deals with the influence in the SC configuration of assessing the environmental impacts through different LCIA methods. All the developments were done based on the model developed by d'Amore and Bezzo [4].

This chapter is divided in four sections: section 4.1 presents an overview of the problem studied, defining several characteristics such as objective functions, SC structure and the main variables considered; in section 4.2 the assumptions made and the essential data collected for the model are presented; section 4.3 presents the mathematical formulation implemented in the model; lastly, section 4.4 deals with the chapter conclusions.

4.1 Problem statement

The presented model handles the strategic design and planning of an industrial SC for the production of bioethanol and bioelectricity over a 15-years time horizon. The problem is formulated as a spatially explicit multi-period and multi-echelon modelling framework, where a multi-objective optimization is executed, maximizing the economic performance (in terms of global NPV), while simultaneously minimizing of the environmental impact (in terms of overall GHG emissions). The entire network can be divided into two main substructures: (i) the upstream network, which deals with all biomass related operations, such as growth, pre-treatment and transport to the conversion facilities, and (ii) the downstream network, dealing with products production, distribution and final usage by end user, as presented in Figure 17.

This study integrates the model by d'Amore and Bezzo [4] representing the dynamic evolution of a bioethanol and bio-power SC located in Northern Italy, with the implementation of several new biomasses as feedstock options.

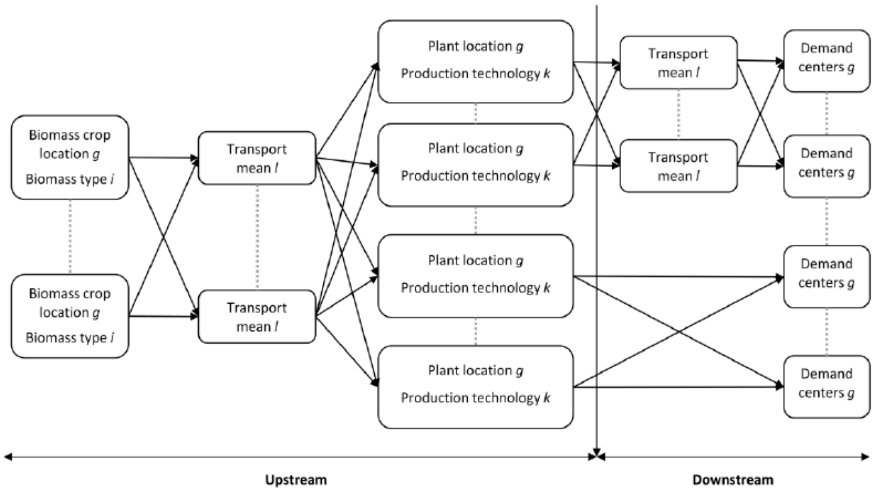


Figure 17 – Bio-power and bioethanol network supply chain [98]

The problem to address can be solved giving the following inputs:

1. Geographical distribution of ethanol demand centers;
2. Bioethanol and bioelectricity demand
3. Biomass availability and production costs in every region
4. Technical and economic parameters as function of biomass type, conversion technology and plant scale;
5. Environmental burdens for the production of each biomass type in each region;
6. Environmental burdens of bioethanol and bioelectricity production for each biomass type and conversion technology;
7. Transport logistics and allowed links;
8. Fuel distribution from terminal to end user;
9. Electricity distribution network efficiency;
10. Ethanol and electricity market prices;
11. AFVs efficiency, costs, consumptions, average distances and emissions.

The key variables to be optimized are:

1. Geographical location of biomass crops, biomass production rate and feedstock mix to the facilities;
2. Bioethanol and bio-power plants selection of technology, location and scale;
3. Characterization of transport logistics;
4. Financial performance of the industrial SC and of the end user economy over the time horizon;
5. Demands quota evolution over the time horizon (instance B);
6. Impact on global warming.

4.2 Model assumptions and data collection

This section deals with the collection and processing of data necessary to the model.

Spatially explicit feature

The geographical region addressed in this study, Northern Italy, was divided in 59 squares of 50 km of length, represented in the model by g, and one extra region (g=60) to represent the import of biomass, as it was proposed by Zamboni et al. [1].

Strategic demand

The model was run for two different instances:

- Instance A, where the demand of both bioethanol and bio-power are set *a priori*. Bio-power demand was calculated based on an averaged EVs market share retrieved from d'Amore and Bezzo [4] of 3.26% by 2030 (t=5). A linear growth-rate was implemented to describe the demand through the time period, and the number of circulating traditional car fleet in Northern Italy is assumed to be constant throughout the 15 years, according to the statistics [98]. Then the number of EVs was converted into actual electricity demand with the factor χ = 1.897 MWh/EV/year [99], which represents the electric energy required to fuel an EV for 1 year, and considering an average trip distance of 45 km/day/vehicle [100, 101]. Although the EVs market share is increasing and therefore reducing the number of bifuel vehicles circulating, the ethanol blending ($etperc_t$) grows during the 15 years period, assuming as mandatory the EU targets for biofuels described by Giarola et al. [3]. The global ethanol demand comes as a percentage of the total gasoline demand at the demand centers, as it was defined by Zamboni et al. [1]. Power demand is not described regionally, because an immediate and region-independent distribution is assumed. The demands of both ethanol and power, as well as the market penetration of EVs and bifuel vehicles are fixed for this instance.
- Instance B, where a global energy demand is set, leaving the decision to the model to calculate the production rates of each product. The global demand is fixed and it is calculated by summing bioethanol and bio-power demands that resulted from instance A.

All these values are presented in Table A1 in Appendix A.

Biomass growth

Regarding biomass cultivation, the data for spatially specific yield ($BY_{i,g}$) for corn and stover was retrieved from the papers of Zamboni et al. [1] and Giarola et al. [3]. The cultivation yields of Arundo Donax, Miscanthus and Poplar were averaged from the values found in the literature [102 – 125], and they are presented in Table A2 in Appendix A. These average values were then linked with the regions *g* according to the grid-dependent differential yields already described for corn and stover by Giarola et al. [3], in order to define the potential production fluctuations among the squares. Once the average yields for the new biomasses were obtained, calculations were made to see how the yield of corn varies for each grid element in the original model, as a fraction of the average corn yield. Then the mean values obtained for the new biomass types were multiplied for these fractions for each grid element, to find the yield of the new biomass types in the respective grid element. In other words, although considering for each biomass *i* its respective yield (according to the different values found in the literature), the dependency of each yield among the regions *g* is assumed for each new biomass the same as for corn and stover.

The implementation of wood residues in terms of biomass availability had to be done in a different way from the other biomass types, since it is not a crop, but a residue. In this sense, its availability is just related to timber production for each region and the percentage that is collected as residues. According to the literature [126, 127] the average yield of fresh biomass collected (moisture content of 60% (M60) when cut) is 0.299 ton biomass M60/m^3 timber. 60% moisture content means that the dry weight of the biomass is 40% of the wet weight [128]. According to the literature, there is an average dry matter loss during drying and storage of 17% [129]. Thus the dry biomass average yield is 0.076 ton d.b./ m^3 timber. In order to apply this yield to find the biomass availability, it was necessary to retrieve the values for yearly timber production, for the regions of Northern Italy considered in the model, from the literature [130]. Afterwards, the biomass availability was calculated for each region and each region was divided in the grid elements (*g*) according to its surface area. It was considered that the woody biomass was only available at mountain regions. The total biomass availability for each region was divided equally for the respective number of grid elements that are mountain regions, so that every grid element that belongs to a region as the same average biomass availability. The values for timber production retrieved from the literature, as well as the biomass yields for the mountain regions are presented in Table A3 and the grid elements *g* considered as mountain regions can be seen in Figure A1, both presented in Appendix A.

The amount of each biomass type that can be used for energy purposes ($quota_i$) is limited, in order to assure sustainability. The values for this parameter regarding corn and stover were obtained in the work by Giarola et al. [3] and for the new biomasses it was assumed to be equal to 1, considering that these biomasses are cultivated only with the objective to produce energy.

Biomass production costs

For the biomass unitary production costs ($UPC_{i,g}$), the values for corn and stover were also found in the works by Zamboni et al. [4] and Giarola et al. [7]. The data related to Arundo Donax, Miscanthus and Poplar was found in the literature [103, 108, 112, 116, 117, 119, 121, 122, 131 - 133] and an average of these values was calculated, as it can be seen in Table A4 in Appendix A. They were then linked to the grid regions *g* the same way it was done for the yield, but this time using the variations in the price of corn between each grid element.

Once again, forestry wood residues data cannot be processed in the same way as the other biomasses. According to the literature [128], the purchase costs of wood chips, with a moisture content of 55% (M55) at the power plants, range from 29 – 38 €/tonM55. These purchase costs represent the price that is paid for wood chips at the power plants, this means that they are calculated based on the entire wood residues supply chain. In the model, the biomass transport costs are a variable, therefore, the transport costs should not be comprised in the wood chips purchase costs. Following this logic, the transport costs, which represent 27.5% of the total costs [134], should be discounted from the purchase costs of biomass. Considering all this information, the average purchase costs of biomass with a moisture content of 55%, without transport costs, are 24.26 €/tonM55. Through Equation (1) [128] it is possible to find the relation between the dry and wet weight of the biomass, where M is the moisture content and W_w and W_0 are the biomass wet and dry weights, respectively:

$$M = \frac{W_w - W_0}{W_w} * 100 \tag{1}$$

The dry weight is 45% of the wet weight, consequently the average dry biomass purchase cost ($UPC_{i,g}$), in the units used in the model, is 53.92 €/ton d.b [128]. This value does not depend on the region, as opposed to the $UPC_{i,g}$ values for the other biomasses, so its value for the wood residues will be the same for every region.

Products market price

Market prices for ethanol, DDGS and power were set, according to d'Amore and Bezzo [4], equal to 710 €/$ton_{ethanol}$, 300 €/ton_{DDGS} and 90 €/MWh, respectively.

Transport

The transport infrastructure includes the biomass distribution, the ethanol transport form the production plants to the demand terminals and final fuel distribution. The transportation can be made by means of truck, rail, barges and ships, tans-ships were also considered as a mean of importing biomass. All the transport related parameters have been based on actual geographic distances between regions *g* and *g'* according to the procedure described in Zamboni et al.[1]. It is assumed that electricity produced is not transported, but directly sent to the grid.

Production technologies

For bioethanol production Poplar and wood residues will not be considered as a feedstock. As reported in Giarola et al. [3], three main technologies were identified in the model by d'Amore and Bezzo [4], but after running the original model and analyzing the results it was possible to conclude that Integrated Grain-Stover Process technology can be neglected, because it was never used to produce ethanol, according to the solver. Therefore only two technologies are considered in this new version of the model: the Dry Grind Process (DGP), where only corn is converted into ethanol through a biological process (*k*=1); and the Ligno-Cellulosic Ethanol Process (LCEP), that does not use corn as a feedstock (*k*=2). The conversion efficiency values for corn and stover were obtained in the work by d'Amore and Bezzo [4], and the values for Arundo Donax and Miscanthus were found in the literature [103, 105, 106, 135] and are presented in Table A5 in Appendix A.

Regarding electricity production, as it was previously done in the model by d'Amore and Bezzo [4], three technologies were considered: biomass direct combustion for Rankine steam cycle (C+R, *k* = 11); biomass gasification for Turbo Gas cycle (G+TG, *k* = 22); and biomass gasification for Internal Combustion Engine (G+MCI, *k* = 33). The data for the efficiency of each technology in converting stover into power ($z_{i,k}$) was collected from the work by d'Amore and Bezzo [4]. For the new biomasses, the values were obtained using the same methodology used in that paper, multiplying the average efficiency of the Italian National grid (0.935) and the average conversion efficiency η_k for each technology *k*. The average conversion efficiency was obtained according to the following equation:

$$Cap_{elec} = \frac{PR.f_c}{\eta_k.LHV_{fuel}} \quad (2)$$

Where *PR* is the electricity generation, Cap_{elec} the biomass input, *fc* is the load factor (assumed to be 8000 h/year), and considering the average values for Lower Heating Value (LHV) for the different biomasses found in the literature [103, 112, 128, 136 - 139]. The values for the different LHVs and conversion efficiencies are presented in Table A6 in Appendix A.

In order to calculate the investment needed to build the plants and the production costs both for ethanol and power, the production plants sizes were divided in six capacity intervals *p*, shown in Table A7, as it was done by d'Amore and Bezzo [4].
Table A8 presents the value of the investment needed to build the plants, and in Table A9 the data related to production costs is exposed, following the work by d'Amore and Bezzo [4].

Environmental performance

As stated before, this thesis contemplates two different environmental performance assessment approaches, the first one was based only on the GHG emissions of all the activities present in the model, and the second one uses five different LCIA methods to measure the total environmental impact: *ReCiPe, Ecological Scarcity 2013, EDIP 2003, EPS 2000* and *Impact 2002+*.

First approach: GHG emissions

The set of LCA stages *s* considered in the evaluation is given by biomass growth (*bg*), biomass pre-treatment (*bpt*), biomass transport (*bt*), bioethanol production (*fp*), bio-power production (*epow*), bioethanol transport (*fd*), fuel distribution (*fdist*), bifuel vehicles usage (*ebifuel*), EVs usage (*ecars*), batteries production (*ebat*) and, emission credits (*ec*) in terms of GHG saving.

It is assumed that the carbon dioxide emissions from the combustion of biofuels by the vehicles and from the combustion of biomass syngas offset the carbon dioxide captured during crop growth.

For the environmental evaluation, the GHG emissions of all these stages are taken into account. All the values for the emissions related to corn and stover, as well as the ones related to bioethanol transport and fuel distribution were retrieved from the work by d'Amore and Bezzo [4]. The emission factors related to biomass pre-treatment for the new biomasses were calculated following the same assumptions made by Giarola et al. [3]. Biomass transport emissions were considered the same as for corn and stover, for the new biomasses, and their values were obtained in the paper by d'Amore and Bezzo [4]. The emissions from ethanol production were calculated following the methodology used by Giarola et al. [3], and the ones related to conversion into electricity also followed the methodology proposed for stover in that paper, but weighting each new biomass for its respective LHV, averaged from the values retrieved from the literature as stated before. All these values can be found in Table A10.

Regarding the biomass production, the new mean values of emission factor for Arundo Donax, Miscanthus and Poplar were found in the literature [112, 114, 123, 140 - 148]. Then, they were linked with the regions *g* according to the same methodology described before for the yield and cost. The average values and the values retrieved from the literature are presented in Table A11.

The mean value for the emissions related to biomass production of forest wood residues was calculated considering only the emissions assigned to the collection of residues and wood chipping processes, since the emissions related to threes growth are charged to industrial timber production. Then the mean value (47.75 kg of CO_2-eq/ton) was linked with the regions *g* in the same way as for the other biomass types. The fuel consumption of the machines and their respective CO_2 equivalent emissions were found in the literature [149, 150]. The mean values for emissions related to collection and chipping were calculated considering a distance to the road side of 200 m [134], and the use of a mobile chipper.

The emissions related to the end user were obtained in the work by d'Amore and Bezzo [4], following the same assumptions: bifuel and traditional vehicles have similar energy efficiency, so the emissions of the bifuel vehicles only depend on the biofuel quota combustion; and it is also assumed that there is practically no difference in terms of emissions related to the production of traditional and electric vehicles, which means it is only necessary to take into account the emissions that come from producing the batteries to be used in the electric vehicles.

Second approach: five different assessment methods

Five different methods (*ReCiPe, Ecological Scarcity 2013, EDIP 2003, EPS 2000* and *Impact 2002+*) to assess the environmental impact of the SC will be applied, which requires access to a significant

amount of data. Several times, this data is not available or is limited, consequentially this approach is restricted to the available data and some assumptions had to be done.
The impact assessment is done based on the LCA stages considered by d'Amore and Bezzo [4], but the biomass pretreatment was excluded because it is already contemplated in the data for biomass growth.
Regarding the biomass growth, data for Arundo Donax, Poplar and stover was not available. For Arundo Donax, the data retrieved was related to sugar cane, as suggested by the support desk of the software *SimaPro* (from where all the data was obtained), whereas for stover an allocation based on the selling price was made considering it to be 24% of corn [3] and therefore the impacts from stover production are 24% of the ones related to corn. For Poplar exploitation it was considered the impacts related to birch, which is also a hardwood type of forestry.
Another alteration made was from spatially explicit to spatially implicit perspective, considering that the existing data does not contemplate the information for each region in Northern Italy, all the regions were considered in the same conditions, once again as suggested by *SimaPro*.
For ethanol conversion it was assumed that the impacts related to both technologies considered were the same, as it was done by d'Amore and Bezzo [4]. For the impacts of the different biomasses in each technology an allocation was made based on the conversion efficiencies used in the model, with corn as base, i.e. the lower the conversion efficiency in comparison to corn, the higher the environmental impacts. When technology DGP is used, DDGP is produced as a by-product, in this sense the impacts from DDGS production were accounted as emission credits.
For power conversion the same logic was followed as it was done for ethanol. Data related to wood combustion and steam turbine power generation, and power production from biogas in a turbo gas cycle was obtained for C+R and G+TG technologies, respectively. Then the allocation was made based on the conversion efficiencies used in the model for the different biomass types and also for the G+MCI technology.
For the transport system, the same impacts were assumed for ship and trans-ship, once they have similar capacities and emissions in the data from original model.
Regarding the production of batteries for the EVs, it was considered an average battery weight of 213 kg [151].
For the bifuel vehicles emissions, since they are very similar to the ones of traditional vehicles [4], the data collected regards the impacts of driving a medium car with a gasoline combustion engine.
The data for the environmental impacts was based on a single score rate obtained in the software *SimaPro 8.2.3.0*. The references used to select the impacts are presented in Table B1 in Appendix B.
The modifications on the model and the implementation of the impacts were developed in this thesis.

