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Strategic Analysis and Optimization of Bioethanol Supply Chains

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To my first teachers, my Parents
To my Beloved Elia

"*The fuel of the future is going to come from fruit like that sumach out by the road, or from apples, weeds, sawdust - almost anything. There is fuel in every bit of vegetable matter that can be fermented. There's enough alcohol in one year's yield of an acre of potatoes to drive the machinery necessary to cultivate the fields for a hundred years.*"

—Henry Ford, *Ford Predicts Fuel from Vegetation Times*, N.Y. Times, 1925.

Foreword

The fulfilment of the research project addressed in this Thesis has involved the financial and intellectual support of many people and institutions, to whom the author is most grateful.

Most of the research activity that led to the achievements outlined and summarized in the Thesis has been developed at the Department of Industrial Engineering under the supervision of Prof. Fabrizio Bezzo. Part of the work has been carried out at the Centre for Process Systems Engineering, Chemical Engineering Department, Imperial College London (UK), with the external advice of Prof. Nilay Shah.

The realization of this study has been made possible thanks to the financial support of the Mexican National Council for Science and Technology (CONACyT) through the PhD scholarship granted.

All the material presented in this Thesis is original, unless explicit references provided by the author. The full list of publications drawn from this research project is reported below.

Publications in International Journals

Ortiz-Gutiérrez, R. A., Giarola, S., Bezzo, F., 2013a. Optimal design of ethanol supply chains considering carbon trading effects and multiple technologies for side-product exploitation. *Environmental Technology* **34** (13-14), 2189–2199. Mazzetto,

F., **Ortiz-Gutiérrez, R. A.**, Manca, D., Bezzo, F., 2013. Strategic design of bioethanol supply chains including commodity market dynamics. *Industrial & Engineering Chemistry Research* **52** (30), 10305–10316.

Mazzetto, F., Simoes-Lucas, G., **Ortiz-Gutiérrez, R. A.**, Manca, D., Bezzo, F., 2015. Impact on the optimal design of bioethanol supply chains by a new European Commission proposal. *Chemical Engineering Research & Design* **93**, 457-463.

Papers Submitted for Publication in Conference Proceedings

Ortiz-Gutiérrez, R. A., Giarola, S., Shah, N., Bezzo, F., 2015. An approach to optimize multi-enterprise biofuel supply chains including nash equilibrium models. In: 12th International Symposium on Process Systems Engineering and 25th European Symposium on Computer Aided Process Engineering. Elsevier.

Publications/Abstracts in Conference Proceedings

Ortiz-Gutiérrez, R. A., Bezzo F. 2014. A game-theory approach for the analysis and optimization of biofuel supply chains. In: 22nd European Biomass Conference and Exhibition, 4DV.3.12, 1616-1620.

Ortiz-Gutiérrez, R. A., Penazzi, S., Bernardi, A., Giarola, S., Bezzo, F., 2013d. A spatially-explicit approach to the design of ethanol supply chains considering multiple technologies and carbon trading effects. In: Kraslawski, A., Turunen, I. (Eds.), 23rd European Symposium on Computer Aided Process Engineering. Vol. 32. Elsevier, 643–648.

Ortiz-Gutiérrez, R. A., Giarola, S., Bezzo, F. 2012. Supply chain optimization for the integrated production of bioethanol and biogas. In: Convegno GRICU 2012 - Ingegneria Chimica: dalla nanoscala alla macroscala. Montesilvano (PE), 16 September 2012, Gruppo di Ingegneria Chimica dell'Università (GRICU).

Ortiz-Gutiérrez, R. A., Bezzo F. 2012. Modelling and Optimization under Spatially-Explicit features of Bioethanol Supply Chains. In: II Symposium of the National Council for Science and Technology (CONACyT) scholarship holders and former scholarship holders together with the Office of the European Parliament, Strasbourg, France, 29-30 November 2012.

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Ricardo Ortiz

Abstract

In modern times, the interest in renewable energy has been increasing considerably in response to the growing energy demand and to the simultaneous concern about global warming effects. The urgency of this issue is related to dissociation between the perspective of a steady growth in demand for fuel and its supply, which is projected to become ever more uncertain and expensive. The phenomenon of climate change is widely recognized as a consequence of the increased concentration of greenhouse gases (GHG) in the atmosphere caused by anthropogenic activity, and to which the transport sector is a significant contributor. Among biofuels, biomass-based ethanol has been in a leading position for substituting petroleum-based road-fuels. Even if its actual carbon footprint is still debated, it is generally acknowledged a reduction in net GHG emissions with respect to oil.

The complexity of the context discussed previously, guides us to the transition towards a more sustainable transport system which requires the adoption of effective quantitative tools able to encompassing the problem to the whole production chain (supply chain), that may help defining a more comprehensive view of biofuels. In dealing with such problems involving high decisional level, the analytical modelling is recognized as the best optimization option, particularly in the initial phase of design of unknown infrastructures in order to cope with a comprehensive management of production systems taking into account all supply chain stages. Mixed Integer Linear Programming (MILP) in particular, emerges as one of the most suitable tools in determining the optimal solutions of complex supply chain design problems where multiple alternatives are to be taken into account. In this sense, the multi-objective MILP (moMILP) enables simultaneous consideration of conflicting criteria (i.e., financial, environmental) to assist the decisions of interested parties on biofuels industry at strategic and tactical levels. Moreover, this complex analysis is addressed effectively by incorporating the principles of Life Cycle Analysis (LCA) within supply chain analysis techniques aiming at a quantitative assessment of the environmental burdens of each supply chain stage.

Accordingly, the main purpose of the research presented in this Thesis is to cover this gap of knowledge in the literature. In the context of the development and adoption of bioenergy

systems, the overall objective of this work is to provide quantitative and deterministic tools to analyze and optimize the supply chain as whole, to thereby identify the most suitable and feasible strategies for the development of future road transport systems.

In this sense, the research design for this Thesis begins with the development and analysis of a multi-period moMILP modelling framework for the design and the optimization of bioethanol supply chain where economics and environmental sustainability (GHG emissions reductions potential) for first generation ethanol is addressed, considering possibilities of several technologies integration (including biogas production). Then, the analysis is focused on the general interactions of market policies under the European Emission Trading System in order to enhance the bioethanol market development trends to boost sustainable production of bioethanol. Next, a comprehensive modelling analysis to predict commodity price evolution dynamics and to extend the price forecasts to other goods related to bioethanol production is addressed. An assessment of the impact on the supply chain design of the recent proposed by the European Commission to amend the existing Directive in terms of accountability technique for biofuels is analyzed and discussed. Besides, multi-criteria decision making tools to support strategic design and planning on biofuel supply chains including several Game Theory features are evaluated. Finally to close up, the main achievements of the Thesis are exposed as well as the main shortfalls and possible future research lines are outlined. Models capabilities in steering decisions on investments for bioenergy systems are evaluated in addressing real world case studies referring to the emerging bioethanol production in Northern Italy.

Riassunto

La domanda energetica mondiale è in continuo aumento. Il sistema energetico attuale è fortemente dominato dai combustibili fossili (petrolio, carbone, gas) e questo determina l'incremento delle emissioni di gas a effetto serra (*greenhouse gases*, GHG). Le crescenti preoccupazioni legate all'incertezza delle forniture energetiche e agli effetti climatici derivanti dall'utilizzo di combustibili fossili spingono verso una necessaria ridefinizione del sistema di approvvigionamento energetico globale. In particolare, il settore dei trasporti è particolarmente critico in quanto presenta un minor numero di alternative disponibili.

In risposta alla crescente domanda energetica, l'interesse per le fonti di energia rinnovabili è cresciuto considerevolmente nell'epoca moderna per cercare di ridurre la dipendenza dai combustibili fossili e contribuire alla mitigazione del riscaldamento globale. Tra i biocarburanti, il bioetanolo da biomassa è ritenuto una delle migliori alternative per la sostituzione dei combustibili fossili.

Attualmente, la produzione di bioetanolo si basa sulla cosiddetta tecnologia di prima generazione, che produce il bioetanolo a partire da mais, canna da zucchero o altre biomasse tradizionalmente utilizzate in campo alimentare. Tuttavia, le preoccupazioni legate alla competizione tra la produzione energetica e la produzione di cibo, assieme a dubbi riguardanti la reale sostenibilità energetica ed ambientale dei processi di prima generazione, ha fortemente limitato lo sviluppo di tale tecnologia e la sua accettazione sociale. In questo contesto i carburanti di seconda generazione, ottenuti a partire da materiale lignocellulosico (non impiegato in ambito alimentare), stanno riscuotendo notevole interesse. La loro applicazione su larga scala è tuttavia limitata dagli alti costi di investimento e di produzione legati a questa tecnologia.