4.3 Model formulation

All the sets, parameters and variables necessary to run the model are presented in this section, as well as the objective functions and its respective constraints. The formulation is based on the model by d'Amore and Bezzo [4], all the changes made are marked.

Sets

- *c* ϵ *C* coefficients for costs linearization, *C* = {*slope, intercept*}
- *g* ϵ *G* grid squares, *G* = {*1,…,60*}
- *g'* ϵ *G* set of square regions different than *g*
- *i* ϵ *I* biomass types, *I* = {*corn, stover, Arundo Donax, Miscanthus, Poplar, wood*}
- *j* ϵ *J* product types, *J* = {*ethanol, DDGS, power}*
- *k* ϵ *K* production technologies, *K* = {*1, 2a, 2b, 2c, 2d, 2e, 11a, 11b, 11c, 11d, 11e, 22a, 22b, 22c, 22d, 22e, 33a, 33b, 33c, 33d, 33e*}
- *l* ϵ *L* transport means, *L* = {*truck, rail, barge, ship, tship*}
- *p* ϵ *P* discretization intervals for plant size linearization, *P* = {*1,…,6*}
- *s* ϵ *S* life cycke stages, *S* = {*bg, bpt, fp, epow, fd, fdist, ebat, ebifuel, ec*}
- *t* ϵ *T* time periods, *T* = {*1,…,5*}

Subsets

- *elec (k) c K* subset of pure power production technologies, *elec* (*k*) = {*11a, 11b, 11c, 11d, 11e, 22a, 22b, 22c, 22d, 22e, 33a, 33b, 33c, 33d, 33e*}
- *tech (k) c K* subset of technologies which involve DDGs sale, *tech* (*k*) = {*1*}

Scalars

- δ conversion factor specific for DDGS, 0.954 ton_{DDGS}/ton_{eth}
- φ fixed costs % over incomes, 0.15
- ψ emission in battery production, 3046.924 kg of CO_2-eq/EV
- ϛ emission in bifuel car driving, 0.005515 kg of CO_2-eq/km_{bifuel}
- ρ ethanol density, 0.7891 kg/l
- Γ MWh to tonne ethanol conversion, 0.133570792 $ton_{ethanol}$/MWh
- χ MWh/year to number of EVs conversion, 1.896918157 MWh/EV/year
- *charg* domestic electric charger 1.4 kW cost, 59.055 €/newEV
- *inc* differential EVs purchasing cost, 5000€/newEV
- *ΔKMcost* differential EVs driving cost, 0.03 €/km_{EV}
- *kmCAR* average daily trip in Italy, 45 km/day

Parameters

- Φ_g average ethanol-petrol distribution diameter, km
- AD_g arable land density, $km^2_{arable\ land}/km^2_{grid\ surface}$
- BCD^{max}_g maximum cultivation density in region *g*, $km^2_{cultivation}/km^2_{arable\ land}$
- $dfTCI_t$ discount factor for investments as time *t*
- $dfTC_t$ discount factor for cash flows as time *t*
- $CFdfCAR_t$ discount factor for cash flows as time *t* for EVs

- $Dterm_g$ fuel demand at the terminals in region g, ton/time period
- $Etperc_t$ ethanol blending percentage at time t
- Θ_t differential EVs purchasing cost reduction at time t
- $gasolTOT_t$ total number of traditional petrol fleet at time t
- $buyCAR1_t$ relative number of old EVs to be substituted with new ones at $t = 4$
- $buyCAR2_t$ relative number of old EVs to be substituted with new ones at $t = 5$
- ω_k exceeding electricity production specific for each conversion technology k, kWh_{el}/l_{EtOH}
- ER_p ethanol production rate for each plant size p, ton_{EtOH}/time period
- PR_p power production rate for each plant size p, MWh/time period
- $\gamma_{i,k}$ conversion factor specific for each biomass type i, $ton_{EtOH}/ ton_{biomass}$
- GS_g grid surface, km^2
- IBF_g internal biomass production feasibility, binary parameter
- MP_j market price for product j [€/ton or €/MWh]
- $quota_i$ maximum biomass quota available for energy conversion
- $BA_{g,i}$ biomass i availability for energy production in region g, ton/time period
- $\beta_{i,k}$ fraction of biomass i used in technology k
- $BY_{g,i}$ biomass yield of product i in region g, $ton_{biomass}$/time period/km^2
- $BYwood_{g,i}$ woody biomass yield in region g, $ton_{biomass}$/time period
- $CI_{p,k}$ capital investment at each linearization interval p and for technology k, M€
- $c_{k,cc}$ coefficients for linear regression of production costs for each technology k, *slope* [€/ton_{EtOH} or €/MWh] and *intercept* [€/time period]
- $fbg_{i,g}$ emission factor for biomass i growth in grid g, kg CO_2-eq/$ton_{biomass}$
- $fbpt_i$ emission factor for biomass i pre-treatment, kg CO_2-eq/$ton_{biomass}$
- fbt_l emission factor for biomass supply via mode l, kg CO_2-eq/$ton_{biomass}$km
- ffp_i emission factor for ethanol production from biomass i, kg CO_2-eq/ton_{EtOH}
- $fpp_{i,k}$ emission factor for power production from biomass i, kg CO_2-eq/MWh
- ffd_l emission factor for ethanol distribution via mode l, kg CO_2-eq/ton_{EtOH}km
- fec_k emission credits for each technology k, kg CO_2-eq/ton_{EtOH}
- $LD_{g,g'}$ local delivery distance between grids g and g', km
- $\tau_{g,l,g'}$ tortuosity factor of transport mode l between g and g'
- $UPC_{i,g}$ unit production costs for biomass type i in grid g, €/$ton_{biomass}$
- $z_{i,k}$ biomass i conversion into electricity by technology k, MWh/$ton_{biomass}$

Continuous variables

- $bifuelCARS_t$ number of bifuel vehicles at time t
- $bifuelKM_t$ total distance traveled by bifuel vehicles at time t, km/time period
- $Cap_{i,k,g,t}$ supply of biomass i to plant of technology k in region g at time t, ton/time period for ethanol production
- $CapElec_{i,k,g,t}$ supply of biomass i to plant of technology k in region g at time t, ton/time period for power production

- BPC_t biomass production cost at time *t*, €t/time period
- *CCF* discounted cumulative cash flow, €
- CF_t cash flow at time *t*, €/time period
- D_t depreciation at time *t*, €/time period
- $Dtot_{g,t}$ ethanol demand at time *t* in grid *g*, ton_{EtOH}/time period
- $Dtoti_{i,g,t}$ biomass *i* demand at region *g* at time *t*, ton/time period
- EPC_t ethanol production cost at time *t*, €/time period
- $ELtot_{k,g,t}$ electricity produced at time *t* by plant of technology *k* in region *g*, MWh/time period
- $Etot_{g,t}$ ethanol demand at time *t* in grid *g*, ton_{EtOH}/time period
- EVm_t EVs market share at time *t*
- $exCO_t$ extra costs for EVs fleet, €/time period
- *FCC* discounted facilities capital costs, €
- FCC_t facilities capital costs at time *t*
- $FixC_t$ fixed costs at time *t*
- $Impact_{s,t}$ impact for life cycle stage *s* at time *t*, kg CO_2-eq/time period
- Inc_t gross earnings at time *t*, €/time period
- $\lambda_{p,k,g,t}$ linearization variable for TCI at interval *p* for technology *k* in region *g* at time *t*
- $\lambda^{plan}_{p,k,g,t}$ linearization variable for TCI at interval *p* for technology *k* in region *g* at time *t*
- *NPV* net present value, €
- NPV_{chain} net present value for SC profit, €
- NPV_{car} net present value for EVs fleet, €
- $nCARS_t$ number of EVs at time *t*
- obj_o objective function expressed as the negative of *NPV*, €, or as overall impact, ton CO_2-eq
- PBT_t profit before taxes at time *t*, €/time period
- $Pb_{i,g,t}$ production rate of biomass *i* in region *g* at time *t*, ton/time period
- $Pp_{i,k,g,t}$ power production rate from biomass *i* through technology *k* in region *g* at time *t*, tee/time period
- PPC_t power production cost at time *t*, €/time period
- $P^{TOT}_{j,k,g,t}$ total production rate for product *j* through technology *k* in region *g* at time *t*, ton_{EtOH}/time period or MWh/month
- $Potot_{g,t}$ energy produced in region *g* at time *t*, tee/time period
- $powerKM_t$ total distance traveled by EVs at time *t*, km/time period
- $Qb_{i,g,l,g',t}$ flow rate of biomass *i* between *g* and *g'* through *l* at time *t*, ton/time period
- $Qf_{g,l,g',t}$ flow rate of ethanol between *g* and *g'* through *l* at time *t*, ton/time period
- $RISP_t$ money saved driving EVs rather than petrol ones in period *t*, €/time period
- TAX_t tax amount at time *t*, €/time period
- TCb_t biomass transport cost at time *t*, €/time period

- TCp_t products transport cost at time *t*, €/time period
- TCI_t total capital investment at time *t*, €/time period
- TD_t total ethanol and power demand at time *t*, ton_{EtOH} /time period
- $TDeth_t$ total ethanol demand at time *t*, ton_{EtOH} /time period
- $TDpow_t$ total power demand at time *t*, tee/time period
- *TGHG* total GHG impact, kg of CO_2-eq
- TI_t total impact at time *t*, kg of CO_2-eq/time period
- TP_t total ethanol and power production at time *t*, ton/time period
- $TPeth_t$ total ethanol production at time *t*, ton_{EtOH} /time period
- $TPpow_t$ total power production at time *t*, tee/time period
- $TPot_{i,t}$ total potential production of biomass *i* at time *t*, ton/time period
- $VarC_t$ variable costs at time *t*, €/time period
- *objective* objective selection variable

Binary variables

- $\Delta_{p,k,g,t}$ 1 if a production facility *k* of size *p* is to be established in region *g* at time *t*, 0 otherwise
- $Y_{k,g,t}$ 1 if a production facility *k* is already established in region *g* at time *t*, 0 otherwise
- $Y_{k,g,t}^{plan}$ 1 if the establishment of a new facility *k* is to be planned in region *g* at time *t*, 0 otherwise
- $Y_{k,g}^{start}$ 1 if the establishment of a new facility *k* is to be planned in region *g* at the beginning, 0 otherwise

Once the sets, parameters and variables are defined, the overall mathematical formulation of the model is presented next.

Objective functions

In this multi-objective model, the first objective function is the maximization of the *NPV* [€], which is expressed as a minimization of its negative form:

$$Obj_{eco} = -NPV \tag{3}$$

The *NPV* is calculated by summing the SC profit (NPV_{chain} [€]) and the cost difference for the end user in driving EVs instead of bifuel vehicles ((NPV_{car} [€]):

$$NPV = NPV_{Chain} + NPV_{Car} \tag{4}$$

NPV_{chain} is calculated by summing up the discounted cumulative cash flows (*CCF* [€]) and subtracting the necessary capital investment to establish the production facilities (*FCC* [€]):

$$NPV_{chain} = CCF - FCC \tag{5}$$

NPV_{car} is calculated by summing up the savings in driving electric instead of bifuel vehicles (*RISP* [€]) and subtracting the extra costs associated to buying the EVs (*exCO* [€]):

$$NPV_{car} = RISP - exCO \tag{6}$$

The purpose of the second objective function is to minimize the total GHG impact (*TGHG* [kg of CO_2-eq]) that results from the SC operation:

$$Obj_{env} = TGHG \tag{7}$$

TGHG is calculated by summing up the total impacts (TI_t [kg of CO_2-eq/time period]) that result from the SC operation and the vehicle utilization by the end user:

$$TGHG = \sum_t TI_t \tag{8}$$

Energy supply chain economics

CCF and *FCC* are calculated as follows:

$$CCF = \sum_t CF_t \cdot dfCF_t \tag{9}$$

$$FCC = \sum_t TCI_t \cdot dfTCI_t \tag{10}$$

Where CF_t [€] is the cash flow and TCI_t [€] is the total capital investment for each time period. $dtCF_t$ and $dtTCI_t$ are the time dependent discount factors, which are calculated as follows:

$$dfTCI_t = \frac{1}{(1+\zeta)^{3(t-1)}} \tag{11}$$

$$dfCF_t = \frac{3 + 3\zeta + \zeta^2}{3(1+\zeta)^{2t}} \tag{12}$$

Where ζ is the future interest rate, assumed to be constant and equal to 10%, as in Giarola et al. [3].
TCI_t is calculated by summing the expenditures needed to establish the facilities, according to their capital investment $CI_{p,k}$:

$$TCI_t = \sum_{p,k,g} \lambda^{plan}_{p,k,g,t} \cdot CI_{p,k} \tag{13}$$

Where $\lambda^{plan}_{p,k,g,t}$ is a linearization variable which is assigned a non-zero value for the period when the investment occurs.
The value of CF_t comes from:

$$CF_t = PBT_t + D_t - TAX_t \tag{14}$$

Where PBT_t [€/time period] represents the profit before taxes, D_t [€/time period] and TAX_t [€/time period] are, respectively, the depreciation charge and tax amount for each time period. TAX_t is defined as total tax amount, and as to be applied only when positive profit is obtained. Being a function of PBT_t would make Eq. (14) non-linear, so it as to be defined as:

$$TAX_t \geq Tr.PBT_t \tag{15}$$

$$TAX_t \geq 0 \tag{16}$$

Where *Tr* is the taxation rate set to 36% as it was done by Giarola et al. [3].

D_t is evaluated adopting the straight line depreciation method, depreciating TCI_t through a fixed quota of 20% (dk_t). Since this model is deals with a multi-period strategy where decisions can occur at each time period, capital depreciations should be evaluated since the time period when the investment decision was made [3]:

$$D_t = \sum_{p,k,g} \lambda_{p,k,g,t}.CI_{p,k}.dk_t \tag{17}$$

Where $\lambda_{p,k,g,t}$ is a linearization variable which has assumed a non-zero value since the moment an investment occurs.

PBT_t is calculated by summing the incomes Inc_t [€/time period] minus the fixed $FixC_t$ [€/time period] and the variable costs $VarC_t$ [€/time period], and minus the depreciation:

$$PBT_t = Inc_t - VarC_t - FixC_t - D_t \tag{18}$$

The incomes are a result of the sum of the revenues from selling the product *j*, which are calculated by multiplying the production rate $P^{TOT}_{j,k,g,t}$ [ton/time period or MWh/time period] by the product market price MP_j [€/ton or €/MWh]:

$$Inc_t = \sum_{j,k,g} P^{TOT}_{j,k,g,t}.MP_j \tag{19}$$

DDGS is only sold if the conversion technology belongs to the subset *tech*(*k*):

$$P^{TOT}_{'DDGS',k,g,t} = 0, \ \ \forall\, k \notin tech(k) \tag{20}$$

The fixed costs are calculated by applying a fixed quota φ set equal to 15% [3] to the incomes:

$$FixC_t = \varphi.Inc_t \tag{21}$$

The variable costs are calculated from:

$$VarC_t = EPC_t + BPC_t + PPC_t + TCb_t + TCf_t \tag{22}$$

Where EPC_t [€/ton] represents ethanol production costs, BPC_t [€/ton] stands for biomass production costs, TCb_t [€/ton] and TCf_t [€/ton] represent biomass and ethanol transport costs and PPC_t [€/tee] represents the electricity generation costs.

BPC_t is evaluated by multiplying the biomass production rate $Pb_{i,g,t}$ [ton/time period] by its unit production costs $UPC_{i,g}$ [€/ton]:

$$BPC_t = \sum_{i,g} Pb_{i,g,t} . UPC_{i,g} \tag{23}$$

EPC_t is defined as the sum of a linear function of the total production rate $P^{TOT}_{'ethanol',k,g,t}$ [ton_{EtOH}/time period] and a fixed quota depending on the technology:

$$EPC_t = \sum_{k,g} (c_{k,'slope'} . P^{TOT}_{'ethanol',k,g,t} + c_{k,'intercept'} . Y_{k,g,t}) \tag{24}$$

Where $c_{k,'slope'}$ [€/ton_{EtOH} or €/MWh] and $c_{k,'intercept'}$ [€/time period] are the arrays of linear coefficients specific for each technology k, and $Y_{k,g,t}$ is the binary variable defining whether a facility is operating or not.

PPC_t is calculated as EPC_t, but as a function of the electricity production rate $ELtot_{k,g,t}$ [MWh/time period]:

$$PPC_t = \sum_{k,g} (c_{k,'slope'} . ELtot_{k,g,t} + c_{k,'intercept'} . Y_{k,g,t}) \tag{25}$$

The transport costs are evaluated as follows:

$$TCb_t = \sum_{i,l} UTCb_l . \left(\sum_{g,g'} Qb_{i,g,l,g',t} . LD_{g,g'} . \tau_{g,l,g'} \right) + \sum_{i,g} UTCl^* . Pb_{i,g,t} . LD_{g,g} \tag{26}$$

$$TCf_t = \sum_{i,l} UTCf_l . \left(\sum_{g,g'} Qf_{g,l,g',t} . LD_{g,g'} . \tau_{g,l,g'} \right) \tag{27}$$

Where $UTCb_l$ and $UTCf_l$ [€/ton.km] are the biomass and ethanol unit transport costs, $Qb_{i,g,l,g',t}$ and $Qf_{g,l,g',t}$ [ton/time period] are the flow rates of biomass and ethanol, $LD_{g,g'}$ and $LD_{g,g}$ [km] are delivery distances, $\tau_{g,l,g'}$ is the tortuosity factor and $UTCl^*$ [€/ton.km] is the unit price for biomass transports within g.