La complessità del contesto precedentemente discusso impone di avviare una transizione verso un sistema di trasporti più sostenibile, che richiede l'adozione di strumenti quantitativi efficaci in grado di rappresentare il problema per l'intera filiera di produzione (*supply chain*). Nell'affrontare questi problemi che coinvolgono un alto livello decisionale, la modellazione analitica è riconosciuta come la migliore opzione di ottimizzazione. Essa è utilizzata

soprattutto nella fase iniziale di progettazione di infrastrutture sconosciute per far fronte ad una gestione completa dei sistemi di produzione, tenendo conto di tutte le fasi della filiera di produzione. Il *Mixed Integer Linear Programming* (MILP) in particolare, costituisce uno degli strumenti più idonei per determinare le soluzioni ottimali di problemi di progettazione delle filiere di produzione complesse in cui devono essere prese in considerazione più alternative. In questo senso, la tecnica multi-obiettivo (MoMILP) consente di studiare in maniera simultanea i criteri in conflitto (i.e., finanziario, ambientale) per agevolare le decisioni a livello strategico e tattico delle parti interessate nell'industria dei biocarburanti. Inoltre, l'analisi è affrontata efficacemente incorporando i principi di analisi del ciclo di vita (*Life Cycle Analysis*, LCA) all'interno dell'analisi della filiera di produzione (*Supply Chain Analysis*, SCA) in modo tale da avere una valutazione quantitativa degli oneri ambientali di ciascuno studio della filiera di produzione.

Di conseguenza, l'obiettivo principale della ricerca presentata in questa Tesi è quello di colmare questo *gap* di conoscenza nella letteratura. Nell'ambito dello sviluppo e dell'adozione di sistemi di bioenergia, lo scopo generale di questo lavoro è quello di fornire strumenti quantitativi e deterministici per analizzare e ottimizzare la filiera di produzione nel suo complesso, al fine di individuare le strategie più idonee e fattibili per lo sviluppo di futuri sistemi di autotrasporto.

La struttura generale di questa Tesi è stata ideata tenendo in considerazione la problematica discussa precedentemente ed stata sviluppata secondo il seguente schema concettuale.

Il Capitolo 2 si propone di offrire uno strumento decisionale per la progettazione del sistema di produzione di bioetanolo da mais, che tenga conto degli aspetti ambientali e che consideri l'integrazione di diverse tecnologie. Il modello si basa su una modellazione multi-periodo e MoMILP per la progettazione e l'ottimizzazione di SC di prima generazione e analizza la sostenibilità economica e ambientale dell'intero processo produttivo. Il modello è in grado di valutare l'effetto dell'introduzione del mercato delle quote di emissione di carbonio e l'effetto di queste ultime sulla sostenibilità economica del bioetanolo di prima generazione. L'analisi è fatta nell'ipotesi che tutti i terreni a riposo presenti nel territorio preso in esame siano impiegati nella produzione di colture energetiche.

Il Capitolo 3 si propone di definire dei modelli per prevedere l'andamento dei prezzi delle *commodity* e di tutti gli altri beni legati alla produzione di bioetanolo. Il sistema di approvvigionamento ottimale è stato identificato per diversi scenari in modo di valutare la robustezza delle prestazioni economiche rispetto alla variazione dei prezzi delle materie prime.

Il Capitolo 4 valuta l'impatto sulla progettazione della filiera di produzione della recente proposta della Commissione Europea di modificare la direttiva esistente. Questa proposta ha cambiato considerevolmente la modalità di conteggio per i biocarburanti, e di conseguenza si prevedono importanti modifiche nella progettazione della filiera di produzione. Le variazioni nella domanda di biocarburanti e nei limiti imposti per ciascuna tecnologia implicano una revisione del modello di filiera di produzione. Infine, il Capitolo discute vantaggi e svantaggi delle modifiche proposte alla Direttiva in vigore.

Il Capitolo 5 estende il framework di modellazione MILP presentato nel Capitolo 2. In particolare, vengono introdotti nel modello alcuni concetti di teoria dei giochi. Lo strumento di supporto decisionale coinvolge agricoltori e produttori di biocarburanti che possono agire in modo cooperativo o competitivo in relazione all'andamento del mercato alimentare e dei combustibili. Una formulazione stocastica sarà implementata per rappresentare l'effetto dell'incertezza sul prezzo della biomassa.

Nel Capitolo 6 si sviluppa una generalizzazione dei concetti di equilibrio di Nash su una generica filiera di produzione *multi-enterprise*. In questo Capitolo viene presentato un approccio generale MILP per determinare quale sia il livello di prezzo di trasferimento tra i siti di produzione di biomassa e i centri di produzione di biocarburanti più appropriato.

Il Capitolo 7 conclude la Tesi riassumendo i principali risultati della ricerca e delineandone le principali lacune. Vengono infine indicate delle prospettive di lavoro futuro.

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Acronyms

ADL autoregressive distributed lag.

CAGR compound annual growth rate.

CHP combined heat and power.

DAP Diluted Acid Prehydrolysis.

DDGS distiller's dried grains with solubles.

DGP Dry Grind Process.

DGP-CHP Dry-Grind Process with a DDGS fuelled CHP station.

DGP-TS Dry-Grind Process with the anaerobic digestion of Thin Stillage.

DGP-TS$_{NG}$ Dry-Grind Process with the anaerobic digestion of Thin Stillage with natural gas compensation.

DGP-TS$_{SC}$ Dry-Grind Process with the anaerobic digestion of Thin Stillage with silage compensation.

DGP-WS Dry-Grind Process with the anaerobic digestion of Whole Stillage.

DGP-WS$_{NG}$ Dry-Grind Process with the anaerobic digestion of Whole Stillage with natural gas compensation.

DGP-WS$_{SC}$ Dry-Grind Process with the anaerobic digestion of Whole Stillage with silage compensation.

dLUC direct land use change.

EC European Commission.

ETS emission trading system.

EU European Union.

EUA European Unit Allowance.

FQD Fuel Quality Directive.

GAMS General Algebraic Modelling System.

GHG greenhouse gas.

GrSCM green supply chain management.

GT game theory.

GWP Global Warming Potential.

iLUC indirect land use change.

ISO International Standards Organization.

KKT Karush-Kuhn-Tucker.

LCA life cycle analysis.

LCEP LignoCellulosic Ethanol Process.

LHV lower heating value.

LP linear programming.

MILP mixed integer linear programming.

MINLP mixed integer non–linear programming.

MIQP mixed integer quadratic programming.

MoMILP multi–objective mixed integer linear programming.

MOO multi–objective optimization.

MP mathematical programming.

MPEC mathematical problem with equilibrium constraints.

NE Nash equilibrium.

NLP non–linear programming.

NPV net present value.

OECD Organisation for Economic Cooperation and Development.

PDF probability density function.

PSE process systems engineering.

RED Renewable Energy Directive.

SC supply chain.

SCM supply chain management.

SCOR supply chain operations reference.

SSF simultaneous saccharification and fermentation.

TS total solids.

TSD time series decomposition.

WTT Well-To-Tank.

List of Symbols

$\Pi^L_{biorefinery}$ minimum profit requirement for biorefinery enterprise [€/GJ_{EtOH}].

$\Pi^L_{farmers}$ minimum profit requirement for farmers enterprise [€/GJ_{EtOH}].

$\beta_{(g)}$ Discount in the biomass price offered by every player in region g [%].

$\Pi_{biorefinery}$ profit for biorefinery enterprise [€/GJ_{EtOH}].

$\epsilon_{CF(t)}$ discount factor for farmers profit at time period t.

$\Pi_{farmers}$ profit for farmers enterprise [€/GJ_{EtOH}].

π_{sc} Probability of the scenario sc [%].

AG_g usable area [ha] per cell g.

BA_g biomass availability for ethanol production in region g [tonnes/time period].

BA^{Sa}_g biomass (from set-aside) availability for ethanol production in region g [tonnes/time period].

$BAy^{Sa}_{g,t}$ biomass (from set-aside) availability in region g considering a land yield of 70% for the first time period [tonnes/time period].

$binl_{(g,s,t)}$ binary variable which takes the value 1 if the s^{th} price level is chosen for the farmer in g at time period t and 0 otherwise.

BPC_t biomass procurement cost at time t [€/time period].

CF_t biorefinery cash flow at time t [€/time period].

$Db^T_{g,t}$ biomass demand in region g at time t [tonnes/time period].

$dfCF_t$ discount factor for cash flow of biorefinery at time t.

$dfTCI_t$ discount factor for capital costs of biorefinery at time t.

$eTFP$ Expected total farmer profit [€].

fec_k emission credits for each technology k [kg of CO_2-eq/t_{EtOH}].

$Fin_{(g,t)}$ Incomes of the players for each farmer in region g for each time period t [€/time period].

FL_g set-aside land for each region in g [ha].

$FPC_{(g,t)}$ Feedstock production cost in region g [€/ha].

$FR_{(i,g,t)}$ farmers incomes from biomass (i = corn) sale in region g at time t [€].

$FTC_{(g,t)}$ Biomass transportation costs in region g at time period t [€/time period].

$g \in G$ Grid squares, $G = \{1, \ldots, 60\}$.

$g' \in G$ Set of square regions different from g.

$GHGg$ emission factor for gasoline [kg of CO_2-eq/GJ].

$GHGr_t$ GHG emissions reduction required from biofuels at time t.

$k \in K$ Set of conversion technologies, K = *{DGP, DGP-CHP, DGP-TS, DGP-WS}*.

$l \in L$ Set of means of transport, L = *{truck, rail, barge, ship, trans-ship}*.

LHV_{EtOH} low heating value of ethanol [GJ/t].

$Lvs_{(i,g,s)}$ price level for biomass (i = corn) in region g at time t [€/tonnes].

$MaxCO2_t$ emissions cap at time t [kg of CO_2-eq/time period].

P_t^{all} purchased permit at time t [kg of CO_2-eq/time period].

$P^T_{\text{"ethanol"},k,g,t}$ total production rate for ethanol through technology k in region g at time t [tonnes/time period].

$Pb_{g,t}$ production rate of biomass in region g at time t [tonnes/time period].

$Pbcum_{g,t}$ production of biomass accumulated over time [tonnes/time period].

$Pbl_{(i,g,s,t)}$ linearized quantity of biomass (i = corn) in region g at time t of the available price levels (s) [tonnes/time period].

$Pr_{(g,t)}$ biomass selling price in region g at time t [€/tonnes].

$Qb_{(g,l,g',t)}$ flow rate of biomass between g and g' via transport mode l at time t [tonnes/time period].

RBE Expenses of the ethanol producer [€].

$s \in S$ Set of life cycle stages, S = *{bp, bt, fp, fd, ec}*.

S_t^{all} sold permits at time t [kg of CO_2-eq/time period].

$sc \in SC$ Set of scenarios, $\text{SC} = \{1, \ldots, 10\}$.

$t \in T$ Set of time intervals, $T = \{1, \ldots, 5\}$.

TCI_t total capital investment at time t [€].

TFP Total farmers profit [€].

TFP_{sc} Total farmer profit of the scenario sc [€].

$TGHG$ total GHG impact [kg of CO_2-eq].

TI_t total impact at time t [kg of CO_2-eq/time period].

$TOC_{(g,t)}$ Total operating cost for each player at time period t [€/time period].

$TPb_{(g,t)}$ Total biomass rate produced by the player in g at time period t [t/time period].

$USC_{(g)}$ Selling cost for biomass by the player in region g [€/t].

$YregFL_r$ specific set-aside surface per hectare per region.

$YregG_{r,g}$ matrix r x g for the regions distributed in 59 cells (g).

CHAPTER 1

Perspective and Motivation

"The beginning is the most important part of the work"

— Plato

THE objective of the discussion presented in this Chapter is to provide the big picture of the motivations as well as the literature survey which supports the research project of this thesis. Current status of global energy supply is first presented focusing on fossil fuels consumption and environmental issues which gradually have led us towards more sustainable energy infrastructures. The present state of biomass-based fuel production as substitutes of fossil fuels is debated here, together with the most promising solutions over the short and medium-long term of the European energy system with a particular view on fuel supply in the transport sector. Successively, an overview of supply chain management and related issues such as biomass-to-biofuels supply chains design are introduced. Next, the theoretical background on the main modelling techniques is outlined by putting particular focus on mixed integer linear programming. The discussion next develops the main aspects concerning with environmental sustainability involved in new biofuels infrastructures design. Finally, motivation and aim of the work are declared and a general overview about the structure of the Thesis conclude the introduction.

1.1 Global energy outlook and biofuels role

As global demand for energy continues to rise, carbon dioxide emissions are expected to reach new record high, increasing from 31 Gt in 2011 to approximately 37 Gt in 2035 (IPCC, 2013). The growth of the world population and its economic expansion are the two main causes for the increase of energy demand. In fact, in the past decades, the global need of energy grew quickly mainly due to the remarkable economic growth of the emergent countries (Bilgen, 2014; Banos et al., 2011). It is estimated that, mainly due to these countries, the world energy consumption will increase 56% in the next 30 years reaching 6.65x10^{30} J in 2020 and 8.65x10^{30} J in 2040 (EIA, 2014). The evolution of the type of energy supply can be summarized as presented in Figure 1.1.

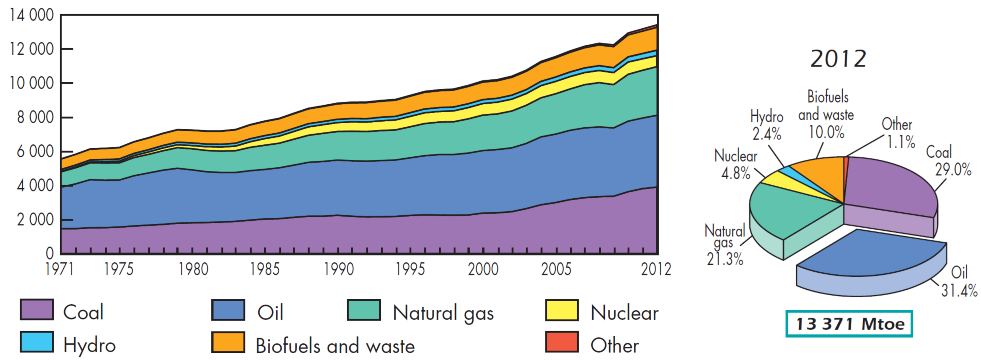


Figure 1.1: *World total primary energy demand from 1971 to 2012 (left) and fuel shares (right). (Source: EIA (2014))*

The total energy demand has steadily increased over the years backed by a huge market of fossil fuels as can be observed in Figure 1.1. The continuing growth of the energy consumption leads to an unsustainable economic and environmental situation caused, mostly, by the increase of the petroleum price and the limited lifetime of fossil fuels (Bilgen, 2014). In an environmental perspective the dependence on this type of fuel is directly related to impacts such as acid rain or the greenhouse effect. Anticipating an extreme scenario, and looking forward to establishing a sustainable development, the dependence on fossil fuels is being fought against with an increasing "bet" in the renewable energy sources (Dincer, 2000). In the market of fossil fuels, petroleum is the major resource and industry (mostly petrochemical) and transports sectors concentrate the bulk of it, as is spotted in the right plot of Figure 1.1 showing that, the oil has almost 32% of fuel shares of the world demand.

In fact, estimates say that in 2030 these two sectors will represent a 93% of global liquid fuels demand. Considering that petroleum and its derivatives represent 93% of the liquid fuels, these two sectors will create a tremendous impact in the fossil market as it can be seen in Figure 1.2 (OECD/IEA, 2013).