AFVs economics

$RISP$ is evaluated through the sum of the potential savings by end users in driving EVs instead of bifuel cars, $RISP_t$ [€/time period] discounted through the $CFdfCAR_t$ factor:

$$RISP = \sum_{t} RISP_t . CFdfCAR_t \tag{28}$$

$RISP_t$ is calculated by multiplying the average distance covered by EVs, $powerKM_t$ [km/time period] for the differential travelling cost with respect to a bifuel vehicle, $\Delta KMcost$ [€/km], of 0.03€ [4]:

$$RISP_t = powerKM_t . \Delta KMcost \tag{29}$$

The discount factor comes from:

$$CFdfCAR_t = \frac{1}{(1+i)^t} \tag{30}$$

Where i represents the interest rate for 3 years and is computed from the yearly interest rate i_0, set equal to 5% [4]:

$$i = (1+i_0)^3 - 1 \tag{31}$$

exCO is calculated from:

$$exCO = \sum_t exCO_t . CFdfCAR_t \tag{32}$$

Where $exCO_t$ [€/time period] represents the additional investment for end user to buy an EV comparing to bifuel:

$$exCO_t = newCARS_t .(charg + inc.\Theta_t) \tag{33}$$

The constant *charg* represents the average cost of an electric charger, set equal to 59 €/new EV [4]. The constant *inc* [€/new EV] evaluates the differential purchasing cost of an EV comparing to a bifuel one, set equal to 5000 €/new EV [4], this constant is decreased for each t by the parameter Θ_t set equal to 0.125 [4]. The number of EVs purchased, $newCARS_t$ comes from:

$$newCARS_t = (nCARS_t - nCARS_{t-1}) + buyCAR1_t . newCARS_{t=1} + buyCAR2_t . newCARS_{t=2} \tag{34}$$

Where $nCARS_t$ stands for the cumulative amount of EVs, and the parameters $buyCAR1_t$ and $buyCAR2_t$ represent, at t = 4 and 5, the substitution of obsolete EVs from t = 1 and 2, since the battery lifetime is 10 years [4].

Constraints: linearization and logical

The linearization variables $\lambda_{p,k,g,t}^{plan}$ and $\lambda_{p,k,g,t}$ are constrained by the binary variables $Y_{k,g,t}^{plan}$ (variable planning the establishment of a new facility) and $Y_{k,g,t}$:

$$\sum_t (\lambda_{p,k,g,t}^{plan}) = Y_{k,g,t}^{plan} \tag{35}$$

$$\sum_t (\lambda_{p,k,g,t}) = Y_{k,g,t} \tag{36}$$

The first year configuration is set by:

$$Y_{k,g,'1'}^{plan} = Y_{k,g}^{start} \tag{37}$$

Once a facility is operating, it will keep like that for the remaining time frame:

$$Y_{k,g,t} = Y_{k,g,t-1} + Y_{k,g,t}^{plan} \tag{38}$$

The variables $\lambda^{plan}_{p,k,g,t}$ and $\lambda_{p,k,g,t}$ are bound by:

$$\lambda^{plan}_{p,k,g,t} = \lambda_{p,k,g,t} - \lambda_{p,k,g,t-1} \tag{39}$$

The binary variable $\Delta_{p,k,g,t}$ binds the selection of the continuous values of the key linearization variables $\lambda^{plan}_{p,k,g,t}$ and $\lambda_{p,k,g,t}$ within a suitable scale range:

$$\lambda^{plan}_{p,k,g,t} \leq \Delta_{p,k,g,t} + \Delta_{p-1,k,g,t} \tag{40}$$

$$\lambda_{p,k,g,t} \leq \Delta_{p,k,g,t} + \Delta_{p-1,k,g,t} \tag{41}$$

Only one conversion plant can operate in a region *g*:

$$\sum_k Y_{k,g,t} \leq 1 \tag{42}$$

The $\Delta_{p,k,g,t}$ variables are subject to the planning decision variable value:

$$\sum_p \Delta_{p,k,g,t} = Y_{k,g,t} \tag{43}$$

Constraints: capacity and production

The amount of ethanol, $P^{TOT}{}_{'ethanol',k,g,t}$ [ton_{EtOH}/time period], and power, $ELtot_{k,g,t}$ [MWh/time period], produced in a region *g* at time *t* are given by the following equations:

$$P^{TOT}_{'ethanol',k,g,t} \leq \sum_p ER_p . \lambda_{p,k,g,t} , \qquad \forall k \notin elec_k \tag{44}$$

$$ELtot_{k,g,t} \leq \sum_p PR_p . \lambda_{p,k,g,t} , \qquad \forall k \in elec_k \tag{45}$$

Where ER_p [ton_{EtOH}/time period] and PR_p [MWh/time period] represent the output rates according to the facility size *p*. The variation of productivity from *t* to *t*+1 is constrained by:

$$P^{TOT}_{'ethanol',k,g,t} \geq 0.8 * \sum_p ER_p . \lambda_{p,k,g,t} , \qquad \forall k \notin elec_k \tag{46}$$

$$ELtot_{k,g,t} \geq 0.7 * \sum_p PR_p . \lambda_{p,k,g,t} , \qquad \forall k \in elec_k \tag{47}$$

Ethanol ($Pf_{i,k,g,t}$ [ton/time period]) and power ($Pp_{i,k,g,t}$ [MWh/time period]) generation from biomass *i*, through technology *k*, in region *g* at time *t* are calculated with:

$$Pf_{i,k,g,t} = \gamma_{i,k} . Cap_{i,k,g,t} \tag{48}$$

$$Pp_{i,k,g,t} = z_{i,k} . CapElec_{i,k,g,t} \tag{49}$$

Where $\gamma_{i,k}$ [ton_{EtOH}/ $ton_{biomass}$] and $z_{i,k}$ [MWh/$ton_{biomass}$] represent the conversion efficiencies from biomass *i*, through technology *k* into ethanol and electricity, respectively. $Cap_{i,k,g,t}$ and $CapElec_{i,k,g,t}$

[ton/time period] represent the supply of biomass *i* to plant of technology *k* in region *g* at time *t*, for ethanol and power production, respectively.

From here, it is possible to evaluate $P^{TOT}_{'ethanol',k,g,t}$ [ton_{EtOH}/time period] and $ELtot_{k,g,t}$ [MWh/time period]:

$$Pf_{i,k,g,t} = P^{TOT}_{'ethanol',k,g,t} \cdot \beta_{i,k} \tag{50}$$

$$Pp_{i,k,g,t} = ELtot_{k,g,t} \cdot \beta_{i,k} \tag{51}$$

Where, in the original model, the parameter $\beta_{i,k}$ sets the type of biomass to be used in each technology, *a priori*, leaving to the model only the decision of which technology to use. In this new approach that would not be possible, since more than two biomass types are available. To get around this problem, the set of technologies *k* is divided, for each technology, according to the number of biomass types that technology can use as an input. Originally, the technologies were defined by *k*={1, 2, 11, 22, 33}, in this new formulation they are defined as *k*={1, 2a, 2b, 2c, 2d, 2e, 11a, 11b, 11c, 11d, 11e, 22a, 22b, 22c, 22d, 22e, 33a, 33b, 33c, 33d, 33e} where all the possible combinations between technologies and biomass types are considered. The numbers represent the conversion technologies (as in the original model) and the letters (a, b, c, d, e) represent the biomass type (stover, Arundo Donax, Miscanthus, poplar and wood, respectively). Then, $\beta_{i,k}$ is set as 1 when the biomass corresponds to the supposed technology and as 0 when that does not happen, like it is possible to see in Table A12 in Appendix A. As stated before, corn can only be used in DGP technology and Poplar and wood residues are only considered for power production. This way the model is allowed to decide the combination between biomass types and technologies to be used. This parameter is presented in this section, since it was one of the modifications made to the original formulation.

The DDGS production is given by:

$$P^{TOT}_{'DDGS',k,g,t} = Pf_{'corn',k,g,t} . \delta \tag{52}$$

Where δ [ton_{DDGS}/ton_{eth}] represents the conversion factor specific for DDGS equal to 0.954 [3].

The production of ethanol in technology *k*=2 also results in electricity generation through the exploitation of DDGS for CHP production. Therefore, the overall electricity generation, $P^{TOT}_{'power',k,g,t}$ [MWh/time period] is given by:

$$P^{TOT}_{'power',k,g,t} = \omega_k . \frac{P^{TOT}_{'ethanol',k,g,t}}{\rho} + ELtot_{k,g,t} \tag{53}$$

Where ω_k [kWh/l_{EtOH}] represents the production of electricity from CHP and ρ [kg/l] stands for ethanol density equal to 0.7891.

Mass balances are necessary to constrain the commodities production rates. A global mass balance on ethanol is given by:

$$\sum_k P^{TOT}_{'ethanol',k,g,t} = Etot_{g,t} + \sum_{l,g'} (Qf_{g,l,g',t} - Qf_{g',l,g,t}) \tag{54}$$

Where $Etot_{g,t}$ [ton_{EtOH}/time period] represents the ethanol demand at time t in region g. The mass balance for biomass is given by:

$$Pb_{i,g,t} = Dtoti_{i,g,t} + \sum_{l,g'} (Qb_{i,g,l,g',t} - Qb_{i,g',l,g,t}) \tag{55}$$

Where $Dtoti_{i,g,t}$ [ton/time period] represents the demand for biomass i at region g at time t and depends on the biomass to be converted in fuel and on the biomass to be converted in electricity:

$$Dtoti_{i,g,t} = \sum_{k} (Cap_{i,k,g,t} + CapElec_{i,k,g,t}) \tag{56}$$

The biomass production must be upper-bounded according to the limits imposed by the production capability:

$$Pb_{i,g,t} \leq BA_{g,i} \tag{57}$$

Where $BA_{i,g}$ [ton/time period] represents the biomass availability and depends on agronomic-related factors such as maximum biomass cultivation fractions $BCD^{max}{}_{g}$ [$km^2_{cultivation}/km^2_{arable\ land}$] over arable land AD_g [$km^2_{arable\ land}/km^2_{grid\ surface}$], the biomass yield $BY_{g,l}$ [$ton_{biomass}$/time period/km^2] and the surface of a region g GS_g [km^2]:

$$BA_{g,i} = GS_g \cdot BY_{i,g} \cdot AD_g \cdot BCD_g^{max} + BYwood_{i,g} \tag{58}$$

Equation (58) is a new equation added to the model. The difference from the original formulation is the addition of $BYwood_{i,g}$ [ton/time period], which represents the yield of recovered wood residues, that does not depend on the agronomic-related factors like the other biomasses, since it is not a crop, but a residue from another activity.

To ensure a sustainable biomass production an utilization factor $quota_i$, that fixes the maximum amount of biomass available for energy production, is applied to the potential biomass production $TPot_{i,t}$ [ton/time period]:

$$TPot_{i,t}.quota_i \geq \sum_{g} Pb_{i,g,t}.IBF_g \tag{59}$$

Where:

$$TPot_{i,t} = \sum_{g} BA_{i,g}.IBF_g \tag{60}$$

With IBF_g being a binary parameter that establishes whether cultivation exists on a certain region g.

Demand evolution

The total transport energy demand is assumed to be constant and the renewable transport energy is assumed to grow as explained in section 4.2. It is assumed that there is no storage of the production, therefore the global production rates of ethanol, $TPeth_t$ [ton_{EtOH}/time period], and power, $TPpow_t$

[tee/time period], should meet exactly the ethanol, $TDeth_t$ [ton_{EtOH}/time period], and power, $TDpow_t$ [tee/time period], demands:

$$TPeth_t = TDeth_t \tag{61}$$

$$TPpow_t = TDpow_t \tag{62}$$

Productions are given by:

$$TPeth_t = \sum_{k,g} P^{TOT}_{\prime ethanol\prime,k,g,t} \tag{63}$$

$$TPpow_t = \sum_{k,g} P^{TOT}_{\prime power\prime,k,g,t}.\Gamma \tag{64}$$

Where Γ [$ton_{ethanol}$/MWh] converts the units of power from MWh to tee and is equal to 0.133570792.

The global ethanol demand comes as the sum of the demands in all the regions g:

$$TDeth_t = \sum_{g} Etot_{g,t} \tag{65}$$

In each region the demand $Etot_{g,t}$ is set by $Dtot_{i,g}$:

$$Etot_{g,t} = Dtot_{g,t} \tag{66}$$

$Dtot_{i,g}$ is set by the fuel demand at the terminals $Dterm_g$ [ton/time period] and the ethanol blending $etperc_t$ [%]:

$$Dtot_{g,t} = Dterm_g.etperc_t \tag{67}$$

The number of EVs $nCARS_t$ is calculated from the power demand and the parameter χ=1.897 MWh/EV/year, that represents the energy necessary to fuel an EV for an year assuming an average of 45 km/day/vehicle:

$$nCARS_t = \frac{TDpow_t}{\Gamma.\chi.3} \tag{68}$$

Bifuel vehicles market penetration, $bifuelCARS_t$, is computed by summing up traditional vehicles fleet, $gasolTOT_t$, minus the EVs fleet, $nCARS_t$:

$$bifuelCARS_t = gasolCARS_t - nCARS_t \tag{69}$$

The total distance covered by bifuel vehicles, $bifuelKM_t$ [km/time period], is set considering an average trip distance of 45 km:

$$bifuelKM_t = bifuelCARS_t * 45 * 365 * 3 \tag{70}$$

On the other hand, the total distance covered by EVs, $powerKM_t$ [km/time period], is given by:

$$powerKM_t = nCARS_t * 45 * 365 * 3 \tag{71}$$

For instance B, as stated before, the demand comes as a total energy demand given by:

$$TD_t = TDeth_t + TDpow_t \tag{72}$$

In this way a total demand is fixed, leaving to the solver the decision of adjusting the production rates of ethanol and power, as well as the market penetration of electric and bifuel vehicles.

The global demands of ethanol and power are given by the sum of their regional demands:

$$TDeth_t = \sum_g Etot_{g,t} \tag{73}$$

$$TDpow_t = \sum_g Potot_{g,t} \tag{74}$$

Which compose the overall regional demand:

$$Dtot_{g,t} = Etot_{g,t} + Potot_{g,t} \tag{75}$$

The only variable which has a fixed value is the overall regional demand:

$$Dtot_{g,t} = Dterm_g . etperc_t \tag{76}$$

Which considers a different *etperc*$_t$ than before, so that *Dtot*$_{i,g}$ takes also the power demand into account, meaning that *Dtot*$_{i,g}$ is no longer the ethanol demand, but the overall demand.

Transport constraints

It is necessary to assure that the flow rate of a biomass or product does not go through internal loops:

$$Qb_{i,g,l,g,t} = 0 \quad \text{and} \quad Qf_{g,l,g,t} = 0 \tag{77}$$

The transport network must respect a transport feasibility condition, considering that some transportation modes cannot be used to link some regions:

$$Qb_{i,g,l,g',t} = 0 \quad \text{and} \quad Qf_{g,l,g',t} = 0 : \qquad (g,l,g') \neq Total_{g,l,g'} \tag{78}$$

Where *Total*$_{g,l,g'}$ represents the total transport links allowed.

Non-negativity constraints

$$Cap_{i,k,g,t} \geq 0 \tag{79}$$

$$CapElec_{i,k,g,t} \geq 0 \tag{80}$$

$$\lambda^{plan}_{p,k,g,t} \geq 0 \tag{81}$$

$$\lambda_{p,k,g,t} \geq 0 \tag{82}$$

$$Pb_{i,g,t} \geq 0 \tag{83}$$

$$P^{TOT}_{'ethanol',k,g,t} \geq 0 \tag{84}$$

$$Potot_{g,t} \geq 0 \tag{85}$$

$$ELtot_{k,g,t} \geq 0 \quad (86)$$

$$Etot_{g,t} \geq 0 \quad (87)$$

$$Dtot_{g,t} \geq 0 \quad (88)$$

$$Qb_{i,g,l,g',t} \geq 0 \quad (89)$$

$$Qf_{g,l,g,t} \geq 0 \quad (90)$$

Environmental impact

TI_t (eq. (8)) is defined as:

$$TI_t = \sum_{s} Impact_{s,t} \quad (91)$$

Where $Impact_{s,t}$ [kg of CO_2-eq/time period] is the GHG emissions resulting from each life cycle stage *s*. The impact related to biomass growth is given by:

$$Impact_{'bg',t} = \sum_{i,g} fbg_{i,g}.Pb_{i,g,t} \quad (92)$$

The impact from biomass pre-treatment is defined as:

$$Impact_{'bpt',t} = \sum_{i,g} fbpt_{i,g}.Pb_{i,g,t} \quad (93)$$

The impacts related to the transport system (biomass supply, ethanol distribution to the blending terminals and the final biofuel distribution to the end users) are given by:

$$Impact_{'bt',t} = \sum_{i,l} fbt_l.\left(\sum_{g,g'} Qb_{i,g,l,g',t}.LD_{g,g'}.\tau_{g,l,g'}\right) + \sum_{i,g} fbtl^*.Pb_{i,g,t}.LD_{g,g} \quad (94)$$

$$Impact_{'ft',t} = \sum_{i,l} ffd_l.\left(\sum_{g,g'} Qf_{g,l,g',t}.LD_{g,g'}.\tau_{g,l,g'}\right) \quad (95)$$

$$Impact_{'fdist',t} = ffd_{'truck'}.\sum_{i,g} \Phi_g.Etot_{g,t} \quad (96)$$

Where Φ_g [km] is the average distribution diameter for the blending terminal at *g*.
The impact related to ethanol production is defined as:

$$Impact_{'fp',t} = \sum_{i,k,g} ffp_i.Pf_{i,k,g,t} \quad (97)$$

The impact resulting from electricity generation is given by:

$$Impact_{'epow',t} = \sum_{i,k,g} fpp_{i,k}.Pp_{i,k,g,t} \quad (98)$$

The impact relate to EV battery production is defined as:

$$Impact_{'ebat',t} = \psi . newCARS_t \tag{99}$$

Where ψ is the differential emission factor between traditional and EVs manufacturing that accounts for battery production and lack of internal combustion engine and is set equal to 3046.9 kg of CO_2-eq/new EV [4]. It is assumed that for the EVs utilization there are no emissions.
The emissions related to the utilization of bifuel vehicles are given by:

$$Impact_{'ebifuel',t} = \varsigma . bifuelKM_t \tag{100}$$

Where ς is the emission factor for driving a bifuel vehicle and is equal to 0.005515 kg of CO_2-eq/$km_{bifuel\ car}$ [4]. Finally, emission credits for by products (DDGS or electricity from CHP) are considered in the formulation as a negative contribution to the impact calculation:

$$Impact_{'ec',t} = -\sum_{k,g} ffp_i . P^{TOT}_{'ethanol',k,g,t} \tag{101}$$

4.4 Chapter conclusions

The MILP model presented addresses the optimization of the economic and environmental performance of a bioethanol and bio-power SC design in Northern Italy. It is based on several models developed in CAPE-Lab at University of Padova and contains a level of information that is not provided in this thesis, due to its extension. The technical and economical modeling parameters can be consulted in the works by d'Amore and Bezzo [4], Zamboni et al. [1,2] and Giarola et al [3].