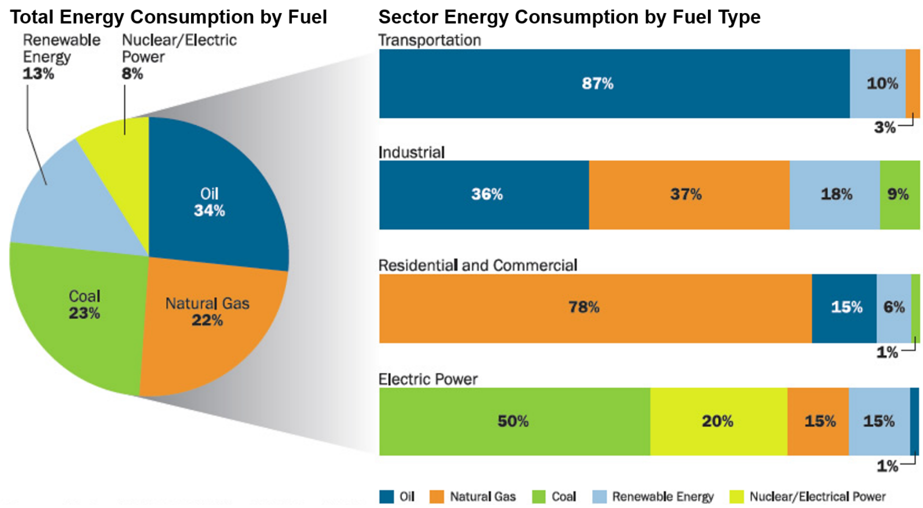


Figure 1.2: *Energy consumption by sector in 2030. (Source: OECD/IEA (2013))*

The medium-term forecasted with a dependency on fossil fuels of about 90% represents an attractive target for improving energy consumption and contributing a more sustainable development. In order to simultaneously reduce the dependence on oil and mitigate climate change in transport and chemical sectors, alternative production chains are necessary. It is increasingly recognized that there is not a single solution to these problems and that combined actions are needed, including changes in behaviour, changes in vehicle technologies, expansion of public transport and introduction of innovative fuels and technologies (Pickett et al., 2008). Today, renewable energy contributes 13% of the total global energy consumption, in which bioenergy accounts for approximately 10% (Figure 1.1). The need for climate change adaptation and the growing concerns over energy security are the main drivers behind the policies of many countries (belonging to the Organisation for Economic Cooperation and Development (OECD)) that encourage the growth of renewable energy.

1.2 Renewable Fuels in the transportation sector

Bioenergy refers to the energy content in solid, liquid and gaseous products derived from biological raw materials (biomass) (IEA, 2010). This includes biofuels for transport (e.g. bioethanol and biodiesel), products to produce electricity and heat (e.g. wood chips and pellets), as well as biogas (e.g. biomethane) produced from processing of biological materials from municipal and industrial waste (OECD/IEA, 2013). Biofuels for transport represent the major fraction of bioenergy production worldwide. Biofuels are primarily produced from food crops with high content of sugar and starch, such as corn and sugarcane to produce ethanol, and oil seeds to produce biodiesel (IEA, 2010). These first generation technologies have been the first significant step of transition away from the traditional fossil fuels. It has then moved forward to the next generations of biofuels produced from non-food biomass, including residues of crops or forestry production (e.g. forest thinning, sawdust, etc.), dedicated energy crops (e.g. switchgrass, poplar, and miscanthus), lignocellulosic fraction of municipal and industrial solid waste, and algal biomass (Sims et al., 2010; Gupta et al., 2014). More than two-thirds of bioenergy comes from the first generation land-based feedstocks (OECD/IEA, 2013), leading to growing concerns over competition for land and water for food and fibre production and other environmental issues related to land-use changes (Gasparatos et al., 2013). Therefore, the use of residues and wastes for bioenergy production has attracted more interest as they are often readily and locally available in most of the countries. Potential of lignocellulosic biomass varies and depends on the type, abundance and cost of biomass feedstocks, efficiency of the available processing technologies, and the pattern of energy demand.

1.2.1 Bioethanol production processes

1.2.1.1 First Generation Bioethanol

Bioethanol is the most used biofuel around the world. It can be obtained from biomass according to two types of technologies:

i) First generation ones, which use biomasses rich in simple sugars or starch: their production process is generally well established; however, one key issue is that raw materials are often used for alimentary purposes, too;

ii) Second generation ones, that use lignocellulosic materials and therefore do not compete directly with alimentary crops: technology is not at the industrial scale yet, but they are considered the real sustainable alternative to fossil fuels.

The present work focuses mainly on first generation technology, because it is already available on industrial scale and its know-how is widespread. An overview on second generation technologies is presented in Chapter 4, where the supply chain design is simulated including also second generation plants.

First generation bioethanol is produced from fermentation of simple sugars: the process has similarities with the alcoholic beverage processes, but it is pushed to obtain fuel-grade ethanol, that is pure at 99.8%, and other valuable by-products to improve the economic performance. The main biomasses for bioethanol production are corn (in the U.S.A. and Europe), sugarcane (in Brazil). In this Thesis the attention is focused on the process for bioethanol from corn, which is the most economical type of process on industrial scale at the European latitudes.

The most used process from corn is the Dry Grind Process (DGP), that produces ethanol as well as distiller's dried grains with solubles (DDGS), which is a valuable animal fodder. The DGP entails several key steps, including:

i) Grinding, cooking and liquefaction

ii) Saccharification and fermentation

iii) Distillation and dehydration

iv) Water evaporation and recycling

v) Drying of the non-fermentable fraction

Figure 1.3 depicts how all of these pieces fit together in a commercial plant. In the first plant section, the corn is milled down to the proper particle size ($\leq$2 mm) in order to facilitate the subsequent penetration of water and is sent to a slurry tank together with process water. The slurry is "cooked" by using steam at 4 bar: the process temperature (110°C) allows the sterilization of the slurry and breaks the starch hydrogen bonds so that water can be absorbed. This step is termed "gelatinization" because the resulting mixture has a highly viscous, gelatinous consistency. The following liquefaction step (85°C)

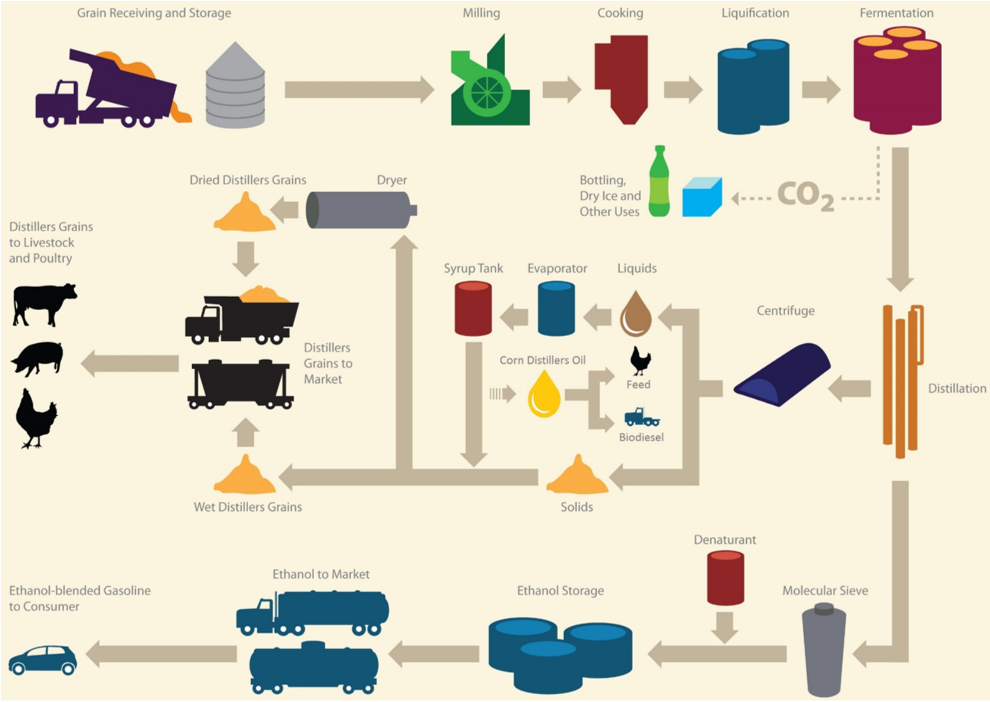


Figure 1.3: *Flow chart of typical corn dry grind fuel ethanol and coproducts processing (from RFA, 2011).*

is accomplished by the action of α-amylase enzyme on the exposed starch molecules: the effect is a random breakage of the α-1, 4 glucosidic amylose and amylopectin linkages, thus decreasing the viscosity (Franceschin et al., 2008). The mash from the liquefaction vessel is added to a backset stream and cooled down to 35°C, ready for the fermentation step.

In the fermentation reactor, a simultaneous saccharification and fermentation (SSF) occurs: starch oligosaccharides are almost completely hydrolyzed (99%) into glucose molecules by glucoamylase enzyme and the yeasts (Saccharomyces cerevisiae) catalyze the reaction of "fermentation" giving a "beer", whose ethanol content is about 12% w/w, is sent to the distillation section. Usually three distillation columns at different pressure conditions are used: this is designed to obtain a 92% w/w ethanol purity in the distillate, so that a molecular sieve section downstream can dehydrate ethanol up to the required fuel grade (99.8%) (Franceschin et al., 2008). The non-fermentable products of the feedstock (known as whole stillage), consisting of suspended grain solids, dissolved materials (both solids and liquids) and water, are sent to a centrifuge where a wet cake (35% of solids by weight) and a thin stillage (8% of solids by weight) are obtained. Part of this last stream is recycled as the above mentioned backset, while the rest is sent to a multiple-effect evaporator. The evaporation units concentrate the stream up to a final solid content of 35% by weight (syrup).

The syrup and the wet cake are mixed together and dried up to produce the DDGS, with a moisture content of about 10%, suitable for animal feeding (Franceschin et al., 2008).

1.2.1.2 Second Generation Bioethanol

Biofuels produced by non-alimentary competitive feedstock are generally referred to as "second generation biofuels": those fuels are generally based on lignocellulosic raw materials. These raw materials can be wastes from agricultural and industrial processes or can be obtained from "energy crops" grown for that purpose. In fact, energy crops are in indirect competition with alimentary feedstock, since they can occupy a surface which could be used for alimentary crops. Nevertheless, biomasses have been selected so that energy crops can be grown on marginal lands, that are not apt to alimentary crops, thus minimizing also indirect competition between the two types of crops. This can also help to increase the value of marginal lands that otherwise would be abandoned or left in degradation. The most frequent energy crops for bioethanol production are miscanthus (*Miscanthus giganteus*), common cane (*Arundo donax*), eucalyptus (*Eucalyptus globulus*) and poplar (*Liriodendron tulipifera*). On the other hand, the use of agricultural residues presents the risk of subtracting the land of their minerals and other factors that allow the successive crops to grow. The problem has been raised for corn stover, which is currently left in the field after the harvest, and whose removal has to be reintegrated by additional fertilizers. Furthermore, corn stover have an important role in limiting soil erosion, therefore it cannot be completely removed from a corn field.

All technologies using lignocellulosic materials are based on the same type of process, which is usually referred to as LignoCellulosic Ethanol Process (LCEP). This process can be found in multiple variants, but the most used one is the Diluted Acid Prehydrolysis (DAP) process, whose diagram is reported in Figure 1.4. This process allows the enzymes to produce ethanol from the monomeric sugars obtained from the scission of the long chains of cellulose and hemicellulose that, together with lignin, make up the raw material structure. Pretreatment, also called prehydrolysis, consists on treating biomass with a diluted sulfuric acid solution (1.1%) at high temperature (190°C) for a short time (not more than 10 minutes): this transforms hemicellulose in soluble sugars; after that enzymatic hydrolysis (that is saccharification) is carried out. Fermentation occurs simultaneously with

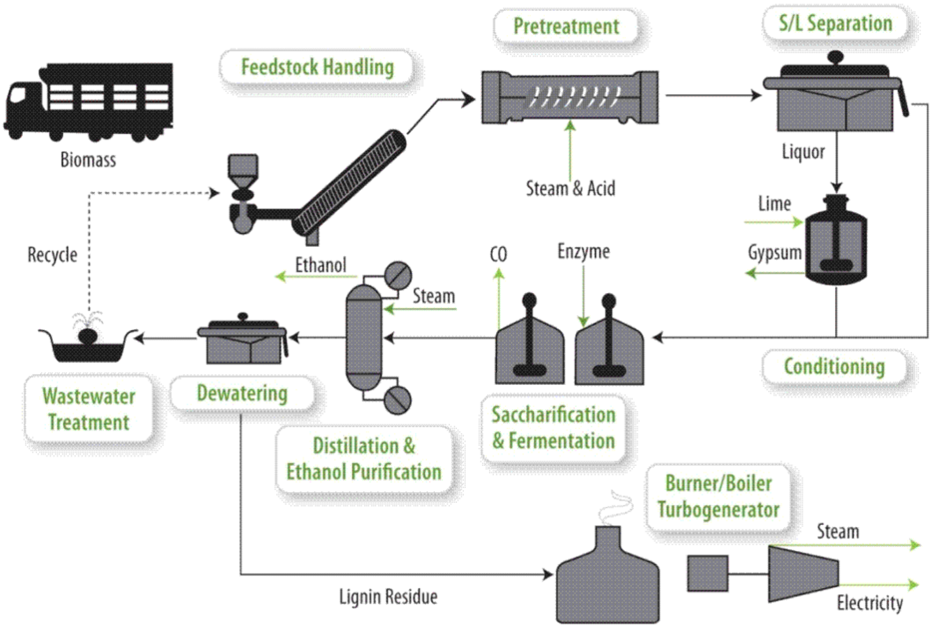


Figure 1.4: *Scheme of the Diluted Acid Prehydrolysis process for ethanol and electricity production from lignocellulosic biomass (from Foust et al. (2009)).*

saccharification in most advanced processes. The final syrup contains about 6% (w/w) of ethanol, and therefore it has to be purified and rectified before dehydration to obtain fuel-grade ethanol. Solid residues (mostly lignin) are burnt in a combined heat and power (CHP) station that allows the whole plant not only to be self-sufficient of heat and electricity, but also to produce excess electricity. The technologies using this process have been included in the supply chain design simulation (Wooley et al., 1999).

By way of conclusion, it is more than obvious that the challenge for the establishment of future biofuels systems is driven by several and interlinked framework of causes and effects, such as energy, resource depletion, food production, climate change mitigation efficiency. In this sense, the biofuels assessment has to comprise all of these aspects to encourage and drive towards a sustainable energy systems. Therefore, the transition from an oil-based fuel system to a biomass-based one, which represents a complex design problem, must be supported by properly devised mathematical modelling tools. There is the need for holistic analyses covering each aspect of the provision network and capable of evaluating several alternative configurations that may help defining a more comprehensive view of the biofuels production systems.

1.3 Supply Chain Management

A supply chain (SC) (Figure 1.5) is a network of facilities or manufacturing process and distribution options that performs the functions of procurement of materials (suppliers), transformation of these materials into intermediate and finished products (manufacturers), and the distribution of these finished products to customers. More generally, a SC may be defined as the set of parties and agents (such as suppliers, manufacturers, transporters, retailers, etc.) involved, directly or indirectly, in fulfilling a customer's request (Chopra and Meindl, 2007; Sarmah et al., 2006). For years each step of the chain has been seen and optimized individually. In fact, supply chains exist in both service and manufacturing organizations, although the complexity of the chain may vary greatly from industry to industry and from firm to firm.

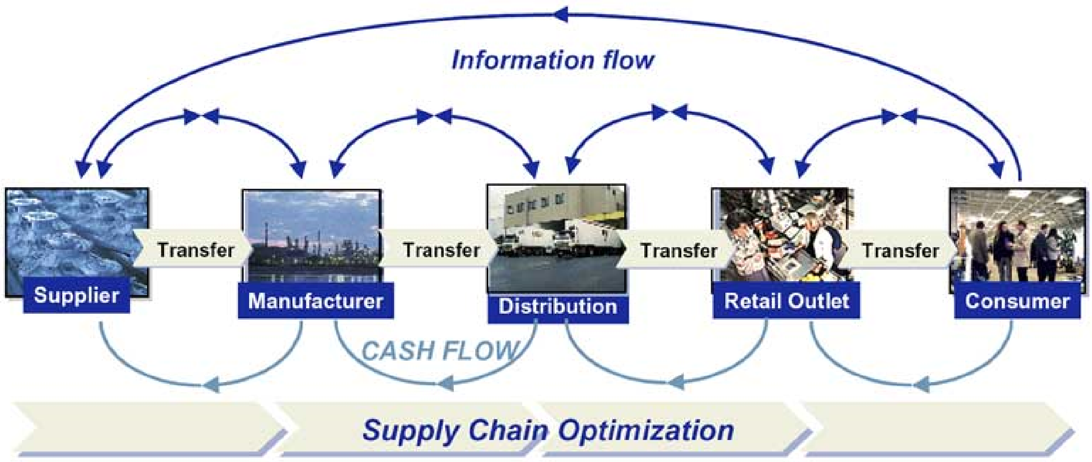


Figure 1.5: *A simple supply chain illustration.*

Recently there has been an increasing attention on the assessment and optimization of the supply chain as a whole entity, characterised by forwards flow of materials and backwards flow of information (Beamon, 1998). The objective of each supply chain is to maximize the overall generated value. The value a supply chain generates is the difference between what the final product is worth to the customer and the costs the supply chain incurs in filling the customer's requests. At the same time, other objective would be the increase of the customer's service level in order to satisfy its requirements in an optimal manner. Both objectives could of course be connected via some costs (Simchi-Levi et al., 2003).