5. Model results

This chapter presents the results obtained from the model explained above. It is divided in four sections: 5.1 and 5.2 present, respectively, the economic and the environmental optimizations both for instance A and B; in section 5.3 the results regarding the multi-objective optimization are presented for instance B; section 5.4 contains the conclusions taken after analyzing the results presented in this chapter.

5.1 Economic optimization

The economic optimization results present the best SC design considering only the economic performance, disregarding the environmental impacts. All the decisions regarding the SC structure are determined by the maximization of the SC NPV.

5.1.1 Instance A

In instance A, as stated before, ethanol and power demands are set *a priori*, which means that the output rates are fixed, leaving to the solver to optimize the SC structure based on the most profitable combination between biomass types and technologies to be used to satisfy that demand. From Table 1 it is possible to verify the positive influence of adding new biomass types to the model, given the increase on an already very promising NPV.

Table 1 – Original and new model results for instance A under economic optimization

	NPV [€]	*NPV* per energy [€/GJ]	GHG emissions [ton of CO_2-eq]	GHG emissions per energy [kg of CO_2-eq/GJ]
Original [4]	6.28×10^8	1.79	3.27×10^7	93.30
New	6.67×10^8	1.90	3.30×10^7	94.29

This *NPV* is highly supported by the NPV_{chain} of 4.69×10^8 €, whereas the NPV_{car} is equal to the one on the original model, 1.98×10^8 €, given that the EVs market share is fixed and equal from one model to the other.

From the investors point of view, the payback time is situated in the first three years of operation, once that when period t=1 ends NPV_{chain} is already positive. On the other hand, considering the end users perspective, only in t=5 the NPV_{car} becomes positive, meaning that only after that time the consumer will have economic advantages in using EVs. Considering the whole problem, the value of *NPV* only becomes positive after 9 years, at the end of t=3, as it is presented in Table 2.

Table 2 – *NPV* evolution in *t* for instance A under economic optimization

t	1	2	3	4	5
NPV_{car} [€]	-4.40×10^{8}	-5.51×10^{8}	-4.07×10^{8}	-2.19×10^{8}	1.98×10^{8}
NPV_{chain} [€]	-6.12×10^{7}	1.18×10^{8}	2.65×10^{8}	3.63×10^{8}	4.70×10^{8}
NPV [€]	-5.05×10^{8}	-4.33×10^{8}	-1.42×10^{8}	1.44×10^{8}	6.67×10^{8}

The good SC economic performance is a result of the total production of 1.14×10^{7} tons of ethanol and 1.08×10^{7} tons of DDGS using corn in a total of six DGP (*k*=1) plants, and a global power production of 1.23×10^{6} MWh from Arundo Donax in one G+TG (*k*=22) and twelve G+MCI (*k*=33) plants. This results in a total income of 1.24×10^{10} € and a total variable costs of 6.43×10^{9} €. The distributions of the incomes and the variable costs are presented in Figures 18 and 19. The share of the ethanol distribution it comes as zero because its value is very small when compared with the total costs.

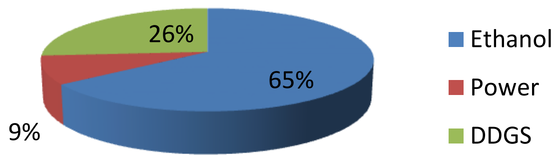


Figure 18 – Share of the incomes by product sold stage for instance A under economic optimization

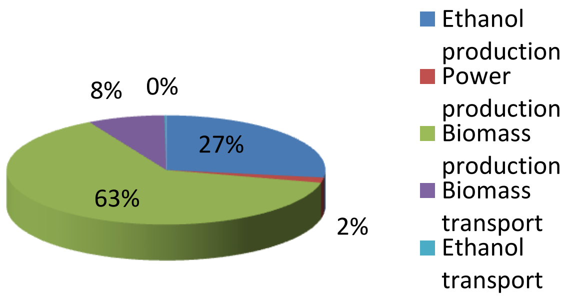


Figure 19 – Share of the variable costs per SC for instance A under economic optimization

The 3.42×10^{7} tons of corn used are all imported (*g*=60) and are transported by trans-ship into Italy and by rail to the conversion facilities, from where the ethanol is sent to the blending terminals by rail or barge. The total production of 7.33 $\times10^{6}$ tons of Arundo Donax is made in only one plantation site and is transported to the power plants by barge, ship and rail. The final configuration (at *t*=5) is presented in Figure 20.

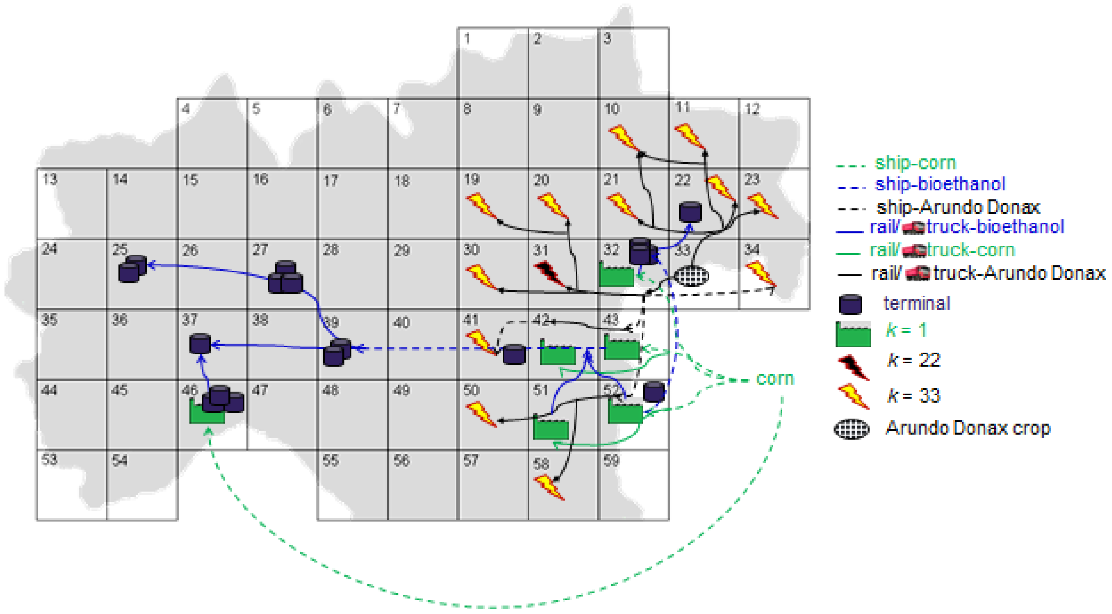


Figure 20 – SC configuration for instance A under economic optimization

Even though this optimization presents a very good NPV, this solution is environmentally unfeasible given the fact that its GHG emissions are higher than the ones related to petrol production and utilization, 85.8 kg of CO_2-eq/GJ [152].

5.1.2 Instance B

In instance B the energy demand comes as an overall energy demand, given by the sum of ethanol and power demands from instance A. In this case the solver optimizes the SC design considering the most profitable combination between the production rates of each product. In Table 3 is possible to see how the new biomasses slightly improved the model's economic results.

Table 3 – Original and new model results for instance B under economic optimization

	NPV [€]	*NPV* per energy [€/GJ]	GHG emissions [ton of CO_2-eq]	GHG emissions per energy [kg of CO_2-eq/GJ]
Original [4]	$1.71\text{x}10^9$	4.88	$3.17\text{x}10^7$	90.43
New	$1.77\text{x}10^9$	5.04	$3.27\text{x}10^7$	93.25

Although the value for the NPV_{chain} is similar to the one of instance A, $4.75\text{x}10^8$ €, this *NPV* is highly supported by an NPV_{car} of $1.29\text{x}10^9$ €, which is a consequence of an EV market penetration much higher than the minimum imposed, of about 12% in t=5. However, as happened for instance A, only in period t=5 the use of EVs starts being advantageous for the end user, since only then NPV_{car} shows positive values. This means that the first EV users would only be a mean to reach a profitable situation and would not get any return, which is unlikely unless it is supported by some government policies. On the other hand, the investment for establishing new facilities has a payback time that comes only in period t=2. Regarding the whole problem, it takes less time to become profitable, since the value for the *NPV* becomes positive in t=2, as it is presented in Table 4.

Table 4 – *NPV* evolution in *t* for instance B under economic optimization

t	1	2	3	4	5
NPV_{car} [€]	0	-9.97×10^{8}	-1.40×10^{9}	-2.07×10^{8}	1.29×10^{9}
NPV_{chain} [€]	-5.68×10^{7}	1.20×10^{8}	2.51×10^{8}	3.60×10^{8}	4.75×10^{8}
NPV	-5.68×10^{7}	-8.77×10^{8}	-1.15×10^{9}	1.53×10^{8}	1.77×10^{9}

In this scenario more importance is given to the production of power instead of ethanol, as opposed to what happened in instance A, since in this case the production rates are not fixed, which means that a higher electricity production promotes a higher *NPV* mainly due to the increase of EVs circulating and the consequential growth of NPV_{car} . The total power production is 3.85×10^{7} MWh, and the productions of ethanol and DDGS are 7.86×10^{6} and 7.5×10^{6} tons, respectively. Ethanol and DDGS are produced in 3 DGP (k=1) facilities, whereas the power production is done in 7 G+TG (k=22) and 20 G+MCI (k=33) plants. This results in a total income of 1.13×10^{10} €, which is smaller than the one from instance A, but is compensated by an also smaller total of variable costs of 5.23×10^{9} €. The distributions of the incomes and the variable costs are presented in Figures 21 and 22.

As opposed to what happened for instance A, the amounts of biomasses used are similar to each other. The 2.37×10^{7} tons of corn used are all imported (g=60) and are transported by trans-ship into Italy and by rail to the conversion facilities, from where the ethanol is sent to the blending terminals by rail or barge. The total production of 2.25×10^{7} tons of Arundo Donax is made in three different crops and is transported to the power plants by barge, ship, rail and truck. The final configuration (at t=5) is presented in Figure 23.

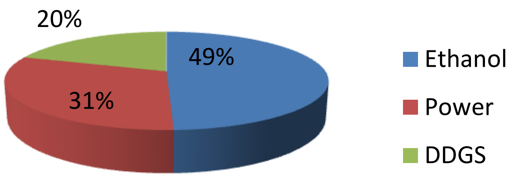


Figure 21 – Share of the incomes by product sold for instance B under economic optimization

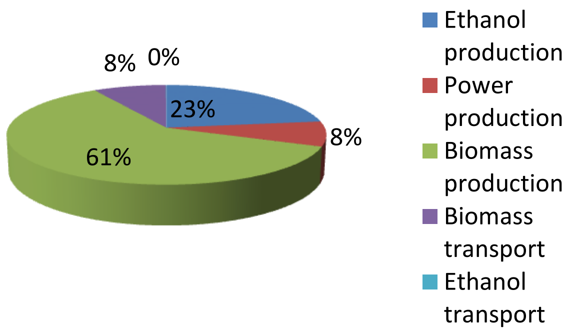


Figure 22 – Share of the variable cost per SC stage for instance B under economic optimization

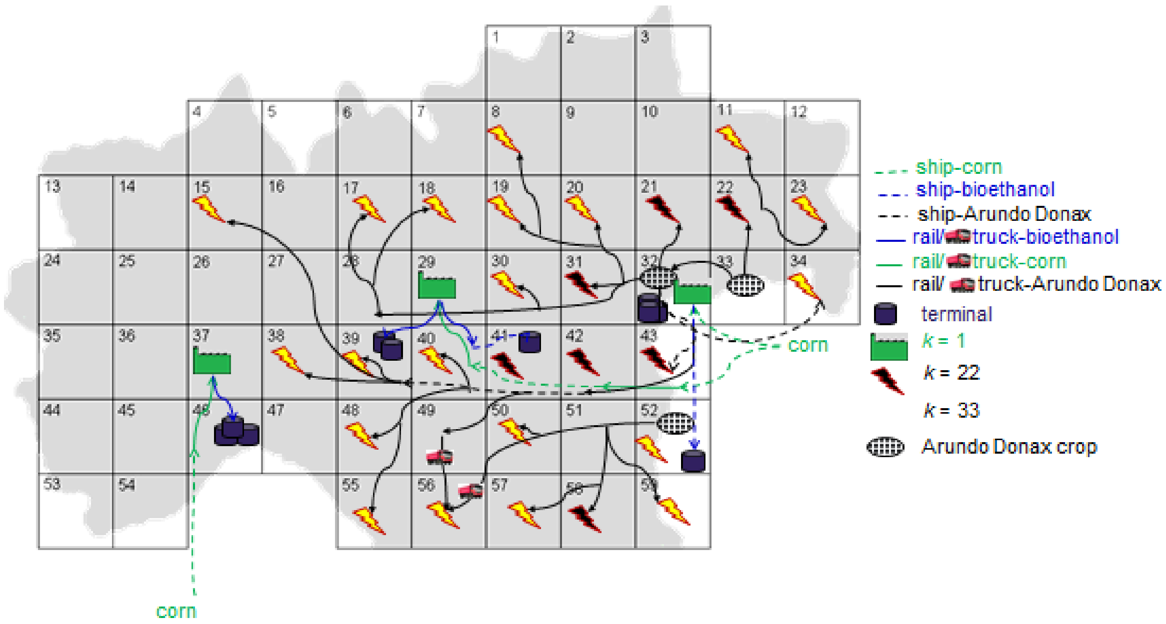


Figure 23 – SC configuration for instance B under economic optimization

Although the total GHG emissions are inferior to the ones of instance A, as it happened then, the configuration obtained is not environmentally feasible given the fact that its GHG emissions are 8% higher than the ones related to petrol (85.8 kg of CO_2-eq/GJ).
The configurations with better environmental performance will be presented in the next section for both instances.

5.2 Environmental optimization

The environmental optimization solution presents the best SC configuration considering only the environmental performance, disregarding the NPV. All the decisions regarding the SC design are determined by the minimization of the total GHG emissions.

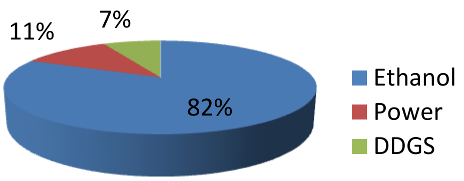
5.2.1 Instance A

As opposed to what happened before, there is no noticeable influence in the addition of the new biomasses in the results, comparing to the original model. For the environmental optimization the economic results are very poor, even though they show a great environmental performance, as presented in Table 5.

Table 5 – Original and new model results for instance A under environmental optimization

	NPV [€]	*NPV* per energy [€/GJ]	GHG emissions [ton of CO_2-eq]	GHG emissions per energy [kg of CO_2-eq/GJ]
Original [4]	$-1.17x10^9$	-3.35	$1.14x10^7$	32.54
New	$-1.17x10^9$	-3.35	$1.14x10^7$	32.54

Although the value for NPV_{car} is equal to the one from the economic optimization, 1.98×10^{8} €, consequence of the fixed EVs market share, this low *NPV* is explained by a -1.37×10^{9} € value for the NPV_{chain}. This poor economic result is a consequence of the great environmental performance, as it can be seen in Table 5, the total GHG emissions are about 38% of the ones related to petrol. Even though the output rates of power and ethanol are the same as for the economic optimization, this difference on the performance is a consequence of the utilization of different biomass types in different technologies. In this case ethanol is not produced only from corn in 1 DGP (k=1) facility, but also from stover in 6 LCEP (k=2) plants, which also produce power as a by-product. The remaining power production is done from stover in 7 G+TG (k=22) plants. This results in a total income of 9.89×10^{9} € and a total of variable costs of 5.44×10^{9} €. The distributions of the incomes and the variable costs are presented in Figures 24 and 25.



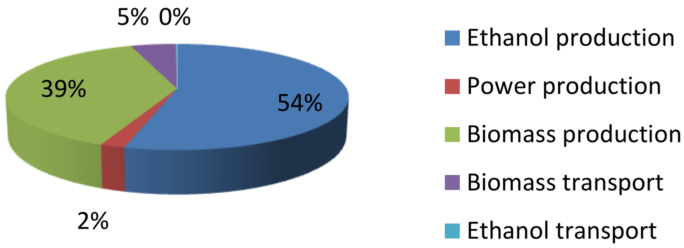


Figure 24 – Share of the incomes by product sold for instance A under environmental optimization

Figure 25 – Share of the variable costs per SC stage for instance A under environmental optimization

Differently from the other cases, here the production of the 7.61×10^{6} tons of corn is done in two crops within Northern Italy, which is then transported by rail to the conversion facility, from where the ethanol is sent to the blending terminals by rail or barge. The 3.65×10^{7} tons of stover are produced in 14 different sites and the biomass is then transported by rail, truck, barge and ship. The final SC configuration (at t=5) is presented in Figure 26.

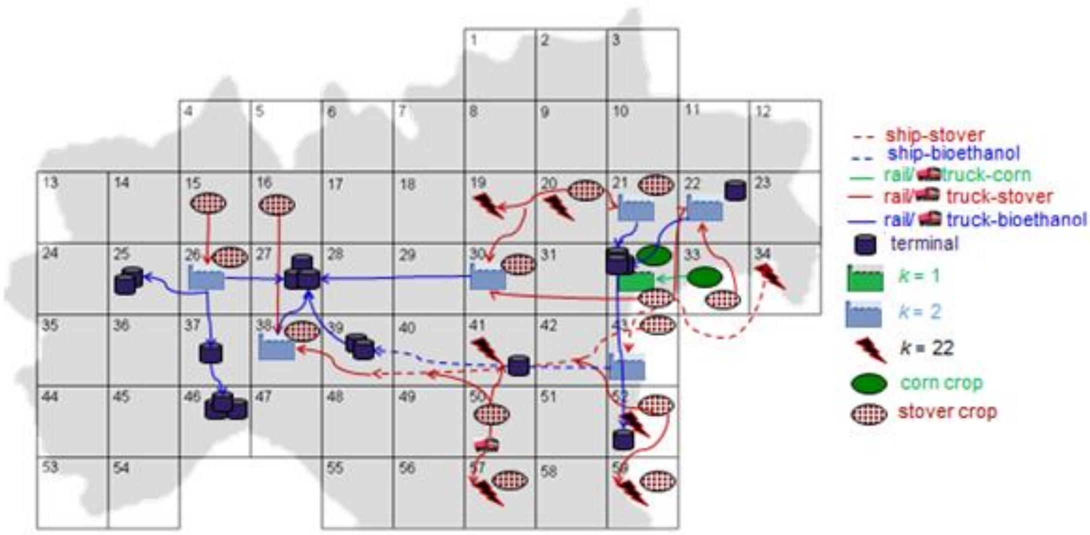


Figure 26 – SC configuration for instance A under environmental optimization

Although this configuration shows a very promising environmental performance, considering the negative economic results, it would only be a feasible solution under a support policy, government subsidy should account for at least 3.35 €/GJ, which adds up to a total of 1.17×10^9 € over the 15 years.

5.2.2 Instance B

Once again, the results from the new and the original models are very similar, but for instance B even though the *NPV* is lower than in instance A, the environmental performance is even better, as presented in Table 6.

Table 6 – Original and new model results for instance B under environmental optimization

	NPV [€]	*NPV* per energy [€/GJ]	GHG emissions [ton of CO_2-eq]	GHG emissions per energy [kg of CO_2-eq/GJ]
Original [4]	-1.7×10^9	-4.84	4.9×10^6	13.98
New	-1.7×10^9	-4.84	4.9×10^6	13.98

In this instance, not only the total *NPV* and the NPV_{chain} (-1.68×10^9 €) are negative, but also the NPV_{car} (-1.47×10^7), consequence of the low EVs market share at t=5 of 1.8%. This poor economic performance is compensated by the low GHG emissions of about 16% of the ones related to petrol. Since there is no fixed demand for ethanol or power, only the technology LCEP (k=2) is used to produce 1.18×10^7 tons of ethanol and the consequential 9×10^6 MWh of by-product electricity, whereas no DDGS is produced. This results in a total income of 9.19×10^9 € and a total of variable costs of 4.88×10^9 €. The distributions of the incomes and the variable costs are presented in Figures 27 and 28. As opposed to what happened in the other three cases, only one biomass type is used. A total of 4.42×10^7 tons of stover are produced in 13 locations spread throughout Northern Italy, which is then transported by rail, truck, barge and ship to the conversion facility, from where the ethanol is sent to the blending terminals by rail or barge. The final SC configuration (at t=5) is presented in Figure 29.

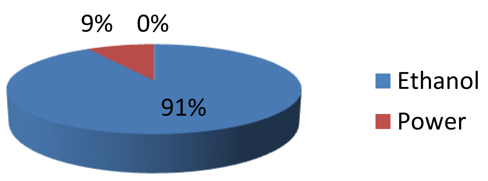


Figure 27 – Share of the incomes by product sold for instance B under environmental optimization

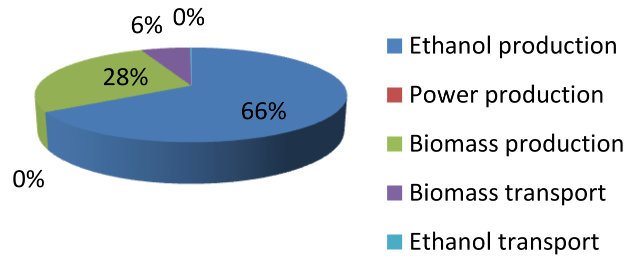


Figure 28 – Share of the variable costs per SC stage for instance B under environmental optimization

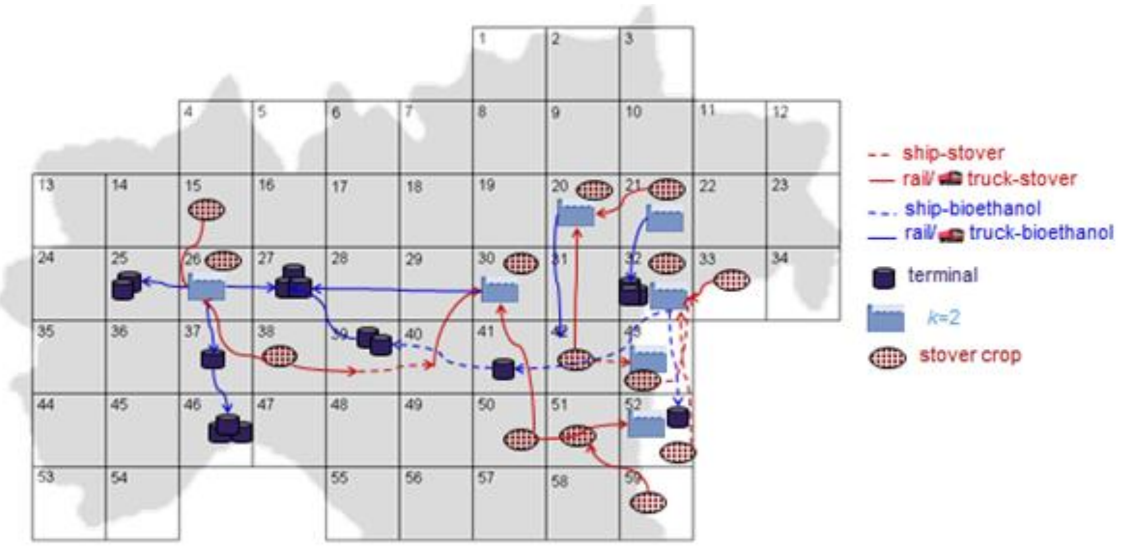


Figure 29 – SC configuration for instance B under environmental optimization

Although this configuration shows a very promising environmental performance, considering the negative economic results, it would only be a feasible solution under a support policy, government subsidy should account for at least 4.84 €/GJ, which adds up to a total of 1.70×10^9 € over the 15 years.

5.3 Multi-objective optimization

The multi-objective optimization joins the economic and the environmental optimizations in one objective function, and presents the multiple SC configurations and results from the different solutions as the weight of one objective grows and the other one decreases in the objective function.

To develop the multi-objective optimization for this model the ε-constraint method was applied. The Pareto curve was obtained for instance B and is presented in Figure 30.

As expected the Pareto curve shows a trade-off between environmental and economic performance. The extreme cases were reported in the previous sections. In the environmental optimization only stover is used to produce mostly ethanol (91% of total energy production) in LCEP facilities. As the objective function moves towards the economic optimization, the production of power becomes more relevant (reaching 40% of global energy production). As this happens, ethanol production is done via DGP from corn instead of stover and power production is done in G+TG and G+MCI from Arundo Donax.

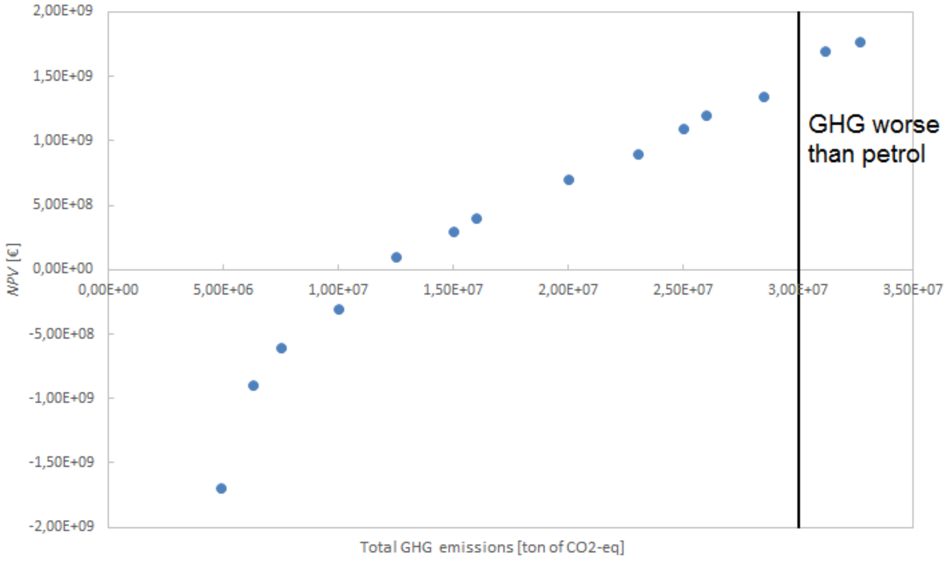


Figure 30 – Pareto curve under multi-objective optimization for instance B

5.4 Chapter conclusions

The first objective of this thesis is to study the profitability and environmental impact of a bioenergy SC that has bioethanol and bio-power as outputs to supply the vehicles market, considering several different biomass feedstocks and conversion technologies, while understanding how the addition of several types of biomasses can influence the economic and environmental performances of a bioethanol and bio-power SC. The model was run for optimizing both performances, considering a fixed ethanol and power demand (instance A) and a global energy demand leaving the output rates as a decision variable (instance B). From the solutions obtained several conclusions were made.

When the economic performance is optimized, the economic results are very promising, especially for instance B as can be seen in Figure 31.

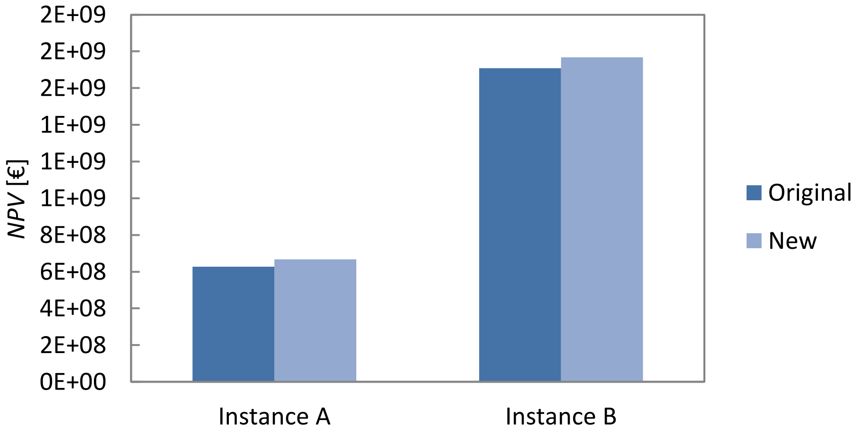


Figure 31 – Economic performance for instance A and B, for the new and the original models, under economic optimization

Table 7 – SC structure summary for the main model results

	Biomass [ton]	Technology	Number of plants	Power [MWh]	Ethanol [ton]
Instace A Economic optimization	Corn $3.42x10^7$ Arundo Donax $7.33x10^6$	k=1 k=22 k=33	6 1 12	$1.23x10^7$	$1.14x10^7$
Instace B Economic optimization	Corn $2.37x10^7$ Arundo Donax $2.25x10^7$	k=1 k=22 k=33	3 7 20	$3.85x10^7$	$7.86x10^6$
Instace A Environmental optimization	Corn $7.61x10^6$ Stover $3.65x10^7$	k=1 k=2 k=22	1 6 7	$1.23x10^7$	$1.14x10^7$
Instace B Environmental optimization	Stover $4.42x10^7$	k=2	7	$9.00x10^6$	$1.18x10^7$

The inclusion of new different biomass types as feedstock option in the model had a positive influence in the results, with an increase on the *NPV* of 6% and 3% on instances A and B, respectively, when compared to the original formulation. The main difference between the new and the original SC designs is the use of Arundo Donax instead of stover to produce power.

In terms of SC configuration, for both instances the solution presented a mix between first generation biorefineries (*k*=1) for ethanol production and gasification plants (*k*= 22, 33) for electricity generation.

A summary of the results regarding the SCs configurations is presented in Table 7.

Although the values for NPV_{chain} of both instances are quite similar, the big difference in the *NPV* value is a consequence of the result for the NPV_{car}, which is much higher in instance B, supported by a big EVs market share of about 12% at *t*=5 against the 3.26% of instance A.

The downside of these configurations is their environmental performance. The total GHG emissions both for instance A and B are, respectively, 10% and 9% superior to the ones related to petrol (85.8 kg of CO_2/GJ).

Regarding the environmental optimization, the addition of the new biomasses did not have any noticeable consequences on the performance, as it is shown in Figure 32. Even though one of these new biomasses is considered to be a residue from forestry activities, as it happened in the original model the preferred biomass for power production is still stover, which is also a residue. This happened because, since there is no fixed demand for power and ethanol, the production of ethanol was promoted by the solver in DGP (*k*=1) and LCEP (*k*=2) technologies, which bury fewer environmental impacts. Electricity production is only done in LCEP as a by-product.

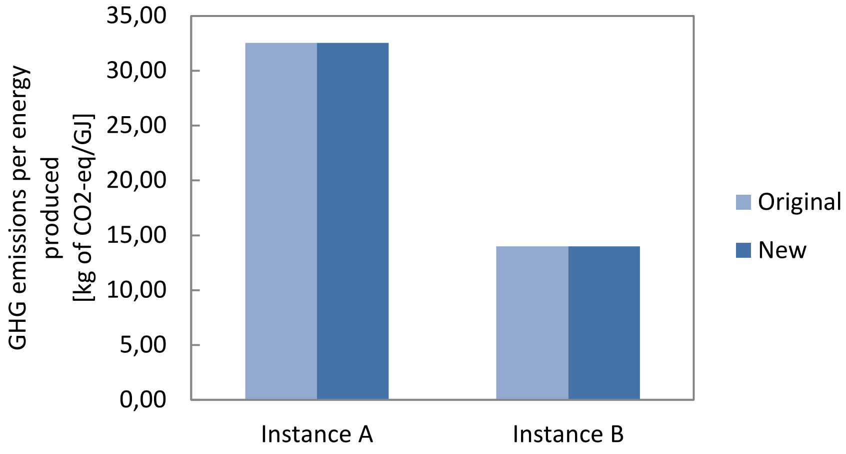


Figure 32 – Environmental performance for instance A and B, for the new and the original models, under environmental optimization

Although both instances present very good environmental performances with GHG emissions much lower than the ones associated to petrol, these configurations are unfeasible, given the fact that their *NPV* is negative. The operation of these systems would only be possible under a strong support policy, with governmental incentives of 3.35 €/GJ for instance A and 4.84 €/GJ for instance B, which adds up to a total of 1.17×10^9 € and 1.70×10^9 € over the 15 years, respectively.

In the multi-objective optimization for instance B, starting with the best environmental performance, only stover is used to produce mostly ethanol in LCEP facilities. Moving towards the economic optimization, the production of power becomes more relevant, the biomass types selected change from only stover to stover in technologies LCEP and G+TG, and wood in G+MCI. Afterwards the ethanol production is done via DGP from corn instead of stover and power production is done in G+TG and G+MCI from Arundo Donax. Direct combustion (*k*=11) and Miscanthus and Poplar are never an option for the solver.

6. Application of the different environmental impact assessment methods

This chapter analyzes the influence of applying different methods to assess the environmental impacts on the SC design and economic performance. Five different LCIA methods (*ReCiPe, Ecological Scarcity 2013, EDIP 2003, EPS 2000* and *Impact 2002+*), that were presented in the chapter dedicated to the state of the art (section 3.3), were applied and the model was solved under environmental optimization for instance B, once it has the most flexible formulation and therefore might present more significant differences between the five solutions. The solutions presented result from the environmental optimization, since the economic aspects of the formulation were not modified.