The term supply chain management (SCM) is over 30 years old, first appearing in the practitioner literature in 1982 (Oliver and Webber, 1982) to describe connecting logistics with other functions, and by Houlihan (1985, 1988) to describe the connections between logistics and internal functions and external organizations. The earliest articles on SCM were written primarily by consultants (Houlihan, 1985, 1988; Stevens, 1989), who viewed supply chain management as a way to better manage resources and assets as well as a powerful competitive weapon in the marketplace (Jones and Riley, 1985; Stevens, 1989), reducing inventory and other costs while more effectively meeting customer demand. It was not until several years later that academics began to adopt the term and explore its meaning and implementation (Stevens, 1990). Even as academics began to use the term SCM, they realized it did not fully or accurately describe the complex web or network of relationships and processes moving in many directions and connecting companies to make products and services more effectively available to customers (Ellram, 1991).

Around 1990, academics first described SCM from a theoretical standpoint to clarify the difference from more traditional approaches to managing the flow of materials and the associated flow of information (Ellram and Cooper, 1990; Lambert, 1992; Lee and Billington, 1992; McKinnon, 1990). Academics described its complexity early on: "It is precisely the broad perspective and coverage of supply chain management that makes the concept so difficult to study" (Ellram, 1991), and noted that these "chains" were really "networks" whose best practices could be informed by industrial organization theory. As the research began to evolve, the goals of the research expanded. In fact, the Global Supply Chain Forum, a partnership between researchers and executives, established a goal of building theory and, "developing a normative model that executives can use to capture the full potential of successful SCM" (Cooper et al., 1997). A practitioner initiative, the supply chain operations reference (SCOR) model, was also developed in the late 1990s as a guideline (Council, 2013). At this point, with this evolution and reinforcement of the cross-functional nature of SCM, the scientific community together with the industrial practitioners were forming conceptual frameworks with extensive application of SCM in practice or research. The International Center for Competitive Excellence (University of North Florida) conceptualised the SCM as "the integration of business processes from end user through original suppliers that provides products, services and information that add value for customers", given that, for the manufacturing of a new product all the aspects of business are ideally involved, *i.e.* marketing, research and development, manufacturing, logistics and finance, therefore there is a higher importance to the level of integration rather than the logistical. Consequently, Cooper et al. (1997) gave a more comprehensive definition of SCM describing it as the integration of business processes across the supply chain. The different entities and agents appear to be somewhat disparate, because in most cases, they are owned by several individuals/organisations. Nevertheless, they are all linked by the integrated nature of the supply chain business.

This strategic viewpoint has created the challenge of coordinating effectively the entire supply chain, from upstream to downstream activities. A well-integrated supply chain requires coordination among all entities and agents. It should involve coordinating the flows of materials and information between suppliers, manufacturers, and customers (Narasimhan and Carter, 1998). Following the same rout, Simchi-Levi et al. (2003) conceives the SCM as a set of approaches utilized to efficiently integrate 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, and on the other hand, Hugos (2011) adopts a similar definition considering the SCM as the coordination of production, inventory, location, and transportation among the participants in the supply chain to achieve the best mix of responsiveness and efficiency for the market being served.

1.3.1 Integrated Supply Chain Management

With the rapid development of information technology and intense global competition, many manufacturers and service providers are collaborating with their primary suppliers to upgrade the traditional material management functions into part of their corporate strategy (Mentzer et al., 2001). Since its appearance in the nineties, the conception of SCM has evolved from the primary idea that was to align the forecasting, distribution, and manufacturing processes. Recently, the term *Integrated Supply Chain Management* has been formally coined in the work of Varma et al. (2007). They noted that Integrated SCM should encompass in an unified manner strategic and tactical decisions such as raw material procurement contracts, routing to plant sites, capacity planning and lead time management, routing of finished products, warehouse positioning, network inventory management and marketing strategies (Grossmann, 2014). Integrated SCM is understood as an enhanced concept that attempts to break down 'walls' by integrating the decision making across three dimensions:

- Diverse geographically distributed facilities and organizations;
- Different hierarchical levels of decision-making (strategic, tactical and operational);
- Various business functionalities (e.g., operations, finances, R&D, marketing, environmental management).

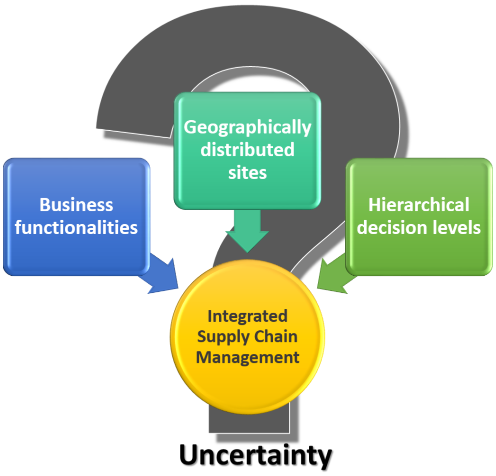


Figure 1.6: *Dimensions of integrated supply chain management.*

Furthermore, as stated by Blanchard (2004) business environment current trends need to be pondered when developing a SC decision support system. Specifically, SC managers need to consider the dynamics of a rapidly changing market environment, such as variability in demand, cancellations and returns, as well as the dynamics of internal SC operations, such as processing times, production capacity pitfalls and the availability of materials. Evidently, market dynamics and uncertainty and internal business operations make it difficult to synchronize the activities of all SC echelons; this causes significant deviations from previous objectives and plans. Therefore, for a SC to be efficiently managed it is important to systematically review variability and to explicitly take it into account in decision making. These actions search for a flexible response to changes in the business environment, increase the decisions accuracy and robustness, and improve business performance. For these reasons, an integrated framework should include the explicit consideration of SC uncertainties and dynamics.

1.4 Biomass–to–Biofuels Supply Chains

The general framework of *Biomass Supply Chain Management* has been defined as the integrated management of bioenergy production from harvesting biomaterials to energy conversion facilities (Gold and Seuring, 2011). The parties involved in a biomass energy supply chain are: the supplier of biomass, transportation and distribution entities, energy production facility developers and operators, the government and utility firms who provide the incentives, and the end-users (Adams et al., 2011). In this sense, a typical bioenergy supply chain is comprised of five major elements; biomass production system as well as its logistics, biomass–to–bioenergy production, biofuel distribution and biofuel end-use. Figure 1.7 shows the general framework of the biofuel supply chain (Iakovou et al., 2010).

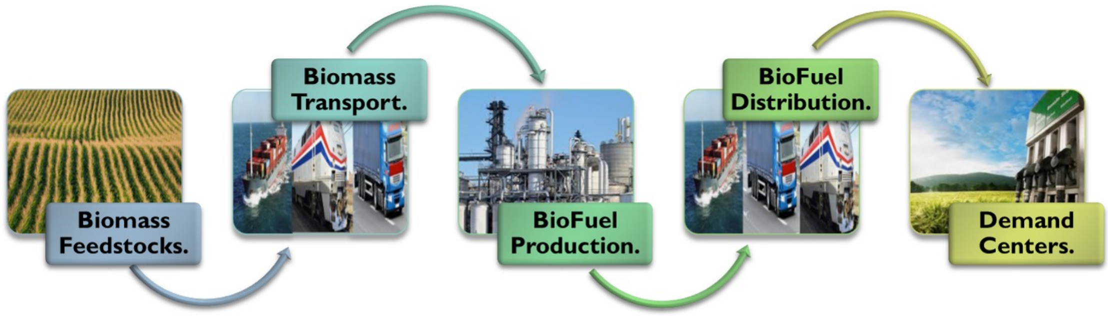


Figure 1.7: *Biofuel supply chain.*

In general, biomass raw materials are transported by trucks or trains from the neighboring farms to the biofuel refinery plant through the farm cooperatives. Cooperatives act as the liaison between the producers and the buyers. Storage facilities are needed between farms and biorefineries. Pre-treatment storage is also provided to ensure raw material freshness and increase the conversion rate. In most cases, the feedstock or raw materials are transported from farms directly to the biorefinery. Biomass raw materials are converted into finished goods such as bioethanol, corn oil and DDGS at the biorefinery. The finished product is transported via trucks to terminals for blending. Blending the ethanol with gasoline is carried out so that the ethanol product will be used for fuel purposes only. This is usually done at the initial stage by denaturing it with other chemicals. The blending of ethanol and gasoline ensures the provision of various grades of ethanol and gasoline combinations such as E85 and E15. The E85 consists of 85% ethanol and 15% of gasoline, while the E15 consists 15% of ethanol and 85% of gasoline. The blended ethanol is subsequently sent to the gasoline retail outlets, where they are sold together with other types of fuel. Some biofuel supply chains have a direct pre-treatment at the refinery or biofuel plants where the raw materials are sent directly as explained previously. Therefore, it is vitally important the integration of production and logistics processes of the biofuel supply chain for the competing biofuel/bioenergy industry.