This chapter is divided in three sections: section 6.1 presents the results obtained regarding the SCs structures and economic performances for the application of the different methods, section 6.2 presents a comparison between the results obtained and section 6.3 presents the chapter conclusions.

6.1 Supply chain structures

To perform this study, some modifications were made to the main model which was used in the previous chapter. All the changes and assumptions made were described in the section 4.2. Each of the five methods considered includes a different set of impact categories, characterizing the diverse environmental areas affected. These impacts were implemented in the model as a normalized value, so that after they have been weighted in the model whit the respective flow it is possible to sum them all into a single score impact for each of the five methods. These normalized values were obtained in similar conditions (Table B1) from the commercial software *SimaPro 8.2.3.0* and are presented in Table B2 in Appendix B.

The solutions obtained considering the environmental optimization are presented in this section. From all the elements of the SCs just the number and type of conversion facility, the output rates and the biomass feedstock are analyzed, due to their considerable impact on the final economic performance, comparing to the other components of the SC. Moreover, only the economic results are compared, since the model uses single impact scores that cannot be compared amongst the different methods, due to the fact that each of them assesses the environmental impacts considering different categories and using different normalization techniques.

Ecological Scarcity 2013

The first results presented are related to the environmental optimization applying *Ecological Scarcity 2013*. The *NPV* of this solution is about -2.31×10^{9} €, which is lower than the solutions obtained previously. As it is possible to see in Figure 33, the best performance comes from producing ethanol (90% of total energy production) and power as a by-product in 8 LCEP (k=2) facilities from

Miscanthus, which is produced in 9 different locations. This configuration clearly promotes ethanol production instead of power, consequence of several aspects such as: slightly higher conversion efficiencies for ethanol; relatively low emissions from Miscanthus growth when compared to the other biomass types that can be used to produce ethanol; the fact that by using LCEP technology power is also being produced, helping to satisfy the energy demand without adding more environmental impacts than the ones that were already accounted for ethanol; and finally, it is trying to avoid the impacts related to battery production, even though this increases the impacts from bifuel vehicles circulation. It is also possible to see that the impacts related to the transportation system are being minimized by placing the crops near to the facilities.

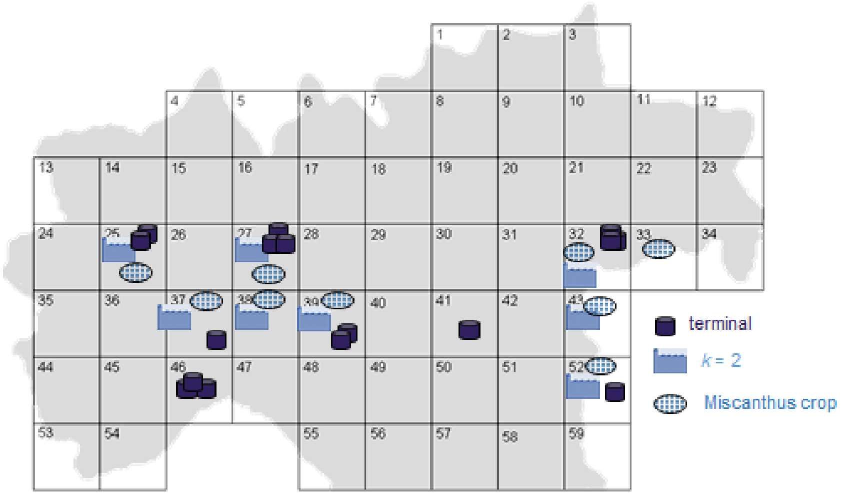


Figure 33 – SC configuration for instance B under environmental optimization applying *Ecological Scarcity 2013*

Figure 34 presents the distribution of the environmental impacts of the SC stages:

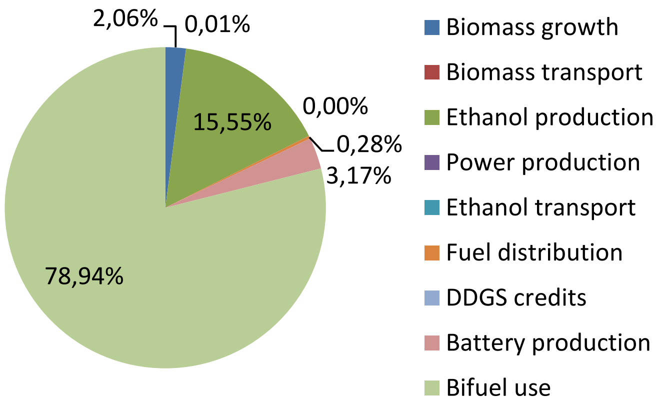


Figure 34 – Impact per SC stage applying *Ecological Scarcity 2013*

It is possible to verify that the activity that produces the biggest impact is driving the bifuel vehicles, followed by ethanol production. These results make sense, considering that in this scenario most of the energy demand is satisfied by ethanol, which results in a low number of EVS and a higher number of bifuel vehicles circulating. DDGS and power production have zero impact in this case, because

DDGS is not produced at all and power is only produced as a by-product, so its emissions are already taken into account.

Regarding the impact categories, as it is possible to see in Table B3 in Appendix B, Global warming, Main air pollutants and Carcinogenic substances into air are the three that contribute mostly to the total impacts, accounting for 80% between them.

EDIP 2003

When *EDIP 2003* is applied the solution presents an *NPV* of -6.66x10^8 €.

The best environmental performance is a result of producing ethanol from corn in two DGP facilities and from stover and Miscanthus in three LCEP (*k*=2) facilities, which also produce power as a by-product. The remaining power production is done in seven G+TG plants (*k*=22), using Arundo Donax as feedstock. Power accounts for 41% of total energy produced. Although the production of ethanol instead of power can bring the same advantages stated before, in this case there is a much higher production of power that can be explained by the fact that using *EDIP 2003* the production of battery has a negative single impact score (see Table B2 in Appendix B), that accounts for emission credits, and therefore the use of EVs is promoted by increasing the power production. The fact that, in this case, several types of biomass and different technologies are used for ethanol production is a result of trying to avoid transportation related impacts by placing the facilities close to the crops, which are situated in the grid elements where the biomass production yields are higher. Meaning that using biomasses that have slightly higher production impacts in this locations is still better that producing a biomass type that presents fewer impacts in grid elements where the yield would be lower and therefore more crops would be needed, as well as more biomass transportation.

The SC structure is presented in Figure 35.

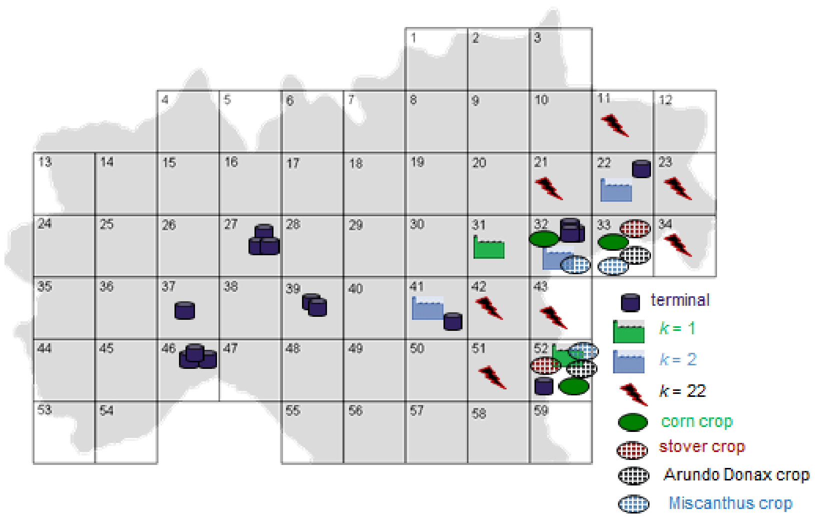


Figure 35 – SC configuration for instance B under environmental optimization applying *EDIP 2003*

Figure 36 presents the distribution of the environmental impacts of the SC stages.

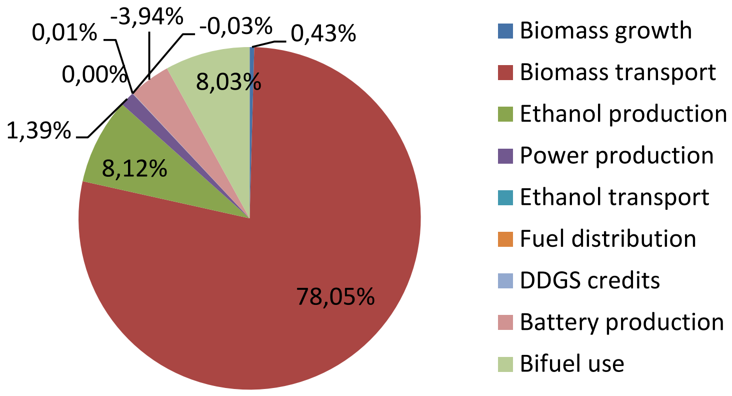


Figure 36 – Impact per SC stage applying *EDIP 2003*

The stage with greater contribution to the global impact is the biomass transport, consequence of the big amount of biomass produced and the distance it needs to travel from the crop location to the conversion sites, even though the facilities are relatively close to the crops. As it is possible to see, battery production accounts for negative impacts, which can be seen as emission credits. The other negative value is related to DDGS production.

As it is shown in Table B4 in Appendix B, the environmental impacts related to each category are balanced, being Ecotoxicity soil chronic, Human toxicity air and Acidification the ones with the highest share, although together they only account for 27% of the total emissions.

EPS 2000

Applying the *EPS 2000* assessment method results in a solution that presents an *NPV* of -1.22×10^{9} €. The best environmental performance with this method is a result of producing ethanol in four DGP and six LCEP facilities, with power, representing only 5% of the total energy production, being produced as a by-product. To feed the DGP (k=1) facilities, corn is produced in six locations and in the LCEP (k=2) facilities, ethanol and power have stover and Miscanthus as feedstock, produced in six and two different sites, respectively. As it happened with *Ecological Scarcity 2013*, there is a clear bet on ethanol production, consequence of the already presented advantages of producing ethanol instead of power, namely, the higher conversion efficiencies, the production of power in LCEP without accounting for its impacts and the avoided impacts related to batteries production. Similarly to the solution obtained using *EDIP 2003*, several types of biomass and different technologies are used for ethanol production, which can be explained as an effort to avoid transportation related impacts by locating the facilities close to the crops, which are situated in the grid elements where the biomass production yields are higher, despite the fact that one DGP facility is located in g=25, which is near a demand center, and therefore helps minimizing the ethanol distribution impacts.

The SC structure is presented in Figure 37.

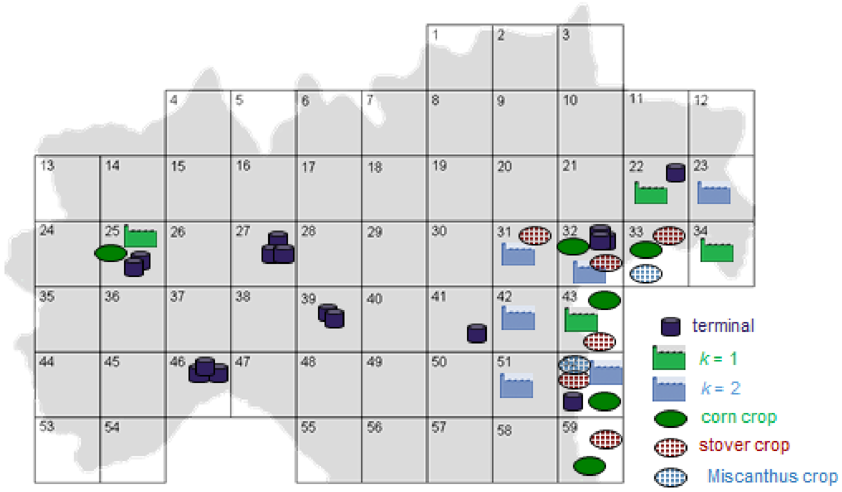


Figure 37 – SC configuration for instance B under environmental optimization applying *EPS 2000*

Figure 38 presents the contribution of each operation to the total environmental impact.

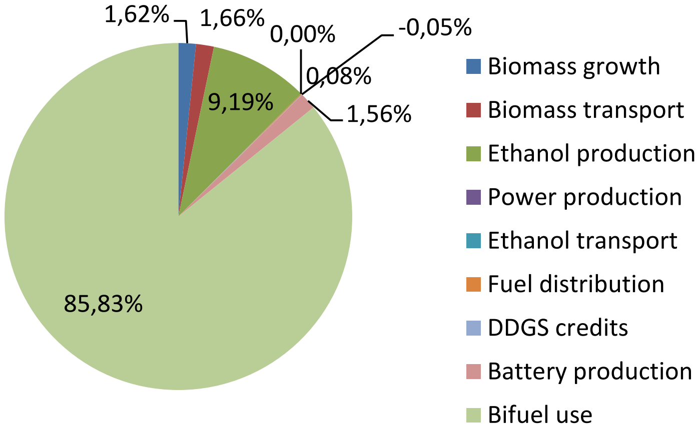


Figure 38 – Impact per SC stage applying *EPS 2000*

As happened for the first method studied, the activity that shows the biggest contribution for the global impact is driving bifuel vehicles, which can be explained by the small quantity of EVs circulating. This results in a huge production of ethanol, which explains why that activity is the second one that generates more environmental impact. Once again the impacts related to power production are considered inexistent because power is only produced as a by-product, so its emissions are taken into account for ethanol production.

Regarding the impact categories, as it is possible to see in Table B5 in Appendix B, Depletion of reserves, Life expectancy and Severe morbidity are the three that contribute mostly to the total impacts, accounting for 98% between them.

Impact 2002+

The application of *Impact 2002+* resulted in an *NPV* of -1.47x10^9 €. This value is a consequence of a SC where ethanol is produced in three DGP (*k*=1) facilities and power, that accounts for 7% of global energy produced, is produced as a by-product in five LCEP (*k*=2) plants along with the remaining ethanol production. The biomass types used as feedstock are the same ones used with the previous method, but this time Arundo Donax is also used, as it is presented in Figure 39.

Once again, there are no facilities that produce only power, consequence of the environmental advantages in producing ethanol already exposed above. As happened before, while trying to reduce the environmental impacts associated with the transportation system, all the crops and facilities are located nearby. The use of different types of biomass and production technologies shows that using biomasses that have slightly higher production impacts is this locations is still better that producing a biomass type that presents fewer impacts in grid elements where the yield would be lower and therefore more crops would be needed, as well as more biomass transportation.

Biomass transportation is the activity that accounts for almost all of the environmental impacts measured with this method. Even though the conversion facilities are relatively close to the crops as an effort to try to minimize the transport impacts, these values come as consequence of the high amount of biomass produced and the distance it needs to travel from the crop location to the conversion sites. Although there is DDGS production, the emissions credits related are almost negligible in the total impact.

As it is shown in Table B6 in Appendix B, the environmental impacts related to each category are quite balanced, being Respiratory inorganics, Global warming and Non-renewable energy the ones with the highest share, although together they only account for 21% of the total emissions.

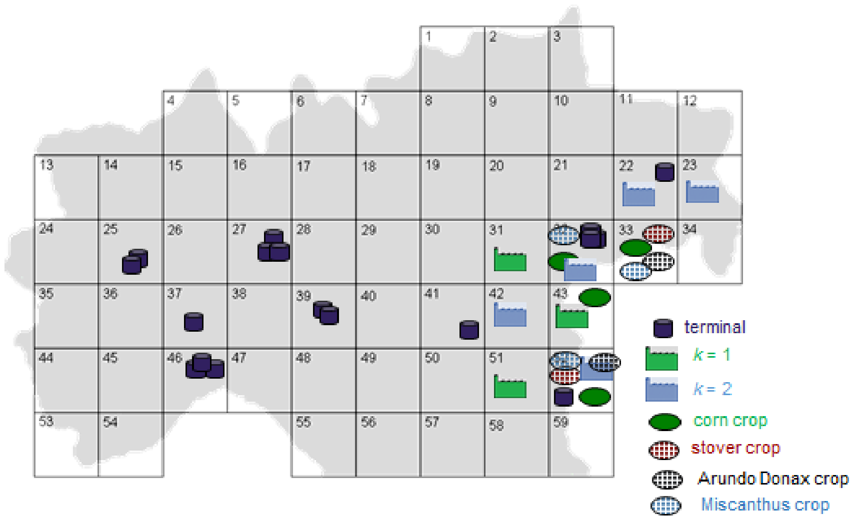


Figure 39 – SC configuration for instance B under environmental optimization applying *Impact 2002+*

Figure 40 presents the contribution of each operation to the total environmental impact.

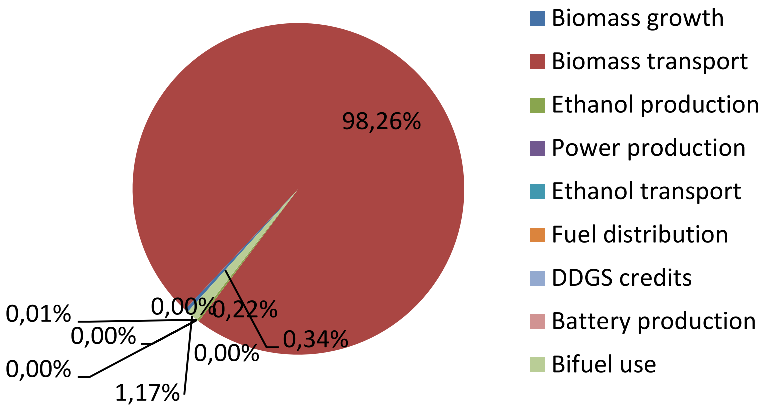


Figure 40 – Impact per SC stage applying *EPS 2000*

ReCiPe

The solution considering the *ReCiPe* method is very similar to the one presented above for *Impact 2002+*, with an *NPV* of -1.69x10^9 €. The conversion technologies and the types of biomass used are the same as in *Impact 2002+* with the difference that in this case there are two DGP (*k*=1) and six LCEP (*k*=2) facilities used to produce the same quantity of each product as before. The SC configuration is presented in Figure 41 and it is a consequence of the reasons already exposed for *Impact 2002+*.

As it is possible to see in Figure 42, once again the biggest share in the total impacts belongs to biomass transportation. Ethanol production and bifuel vehicle use are the activities with the next biggest percentag, which makes sense considering the reduced number of EVs circulating. There are no impacts related to power production because, as before, power is produced only as a by-product.

Regarding the impact categories, as it is possible to see in Table B7 in Appendix B, the contribution of each one is very balanced, Natural land transformation, Human toxicity and terrestrial toxicity are the three that present the highest share, accounting for 24% between them.

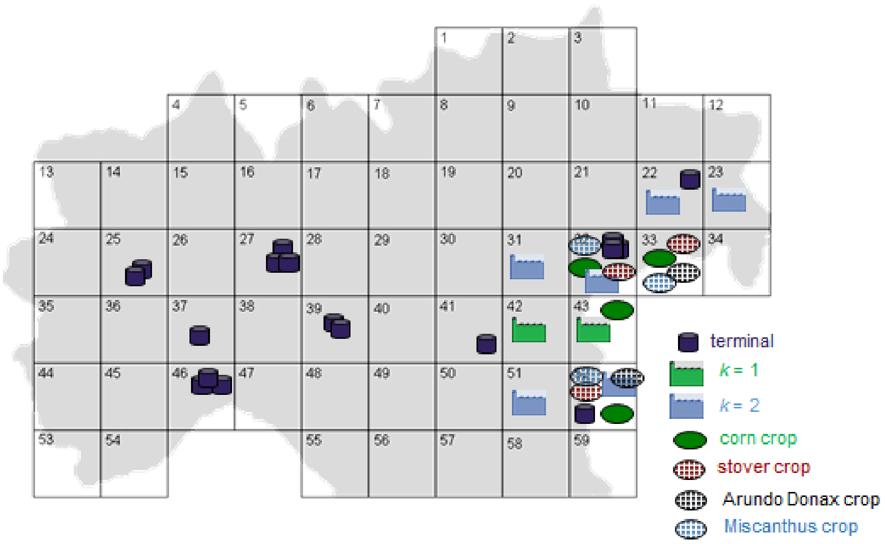


Figure 41 – SC configuration for instance B under environmental optimization applying *ReCiPe*

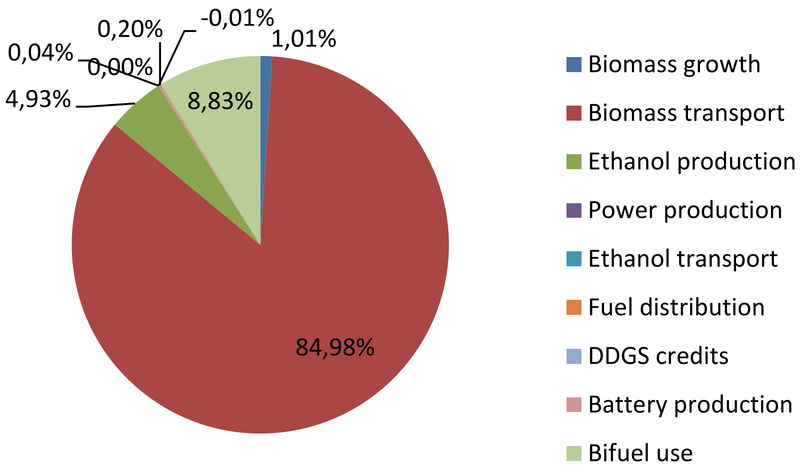


Figure 42 – Impact per SC stage applying *ReCiPe*

6.2 Comparison between the five methods

Comparing the environmental performances of all the solutions from the application of the different methods is not reasonable, once that each method assesses the impacts through different categories and different normalized values, which results in very different final single impact scores from method to method. Therefore, a comparison of the results regarding economic performance and SC structure is presented in this section.

Once the five methods reported in this chapter were applied, it was possible to conclude that the method chosen influences the decisions of the SCs design, since the configuration was different for each method and also different from the results of the previous chapter, where the environmental performance was analyzed only based on the total CO_2-eq emissions.

Not only is the number of plants and type of technologies used different between the solutions, but also the biomass types used as feedstock vary from method to method. In the solution from the original formulation only stover was chosen. With the implementation of the new methods other combinations of biomass were chosen: with *Ecological Scarcity 2013* only Miscanthus is part of the solution; with *EPS 2000* the biomasses used were corn, stover, and Miscanthus; for the remaining methods, corn, stover, Miscanthus and Arundo Donax were the chosen biomass types. However, the SCs structure is not the only issue affected by the implementation of the different methods.
Table 8 presents a summary of the results regarding the SCs configurations and the *NPV*s for the five solutions obtained using the different methods, as well as the one obtained through the original formulation and already presented in the previous chapter, for comparison.

Table 8 – SC structure summary and *NPV* for the different methods

	Biomass type	Technology	Number of plants	Power [MWh]	Ethanol [ton]	*NPV*[€]
Ecological Scarcity 2013	Miscanthus	*k*=2	8	9.00×10^6	1.18×10^7	-2.31×10^9
EDIP 2003	Corn Stover Arundo Donax Miscanthus	*k*=1 *k*=2 *k*=22	2 3 7	3.89×10^7	7.80×10^6	-6.66×10^8
EPS 2000	Corn Stover Miscanthus	*k*=1 *k*=2	4 6	4.84×10^6	1.24×10^7	-1.22×10^9
Impact 2002+	Corn Stover Arundo Donax Miscanthus	*k*=1 *k*=2	3 5	7.04×10^6	1.21×10^7	-1.47×10^9
ReCiPe	Corn Stover Arundo Donax Miscanthus	*k*=1 *k*=2	2 6	7.15×10^6	1.20×10^7	-1.69×10^9
CO_2-eq	Stover	*k*=2	7	9.00×10^6	1.18×10^7	-1.70×10^9

6.3 Chapter conclusions

The second goal of this thesis was to analyze the effect of using different methods to calculate the global environmental impact in the bioenergy SC configuration and economic performance. It was possible to verify that the utilization of the different methods had influence not only on the SC structure, but in the final economic performance as well.
Although all the configurations are different in terms of biomass type, number and type of technologies used, there was a similar criterion in four of the solutions presented, which was promoting ethanol production instead of power, consequence of several aspects such as: slightly higher conversion efficiencies for ethanol; the fact that by using LCEP technology power is also being produced, helping to satisfy the energy demand without adding more environmental impacts than the ones that were already accounted for ethanol; and finally, it is trying to avoid the impacts related to battery production,

even though this increases the impacts from bifuel vehicles circulation. The exception was when *EDIP 2003* was used, where the production rates were more similar to each other, given the fact that in this case the production of batteries had a negative environmental impact, that the model accounted as emission credits and therefore the use of EVs was promoted, increasing the power production.

The differences are not only related to the SCs configurations, in terms of economic performance *NPV* values go from -2.31×10^9 €, obtained using *Ecological Scarcity 2013*, to -6.66×10^8 €, using *EDIP 2003*. This variation of about 1.64×10^9 € cannot be ignored by the decision makers of the SCs design.

The methods applied were not created in the same locations or in the same conditions and furthermore, the values used for the environmental impacts follow a different normalization process for each method. Having this in mind, the decision makers must be rigorous when selecting the environmental impact assessment method to be used, according to the purpose and scope of the project.

7. Price sensitivity analysis

The market prices for ethanol and power were taken from the work by d'Amore and Bezzo [4] and are set to be constant during the time horizon for the problem. This scenario does not correspond to reality, where these values are constantly changing. The goal of this chapter is to test the model's results and reliability and it is divided in two sections: section 7.1 presents the results obtained and in section 7.2 the conclusions regarding the model's robustness are made.

7.1 Price sensitivity analysis results

A sensitivity analysis was made on the prices of ethanol and power, to study how the model solutions change, according to the price fluctuations, in terms of economic performance and SC structure. The model was run four times for instance B, considering all the possible combinations between the prices variation, under economic optimization. The variation of prices was done by increasing and decreasing the prices of ethanol and power in 5% and the values used as well as the combinations considered are presented in Table 9.

Table 9 – Combinations between price variations

Scenario	Ethanol price [€/ton]	Power price [€/MWh]
1	745.5	94.5
2	745.5	85.5
3	674.5	94.5
4	674.5	85.5

The results obtained are presented in Table 10.

Table 10 – Economic results for price sensitivity analysis

Scenario	*NPV* [€]	NPV_{car} [€]	% EV
1	$1.85\text{x}10^9$	$1.27\text{x}10^9$	11.52
2	$1.83\text{x}10^9$	$1.29\text{x}10^9$	11.77
3	$1.69\text{x}10^9$	$1.28\text{x}10^9$	11.66
4	$1.65\text{x}10^9$	$1.28\text{x}10^9$	11.77

As expected, the best result for the *NPV* was achieved when the prices of both products are 5% superior to the ones used in the model, and the worst *NPV* is presented when both prices are 5% lower. When ethanol price is higher and power is lower, a better economic performance was achieved than when the prices are set the other way around, mostly due to the fact that its production rate is always higher than the one of power.

The SCs structures do not change much between the four cases, ethanol is produced in three DGP facilities (k=1) with imported corn (from g=60) as feedstock, and power production is done among a similar number of plants of technologies G+TG (k=22) and G+MCI (k=33), using Arundo Donax as a biomass input. This results in also quite similar production rates and EVs market share between the four cases. A summary of the SCs configurations is presented in Table 11.

Table 11 – SC structure summary for price sensitivity analysis

Scenario	Biomass type	Technology	Number of plants	Power [MWh]	Ethanol [ton]
1	Corn Arundo Donax	k=1 k=22 k=33	3 5 34	$3.69x10^7$	$8.07x10^6$
2	Corn Arundo Donax	k=1 k=22 k=33	3 6 33	$3.84x10^7$	$7.87x10^6$
3	Corn Arundo Donax	k=1 k=22 k=33	3 8 30	$3.81x10^7$	$7.91x10^6$
4	Corn Arundo Donax	k=1 k=22 k=33	3 5 34	$3.78x10^7$	$7.95x10^6$

7.2 Chapter conclusions

A sensitivity analysis on the market prices of ethanol and power was performed, in order to study their effect on the solution presented. The prices were increased and decreased by 5% and all the combinations between these variations were tested in the model. The *NPV* oscillated about 10.8% between $1.85x10^9$ € and $1.65x10^9$ €, with the higher value being achieved when both prices were 5% bigger and the lower value when both prices were 5% smaller, as expected. Comparing to the *NPV* obtained with the original prices, there was a difference of 4.5% and -6.8%. When power price was lower and ethanol was higher, a worse economic performance was achieved than when the prices are set the other way, which means that the fluctuation of ethanol price has a bigger influence on the *NPV*. This happens not only because the original price of ethanol is much higher than the one of power, but also because its production rate is higher.

Regarding the SCs structures, there were not considerable differences between the four cases and the original, which resulted in quite similar production rates and EVs market penetration. In all the cases ethanol is produced from corn in DGP technology (*k*=1), and power production is done with technologies G+TG (*k*=22) and G+MCI (*k*=33), using Arundo Donax as a biomass input.

It is possible to conclude that this variation of the prices has a slightly noticeable impact on the *NPV* mainly due to the variation on the price of ethanol. On the other hand, it does not have much of an influence on the SC design, considering that the production rates and the SC configurations are always very similar. In this sense it is possible to conclude that the model presents robust solutions, considering that the economic performance and the SC structure do not suffer a big variation with the products' market prices fluctuations.

8. Conclusion and future work

This thesis aims to assess if the sustainable production of bioenergy can be competitive. To do so, two objectives must be fulfilled: the maximization of the economic performance and the minimization of the total environmental impacts of a bioenergy SC to supply vehicles as a final market considering bioethanol and bio-power production in Northern Italy; and study the influence of choosing different environmental impact assessment methods in the SC structure and economic performance. To assess these problems a MILP model based on the models previously developed by Zamboni et al. [1, 2], Giarola et al. [3] and d'Amore and Bezzo [4] was applied and implemented in GAMS®.

The problem comes as a consequence of the growing concern about the usage of fossil fuels, mainly in the transport sector, due to the depletion of reserves and mostly because of the environmental impacts associated. The model assesses the best way to supply energy for an alternative vehicles market, in order to be not only environmentally sustainable, but also economically competitive. The supply of energy can be done from ethanol or electricity, which can both be produced in multiple technologies and from a diverse set of biomass feedstock. The problem was studied from two perspectives: in instance A the ethanol and power demands are fixed, and in instance B there is a global energy demand defined, allowing the solver to adjust the production rates of ethanol and power.

The addition of Arundo Donax, Miscanthus, Poplar and wood residues from forestry activities in the model as biomass types as feedstock option had a positive influence in the economic performance, with an increase on the *NPV* of 6% and 3% on instances A and B, respectively, when compared to the original formulation [4]. The main difference between the new and the original SC structure is the use of Arundo Donax instead of stover to produce power. In terms of SC configuration, for both instances the solution presented a mix between first generation biorefineries (k=1) for ethanol production and gasification plants (k=22, 33) for electricity generation, which accounts for 16% of total energy produced in instance A and 40% in instance B . Although the values for NPV_{chain} of both instances are quite similar, the big difference in the *NPV* value is a consequence of the result for the NPV_{car}, which is much higher in instance B, supported by a big EVs market share of about 12% at t=5 against the 3.26% in instance A. The downside of these configurations is their environmental performance. The total GHG emissions both for instance A and B are, respectively, 10% and 9% superior to the ones related to petrol.

Regarding the environmental optimization, the addition of the new biomasses did not have any noticeable consequences on the performance. Even though one of these new biomasses is considered to be a residue from forestry activities, as it happened in the original model the preferred biomass for power production is still stover, which is also a residue. This happened because, since there is no fixed demand for power and ethanol, the production of ethanol was promoted by the solver in DGP (k=1) and LCEP (k=2) technologies, which bury fewer environmental impacts. Electricity production is only done in LCEP as a by-product.

Although both instances present very good environmental performances with GHG emissions of 38% and 16%, respectively for A and B, from the ones associated to petrol, these configurations are unfeasible, given the fact that their *NPV* is negative. The operation of these systems would only be possible under a strong support policy, with governmental incentives of 3.35 €/GJ for instance A and 4.84 €/GJ for instance B, which adds up to a total of 1.17×10^9 € and 1.70×10^9 € over the 15 years, respectively.

The second objective of this thesis was to analyze the effect of using different methods to assess the environmental impacts on the SC structure. Each of these methods uses different impact categories and normalization rules for the values attributed to those categories to assess the total impacts.
Applying the methods, different SC configurations and economic performances were obtained for all of them. Although the SC design varies a lot from method to method, not only in terms of the conversion technologies used, but also in terms of the biomass type used as feedstock, all the solutions presented a higher ethanol production rate. The variation in the economic performance, which goes from -2.31×10^9 € to -6.66×10^8 € cannot be ignored. In this sense, before developing a bioenergy SC project, the decision makers must select the adequate environmental impact assessment method to be used, according to the purpose and scope of the project.

In order to take this SC model further, it could be interesting to implement other conversion technologies, namely second generation biorefineries, and explore further the utilization of organic residues present in agroindustrial, forestry, zootechnical, fishery, and municipal leftovers that could improve biorefineries and bio-power plants competitiveness and the SC environmental performance.
This work also leaves another future research path, where the different LCIA methods should be analyzed in more detail so that some guidelines can be given to the user in terms of the best method to apply for the different situations.