1.4.1 Feedstock supply and Logistics

The feedstock production and logistics stages of the supply chain is responsible for managing issues as land availability, seeding, growing, yield, environmental impact of biomass growing in order to deliver high-quality, stable, and infrastructure-compatible feedstocks from diverse biomass resources to biorefineries. For terrestrial biomass, a main challenge is to develop an efficient feedstock supply system for cost-effective and time-sensitive collection, pre-processing, storage, and transport, in order to deliver diverse consistently high-quality terrestrial biomass for biofuel conversion.

First of all, feedstock is normally harvested during a specific season and the feedstock needs to be stored and preserved to provide steady supply throughout the course of the year, increasing storage and holding costs. Starting from the cheapest option, ambient storage leads to significant cost reduction at the storage and handling stage of the biomass supply chain. If a higher-quality biomass supply is required, a closed warehouse with hot air drying capability can be employed. The material loss in this scenario can be assumed negligible (Cundiff et al., 1997).

In addition to the direct storage of raw biomass, pre-treatment processes on raw biomass materials are also adopted in many practices where thermal and chemical treatments are applied to reduce moisture content, remove contaminants, and improve feedstock quality, stability,and processing performance (Agbor et al., 2011). Moreover, year-to-year production naturally varies, and other agricultural irregularities, such as crop rotation, make producing a predictable amount of supply difficult. Most biomass resources are plant matters, which need to be planted, cultivated, and harvested, going through a growing cycle. Crop residues are usually collected after the harvest of the agricultural crops (Sacks et al., 2010). For instance, the corn stover in the U.S. Corn Belt is mainly harvested from September through November. The wood residues are grown over multiple years, which makes them less seasonal compared to crop residues. They are usually available all year round. However, the yields may vary in different months. For instance, it might be more difficult to collect the wood residues during snowing seasons (USDA, 2010).

In addition, it is also reported that the harvesting timing and frequency may affect the yields of energy crops, thus careful planning and scheduling would be necessary in order to guarantee the quantity and quality of the biomass supply (Sokhansanj et al., 2009). The biomass supply may be discrete due to the seasonality, but the demand for transportation fuels is all-year-round. Therefore, the resulting operational challenge is to manage the biomass storage in order to maintain a continuous supply for the production at biorefineries.

On the other hand, the logistics of biomass has an important role in the bioenergy supply chain, because integrates and coordinates in a dynamic fashion the operations of collection-storage-delivery in an efficient and consistent high quality biomass system. Both the biomass collection and delivery require extensive efforts in equipment selection, shift arrangement, vehicle routing and fleet scheduling (DOE/EERE, 2013).

There are a number of challenges involved in the procurementmanaging of the feedstock for biofuel production. Improving sustainability is a challenge together with many sustainable initiatives can actually reduce cost at the same time. Furthermore, another major challenge is the enhancement of the yield of a feedstock, because this is directly related to unit cost of feedstock. An assessment of the environmental impact of feedstock cultivation of each feedstock is another challenge to be addressed. Environmental implications such as effect of feedstock cultivation on the quality of soil, water, and air should be analyzed because environmental concerns are the main reasons why biofuel is produced in the first place. Improving the net energy balance, which is relationship of maximizing energy output and minimizing the amount of energy input, and net carbon reduction of growing feedstock is also a critical issue (Stitt, 2013).

1.4.2 Biomass–to–Bioenergy Conversion Technologies

This stage includes all the issues related to transformation of the feedstock into commercially viable liquid fuels. This conversion takes place through a biorefinery system, wherein there is a concept of converting plant-based biomass to bioenergy (i.e. biofuels, heat and power), chemicals and materials that, replacing the needs of petroleum, coal, natural gas, and other non-renewable energy and chemical source (Cherubini, 2010). The conception of a biorefinery has similar characteristics to oil refineries of nowadays. The biomass conversion pathways to biofuels have been previously discussed in Section 1.2.1.

1.4.3 Biofuel Distribution and End-use system

The distribution stage as well the end-use system comprise the last components in the biofuel SC ensuring that bioproducts can cost-effectively and sustainably reach their market and be used by consumers, specially the liquid-biofuels as a replacement for oil-based fuels. For delivery, a network of trucks, trains, barges, and, possibly in the long term, pipelines can be utilized. In addition, blending and storage stations are required to mix biofuel with traditional, petroleum based fuel. However, Bunting et al. (2010) establish that in the U.S. dedicated fuel distribution and blending systems for biofuels are necessary, since the biofuels have been banned by most of the U.S. pipeline operators due to their polarity and other corrosion, contamination issues. The biofuel end-use stage focuses on how the consumers access the biofuel. Two significant levers in driving demand are cost efficiency and sustainability. Cost efficiency is the biggest issue, since the current biofuel costs more than its fossil fuel counterpart even with government subsidies. The sustainability of biofuel is being challenged by a significant amount of research particularly at government level. Both government agencies and academy supporting biofuels need to further research in order to improve the sustainability of biofuel in terms of carbon footprint and net energy balance. Research must be performed to make sure higher biofuel blends do not damage existing vehicle engine parts at the end use stage of the supply chain (BRDB, 2008).

1.5 Decision Making in Biofuel SCM

In more recent times, Tang (2006) envisage that the main objectives are to achieve the desired consumer satisfaction levels and the maximum financial returns by synchronizing and coordinating the SC members activities, thus defining the SCM as the management of material, information and financial flows through a SC that aims at producing and delivering goods or services to consumers. In turn Papageorgiou (2009) establishes that the SCM can be classified on different levels, wherein each one is characterised by a well determined time horizon as well as a precise detail level, according to the following categories shown in the Figure 1.8.

Strategic decisions typically involves a long planning horizon and top-level executive participation; examples include market evaluation, business partner selection, capacity

Figure 1.8: *The three levels of supply chain management.*

expansion/contraction, product introduction, and technology adoption. While the extent and frequency of planning are least demanding at the strategic level, their effects are the most significant. Tactical SCM moves forward through business models adopted at the strategic level, with further planning involving yet more details. The planning horizon at this level is shorter (usually weeks or months) than at the other two levels. Tactical SCM sets medium term decisions on demand planning, inventory planning, and master supply planning. It takes into account logistical needs, distribution parties or network and inventory planning levels. Usually tactical decisions are made to provide cost benefit due to the constraints of the strategic decisions. Demand planning helps generating accurate sales forecasts and a sales plan. Inventory planning helps adjusting optimal inventory levels (safety stocks), hedging against variability in demand and the lead times of various activities in the supply chain. Master supply planning involves procurement, production, distribution, and transportation. These decisions are further analyzed, executed, and monitored at the operational level. The operational decisions are short term decisions and the number of people directly involved is the greatest of the three levels. It includes demand fulfillment, the scheduling of procurement, production, transportation, and monitoring, as well as corrective measures in light of changing conditions (Sharma et al., 2013; Papageorgiou, 2009; Dallery, 2000).

The design and management of efficient supply chains in today's competitive environment should focus on optimizing all the decisions to achieve robust and reliable supply chain. Therefore, designing the supply chain of biofuel should focus on optimizing strategic, tactical and operational decisions to reduce system wide total cost or maximize profit for the benefit of the stakeholders.

1.5.1 Strategic decisions in biofuel SC

The strategic decisions are those decisions that have an influence over years and decades, and even beyond the lifetime of the project. Once a strategic decision is made, it is very unlikely to be altered in the short term. Strategic decisions in biofuel supply chain include, but are not limited to; (*1*) selection of energy production technologies, (*2*) network configuration, (*3*) supply and demand contracts, and (*4*) ensuring sustainability (An et al., 2011a).

The selection of the energy production technologies, i.e. conversion of wide range of types and sources feedstocks into energy through diverse conversion methods, end user applications and infrastructure requirements, should be made at the beginning of planning the production of biofuel and thus will not be changed in a short-term period. The reason for this is that there are important factors to be considered when choosing the typology of technology used for the biofuel production, as is indicated by Ekşioğlu et al. (2009a). These issues include the raw material availability, raw material type, cost of building and maintaining the plants, energy and food debate as well as environmental and sustainability issues. Optimal biofuel supply chain network will ensure that the biofuel can be delivered efficiently and effectively to the end-user market. Supply chain network design involves decisions such as sourcing and location of production facilities. One of the most inclusive studies of the design of logistics network is the strategic decision problems that need to be optimized for the long-term efficient operation of a biofuel supply chain (Hamelinck et al., 2005; Atchison and Hettenhaus, 2004).