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Appendixes

Appendix A – Model parameters

Table A1 – Ethanol (*TDeth$_t$*) and power (*TDpow$_t$*) demands, ethanol blending (*etperc$_t$*) and EVs market share (*EVm$_t$*) (instance A) and global demand (*TD$_t$*) (instance B) for each time period *t* [4]

t	Instance A				Instance B
	TDeth$_t$ [kton/year]	*TDpow$_t$* [ktee/year]	*etperc$_t$* [%^{vol}]	*EVm$_t$* [%]	*TD$_t$* [kton/year]
1	557	36	10.20	0.65	593
2	659	73	12.10	1.30	732
3	761	109	14.00	1.95	870
4	857	146	15.80	2.61	1003
5	953	182	17.60	3.26	1135

Table A2 – Biomass yields for Arundo Donax, Miscanthus and Poplar

	Arundo Donax		Miscanthus		Poplar	
	Biomass yield [ton/ha/year]	Reference	Biomass yield [ton/ha/year]	Reference	Biomass yield [ton/ha/year]	Reference
	37.7	[102]	28.7	[102]	9	[103]
	35	[103]	22.1	[104]	20	[103]
	45	[103, 105, 106]	12.39	[107]	11.2	[108]
	15	[109]	13.04	[107]	10	[112]
	41	[109]	16.5	[111]	12	[114]
	21	[109]	13.1	[113]	10	[114]
	49	[109]	16.2	[115]	18.49	[116]
	35	[117]	18.7	[118]	20	[119]
	49	[117]	15.5	[120]	15	[121]
	37.7	[122]	25	[123]	18	[124]
			12.85	[125]		
Mean value	36.54		17.64		14.37	
Mean value [ton/km^2/month]	304.5		147.03		119.74	

Table A3 – Timber and average biomass production in each region

Region	Timber production [m³/y]	Biomass availability [ton d.b./y]	Average biomass availability for each *g* [ton d.b./m]	Grid elements *g*
Valle d'Aosta	25644	1951.79	81.32	13, 14
Piemonte	564921	42996.70	511.87	4, 15, 24, 35, 44, 45, 53
Lombardia	1750248	133213.13	1387.64	5, 6, 7, 8, 16, 17, 18, 19
Liguria	97252	7401.95	205.61	46, 47, 54
Trentino-Alto Adige	898387	68377.13	1899.36	1, 2, 3
Veneto	313520	23862.32	397.71	9, 10, 11, 20, 21
Friuli-Venezia Giulia	222887	16964.15	471.23	12, 22, 23
Emilia-Romagna	582127	44306.27	461.52	48, 49, 50, 55, 56, 57, 58, 59

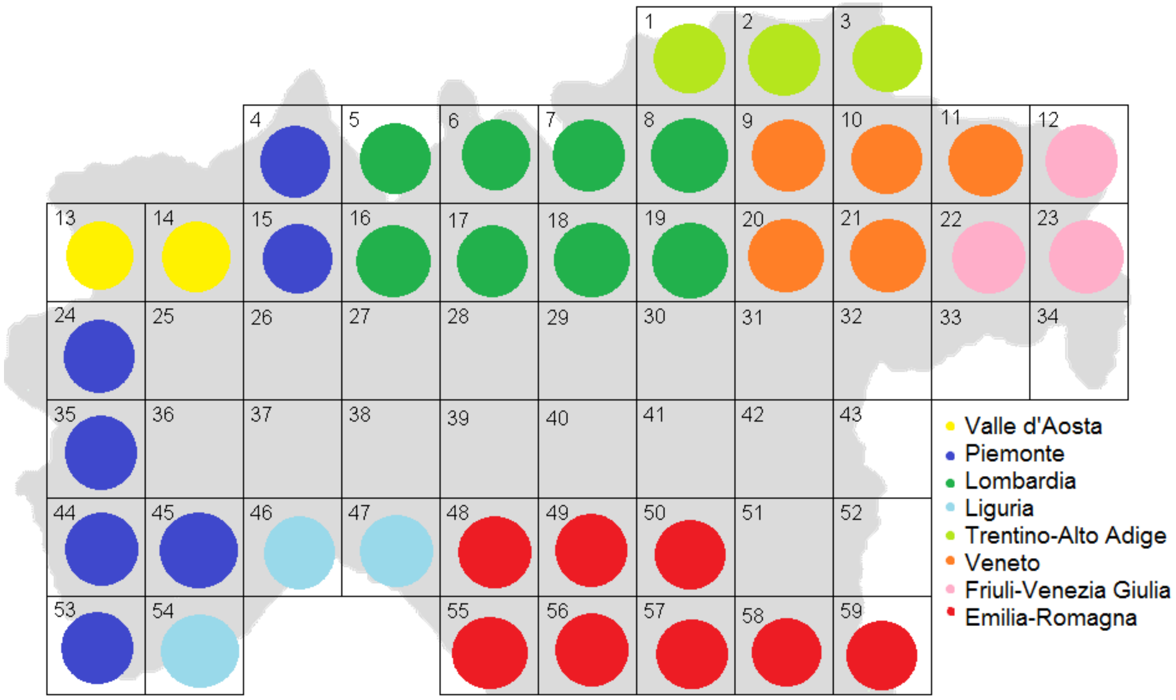

Figure A1 – Grid elements *g* with available woody biomass for each region

Table A4 – Values for purchase costs for Arundo Donax, Miscanthus and Poplar

	Arundo Donax		Miscanthus		Poplar	
	Cost [€/ton]	Reference	Cost [€/ton]	Reference	Cost [€/ton]	Reference
	13	[103]	65.85	[131, 132]	52	[108]
	20	[103]	63	[133]	60	[112]
	23.63	[117]	37.57	[116]	44.1	[116]
	26.53	[122]	59.35	[116]	63.7	[117]
					80	[119]
					100	[120]
Mean value	20.79		56.44		66.63	

Table A5 – Values for ethanol conversion for Arundo Donax and Miscanthus

	Arundo Donax		Miscanthus	
	$\gamma_{i,k}$ [ton eth/ton biomass]	Reference	$\gamma_{i,k}$ [ton eth/ton biomass]	Reference
	0.193 0.223 0.267	[103, 105, 106] [103] [103]	0.315 0.237	[103, 135] [105]
Mean value	0.219		0.276	

Table A6 – Values for LHV and power conversion in all the technologies for Arundo Donax, Miscanthus and Poplar

	Arundo Donax		Miscanthus		Poplar		Wood	
	LHV [MJ/kg]	Reference	LHV [MJ/kg]	Reference	LHV [MJ/kg]	Reference	LHV [MJ/kg]	Reference
	16.8	[103]	17.8	[137]	19.4	[139]	18.5	[128]
	17.5	[136]	18.1	[137]	17.7	[137]		
					21	[112]		
					18.2	[139]		
Mean LHV [MJ/kg]	17.15		17.95		19.08		18.5	
$z_{i,k}$ k=11 [MWh/ton]	1.17		1.23		1.31		1.267	
$z_{i,k}$ k=22 [MWh/ton]	1.76		1.84		1.96		1.899	
$z_{i,k}$ k=33 [MWh/ton]	1.65		1.73		1.84		1.781	

Table A7 – Production capacity, nominal values for each plant size p, ER_p and PR_p

p	ER_p [kton/year]	PR_p [MW]
1	96	1
2	110	5
3	150	10
4	200	15
5	250	30
6	276	60

Table A8 - Capital Investment, values of the linearization parameters, $CI_{p,k}$ [M€]

p	k	1	2	11	22	33
1		62	396	-	4	2
2		70	434	22	10	5
3		91	535	32	14	8
4		115	648	49	21	-
5		139	753	62	26	-
6		151	804	94	39	-

Table A9 – Production Costs, values of the linearization parameters $c_{k,c}$

k	*slope* [€/ton or €/MWh]	*Intercept* [€/month]
1	140.83	169.906
2	202.88	891.755
11	10.71	64.377
22	13.71	45.894
33	2.91	19.805

Table A10 - Emission factors for ethanol ($ffp_{i,k}$) or power ($fpp_{i,k}$) production stages [kg of CO_2-eq/ton of ethanol or MWh]

	$ffp_{i,k}$		$fpp_{i,k}$		
i	k=1	k=2	k=11	k=22	k=33
Arundo Donax	0.00	238.78	1.83	1.36	1.42
Miscanthus	0.00	228.14	1.75	1.30	1.36
Poplar	0.00	0.00	1.64	1.23	1.28
Wood	0.00	0.00	1.69	1.27	1.32

Table A11 - Calculation of mean values of impact factor for biomass *i* production fbg_i [kg of CO2-eq/ton of biomass]

Biomass *i*	GHG balance [kg of CO_2-eq/ha]	Average Yield [ton of biomass/ha]	Emission factor [kg of CO_2-eq/ton]	Reference
Arundo donax	2522	37	68.16	[140]
Arundo donax	2636	18	146.44	[140]
Arundo donax	1080	21	51.43	[112]
Arundo donax	2037	23	88.57	[141]
Arundo donax		Mean value	88.65	
Miscanthus			112.00	[123]
Miscanthus			70.03	[116]
Miscanthus			86.47	[142]
Miscanthus	615	15	41.00	[143]
Miscanthus	1520	10	152.00	[144]
Miscanthus	707	19	37.21	[145]
Miscanthus		Mean value	83.12	
Poplar	325	17	19.12	[146]
Poplar		14	76.94	[147]
Poplar	517	15	34.47	[148]
Poplar		Mean value	43.51	

Table A12 – Parameter $\beta_{i,k}$

Biomass type	Technology *k*																				
	1	2a	2b	2c	2d	2e	11a	11b	11c	11d	11e	22a	22b	22c	22d	22e	33a	33b	33c	33d	33e
Corn	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Stover	0	1	0	0	0	0	1	0	0	0	0	1	0	0	0	0	1	0	0	0	0
Arundo Donax	0	0	1	0	0	0	0	1	0	0	0	0	1	0	0	0	0	1	0	0	0
Miscanthus	0	0	0	1	0	0	0	0	1	0	0	0	0	1	0	0	0	0	1	0	0
Poplar	0	0	0	0	1	0	0	0	0	1	0	0	0	0	1	0	0	0	0	1	0
Wood	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	1	0	0	0	0	1

Appendix B – Application of the different environmental impact assessment methods

Table B1 - Product specifications of data collected from *SimaPro*

Activity	*SimaPro*
Corn production	1 ton Maize, at farm/IT Energy (of project Agri-footprint - gross energy allocation)
Arundo Donax production	1 ton Sugarcane {RoW}| production Conseq, S (of project Ecoinvent 3 - consequential - system)
Miscanthus production	1 ton Miscanthus, chopped {RoW}| miscanthus production Conseq, S (of project Ecoinvent 3 - consequential - system)
Poplar production	1 ton Bundle, energy wood, measured as dry mass {RoW} hardwood forestry, birch, sustainable forest management Conseq, S (of project Ecoinvent 3 - consequential - system)
Wood chips production	1 ton Wood chips, wet, measured as dry mass {CH} hardwood forestry, mixed species, sustainable forest management Conseq, S (of project Ecoinvent 3 - consequential - system)
Truck	1 tkm Transport, freight, lorry 16-32 metric ton, EURO3 {GLO}| market for Conseq, S (of project Ecoinvent 3 - consequential - system)
Barge	1 tkm Transport, freight, inland waterways, barge {GLO}| market for Conseq, S (of project Ecoinvent 3 - consequential - system)
Rail	1 tkm Transport, freight train {Europe without Switzerland}| market for Conseq, S (of project Ecoinvent 3 - consequential - system)
Trans-ship	1 tkm Transport, freight, sea, transoceanic ship {GLO}| market for Conseq, S (of project Ecoinvent 3 - consequential - system)
Ethanol from corn	1 ton Ethanol, without water, in 95% solution state, from fermentation {RoW} ethanol production from maize | Conseq, S (of project Ecoinvent 3 - consequential - system)
Power production direct combustion	1 MWh Electricity, high voltage {IT} heat and power co-generation, wood chips, 6667 kW, state-of-the-art 2014 Alloc Rec, S (of project Ecoinvent 3 - allocation, recycled content - system)
Power production turbo gas	1 MWh Electricity, high voltage {IT}| heat and power co-generation, biogas, gas engine Alloc Rec, S (of project Ecoinvent 3 - allocation, recycled content - system)
DDGS	1 ton Distiller's Dried Grains with Solubles {RoW}| ethanol production from maize Alloc Rec, S (of project Ecoinvent 3 - allocation, recycled content - system)
Batery production	1 kg Battery, Li-ion, rechargeable, prismatic {GLO}| production Conseq, S (of project Ecoinvent 3 - consequential - system)
Bifuel emissions	1 km Transport, passenger car, medium size, petrol, EURO 4 {RER} transport, passenger car, medium size, petrol, EURO 4 Conseq, S (of project Ecoinvent 3 - consequential - system)

Table B2 - Single impact scores per activity per method

Activity	*Ecological Scarcity 2013*	*EDIP 2003*	*EPS 2000*	*Impact 2002+*	*ReCiPe*
Corn growth	1913859.4136	1.6266	171.3678	0.3166	3.9900
Stover growth	459326.2593	0.3904	41.1283	0.0760	0.9576
Arundo Donax growth	242556.3453	0.3502	93.2914	0.5769	0.6427
Miscanthus growth	79962.3082	0.3288	109.3882	-0.1058	0.3414
Poplar growth	225298.9560	0.3848	88.8798	0.5304	0.6543
Wood residues	64323.9491	0.0838	25.7159	0.0262	0.0006
Truck	248.0152	0.0005	0.1163	0.00009	0.0012
Barge	68.3967	0.0001	0.0390	0.00002	0.0004
Rail	73.4073	0.0002	0.0668	0.00002	0.0002
Ship	19.4526	0.00004	0.0074	0.00001	0.0001
Trans-ship	19.4526	0.00004	0.0074	0.00001	0.0001
Ethanol from corn DGP	1820721.8051	57.6409	1912.3064	0.5494	17.2707
Ethanol from stover LCEP	2263968.6865	71.6734	2377.8491	0.6832	21.4752
Ethanol from Arundo LCEP	2760181.0013	87.3826	2899.0216	0.8329	26.1821
Ethanol from Miscanthus LCEP	2190143.6206	69.3362	2300.3106	0.6609	20.7750
Power from stover C+R	296965.3240	0.3718	64.9232	0.1088	0.8804
Power from Arundo C+R	275320.6211	0.3447	60.1912	0.1009	0.8163
Power from Miscanthus C+R	263050.0641	0.3293	57.5086	0.0964	0.7799
Power from Poplar C+R	247471.1033	0.3098	54.1027	0.0907	0.7337
Power from wood C+R	255229.6568	0.3195	55.7988	0.0935	0.7567
Power from stover G+TG	224965.4620	0.3593	178.7550	0.0407	0.3589
Power from Arundo Donax G+TG	208568.5625	0.3331	165.7262	0.0377	0.3328
Power from Miscanthus G+TG	199273.0276	0.3182	158.3401	0.0361	0.3179
Power from Poplar G+TG	187471.2184	0.2994	148.9625	0.0339	0.2991
Power from wood G+TG	193348.6944	0.3088	153.6327	0.0350	0.3085
Power from stover G+MCI	239813.1825	0.3830	190.5528	0.0434	0.3826
Power from Arundo Donax G+MCI	222334.0876	0.3551	176.6641	0.0402	0.3547
Power from Miscanthus G+MCI	212425.0475	0.3393	168.7905	0.0384	0.3389
Power from Poplar G+MCI	199844.3188	0.3192	158.7940	0.0362	0.3188
Power from wood G+MCI	206109.7082	0.3292	163.7724	0.0373	0.3288
DDGS	73282.8753	0.7786	26.4126	0.0131	0.1538
Batery production	7721196.9268	-77.769	11060.688	0.9382	20.2350
Bifuel emissions	403.2306	0.0018	0.7442	0.0001	0.0014

Table B3 - Influence of each impact category in the total impact *Ecological Scarcity 2013*

Category	Percentage of total impact
Global warming	41.48%
Main air pollutants and PM	28.04%
Carcinogenic substances into air	11.00%
Water pollutants	8.39%
Energy resources	5.53%
Heavy metals into air	4.46%
Mineral resources	3.91%
POP into water	2.37%
Heavy metals into water	0.66%
Water resources	0.53%
Pesticides into soil	0.34%
Ozone layer depletion	0.11%
Non-radioactive waste to deposit	0.09%
Radioactive substances into air	0.00%
Noise	0.00%
Radioactive substances into water	-0.02%
Radioactive waste to deposit	-1.80%
Land use	-2.12%
Heavy metals into soil	-2.96%

Table B4 - Influence of each impact category in the total impact *EDIP 2003*

Category	Percentage of total impact
Ecotoxicity soil chronic	13.05%
Human toxicity air	8.21%
Acidification	5.50%
Aquatic eutrophication EP(P)	5.32%
Radioactive waste	5.27%
Ozone formation (Human)	5.07%
Human toxicity water	5.02%
Human toxicity soil	4.97%
Bulk waste	4.92%
Global warming 100a	4.88%
Ozone formation (Vegetation)	4.84%
Aquatic eutrophication EP(N)	4.73%
Terrestrial eutrophication	4.69%
Ecotoxicity water chronic	4.55%
Ecotoxicity water acute	4.53%
Slags/ashes	4.48%
Ozone depletion	4.48%
Hazardous waste	4.47%
Resources (all)	1.00%

Table B5 - Influence of each impact category in the total impact *EPS 2000*

Category	Percentage of total impact
Depletion of reserves	87.95%
Life expectancy	7.85%
Severe morbidity	2.05%
Morbidity	0.55%
Nuisance	0.42%
Species extinction	0.30%
Severe nuisance	0.20%
Crop growth capacity	0.15%
Soil acidification	0.14%
Prod. cap. irrigation Water	0.13%
Prod. cap. drinking water	0.13%
Fish and meat production	0.12%
Wood growth capacity	0.02%

Table B6 - Influence of each impact category in the total impact *Impact 2002+*

Category	Percentage of total impact
Respiratory inorganics	7.00%
Global warming	6.94%
Non-renewable energy	6.93%
Non-carcinogens	6.81%
Carcinogens	6.72%
Terrestrial ecotoxicity	6.60%
Land occupation	6.58%
Terrestrial acid/nutri	6.56%
Aquatic ecotoxicity	6.55%
Respiratory organics	6.55%
Ionizing radiation	6.55%
Ozone layer depletion	6.55%
Aquatic acidification	6.55%
Aquatic eutrophication	6.55%
Mineral extraction	6.55%

Table B7 - Influence of each impact category in the total impact *ReCiPe*

Category	Percentage of total impact
Natural land transformation	11.03%
Human toxicity	6.59%
Terrestrial ecotoxicity	5.95%
Marine ecotoxicity	5.78%
Freshwater ecotoxicity	5.52%
Freshwater eutrophication	5.49%
Terrestrial acidification	5.42%
Fossil depletion	5.36%
Particulate matter formation	5.17%
Climate change	5.00%
Marine eutrophication	4.99%
Urban land occupation	4.94%
Photochemical oxidant formation	4.87%
Agricultural land occupation	4.87%
Metal depletion	4.81%
Ozone depletion	4.74%
Ionising radiation	4.73%
Water depletion	4.72%