The contracts of supply and demand imply decisions such as the agreed terms of delivery and payment between the producer and the supplier. Some of these measures include governmental R&D programs, tax cuts and exemptions, investment subsidies, feed-in tariffs for renewable electricity and mandatory blending for biofuels quotas (Bai et al., 2011). In providing renewable energy policies to a changing market demand for bioenergy, a collaborative effort among agricultural, governmental and consumer organizations should be established to fully utilize the varied expertise that each team brings in the overall objective (Ekşioğlu et al., 2010). Sustainability on the other hand ensures that the social, economic and environmental impacts of the supply chain are adequately addressed.

1.5.2 Tactical decisions in biofuel SC

Tactical decisions are medium term decisions that involve sourcing decisions, production decisions, scheduling, transportation and logistical contracts, and planning process definition. Inventory decisions such as location, quality and quantity of inventory are also considered (Shapiro, 2004). Decisions taken at the tactical decision level are planned towards achieving and executing the strategic decisions (Sharma et al., 2013).

Biomass sourcing decisions are crucial in the biofuel SC in order to minimize the geographical distance and increase accessibility to the raw material sources among other factors. This ensures that the rather isolated geographical allotment of significant biomass is able to raise the interest of researchers into identifying the available biomass quantities over a region, and subsequently proceeding with the selection of the optimal biomass sources (Sharma et al., 2013).

Production scheduling and inventory decisions in biofuel supply chain represent typical medium term decisions. These decisions are considered as the base of the tactical level in order to streamline the stock of finished products that are produced. Also, the amount of finished goods to be stored are based on the raw material availability and overall strategy of the immediate production plan (Lin et al., 2014).

Transportation involves the movements of people and goods from one location to the other. Logistics on the other hand considers the management of the flow of the goods, information and other resources in order to meet customer requirements (Lin et al., 2014). Transportation and logistics selection or contracting is another important decision in the tactical decision level which seeks to create the link between the various points of processing and delivery. Transportation and logistics usually have a high impact on the efficiency and responsiveness of the entire chain (Bai et al., 2011).

1.5.3 Operational decisions in biofuel SC

Operational decisions are short term decisions that ensure the continuous operation of the plants and other processes in the SC. These decisions are made daily or weekly and may be reiterated several times to make sure that products are manufactured, moved and sold in a timely and cost effective manner. Some of the operational level decisions are detailed production scheduling, daily fleet management, and daily or weekly inventory review. The focus here is geared towards achieving the plan or framework set by the tactical supply chain decisions. In the biofuel SC, this involves daily activities and planning such as transportation and logistics scheduling, demand forecasting and review to meet the monthly targets. The manufacturing planning for the plants and the detailed production and material requirements planning are usually reviewed at this decision level (Papageorgiou, 2009). Logistics and fleet management involve important decisions that are made within the operational decision level in the biofuel SC. This ensures that adequate provisions are made in the delivery of the products in a timely fashion. In doing this, one of the important factors to consider is the provision of the necessary technical tools to implement the decisions that are chosen. Operational decisions in the biofuel SC impact the material flow, timeliness, efficiency and effectiveness to ensure minimized cost of delivery (Shapiro, 2004).

1.6 Mathematical Programming

The great development of mathematical programming (MP) has been occurring after the mid-20th century as an important tool in decisions science and is that branch of mathematics dealing with techniques for optimizing the performance of a system. The concept as such arises thanks to George B. Dantzig, who as a mathematical advisor part of the US Air Force controller in the Pentagon developed the Simplex algorithm in 1947 as part of a military program to assist various plans, proposed schedules of training, logistical supply and deployment of combat units, (Dantzig, 1998; Gill et al., 2008). Subsequently, the scientific community began to refer to the concept of MP as a mathematical optimization technique in order to determine the values of a set of decision variables to optimize an objective function subject to a number of mathematical constraints (Kallrath and Wilson, 1997; Lev and Weiss, 1982). Also, the optimization-based mathematical programming approaches came into use to obtain the optimal allocations of limited resources among competing activities, under a number of constraints imposed by the nature of the problem being studied (Bradley et al., 1977). As one of the most important branches in the area of operational research (or management science), it has been widely studied in the research literature and commonly applied in the real world, e.g. engineering, business, management, and social sciences. On the other hand, the process industry SCM began using it as a main methodology to assist in the operation and design of chemical processes at production stage level (Papageorgiou, 2009). Despite the multiple range of use, a typical representation of a MP problem is as follows:

$$\begin{aligned} min = & f(x) \\ s.t. \quad & g(x) \leq 0 \\ & h(x) = 0 \end{aligned} \tag{1.1}$$

where $x \in X \subseteq \mathbb{R}^n$, $f : \mathbb{R}^n \longrightarrow \mathbb{R}$, $h : \mathbb{R}^n \longrightarrow \mathbb{R}^l$, $g : \mathbb{R}^n \longrightarrow \mathbb{R}^m$

Its main components are:

- The *objective function*, i.e. a quantitative measure of the performance of the system under study (i.e., f).
- The *Variables*, i.e. the unknowns whose values are to be determined such that the objective function is optimized (i.e., x).
- The *Constraints*, i.e. any restriction the decision variables must satisfy (i.e., $h \wedge g$).

Based on the nature of equations for the objective function and the constraints, the MP problems can be classified as:

- *Linear programming (LP)* If the set X is continuous and the functions f, h, and g are linear.
- *Non–linear programming (NLP)* If the set X is continuous and at least one of the functions f, h, and g is nonlinear.
- *Mixed integer linear programming (MILP)* If the set X requires at least some of the variables x to take integer values only; and the functions f, h, and g are linear.
- *Mixed integer non–linear programming (MINLP)* If the set X requires at least some of the variables x to take integer values only; and at least one of the functions f, h, and g is nonlinear.

Among the MP techniques, MILP is the most frequent optimization technique and is applied at all decision levels above mentioned. The work presented in this Thesis will use MILP-based models and approaches to model and solve the considered SCM problems.

1.6.1 Mixed Integer Linear Programming

Currently, the optimization-based mathematical programming approaches are the main methodologies used in the process industry SCM especially when the different enterprises are confronted with the need for adopting a comprehensive approach considering all the stages belonging to the entire production and distribution SC (Papageorgiou, 2009). In particular, as stated by Kallrath (2000) the MILP approach combine the characteristics of the mathematical models described above, i.e. some (or all) decision variables are integers and the objective function and all constraints are linear, thus representing one of the most suitable tools in determining the optimal solutions of complex SC design problems where multiple alternatives are to be taken into account. In dealing with SC networks design and planning, many of the decision that must be taken might be represented through discrete variables. Thus, MILP problems might capture investors' decisions through purposed devised Boolean variables (i.e. representing whether an activity exists within a SC node, or a transportation link has to be established between different nodes). If this task is addressed through algorithmic approaches, it raises the need to represent these discrete choices, along with the continuous ones (e.g., production rate, profits, taxes). Hence, a combination of discrete and continuous variables must be embodied within the general mathematical formulation. Because of wide application of such models covering a diverse variety of fields, the corresponding literature survey is organized according to the decision levels described in section 1.5.

1.6.1.1 Strategic decision making

The decision makers and investors often exhibit their concern regarding with the interaction between the biomass allocation and the design of the SC infrastructure, therefore, exist a great interest in identifying the optimal facility locations (whether or not in combination with the capacity and technology) simultaneously with the determination of the optimal flow of biomass (and eventually bioenergy) among the various nodes of the network (Melo et al., 2009).

Recently Yue et al. (2014) have presented a literature survey that covers the challenges biofuel production is currently facing. The work gives an overview of biofuel technologies and different approaches to their implementation. It also reviews many papers regarding current studies in the biofuels area. Consequently, there is a large compendium of works tackling strategic decisions in the field of biomass SC optimization describe the upstream biomass SC as a network structure in which nodes correspond with source locations, collection sites, transhipment sites, pre-treatment sites and/or conversion sites while arcs correspond with the product flow and transport operations (Bowling et al., 2011). Indeed, both Bowling et al. (2011) and Mol et al. (1997) use a MILP model in order to optimize the network structure together with the biomass flows according to a specified economic, energetic and/or environmental objective with the mass balances, capacities and demands as constraints. Into the models exists a set binary variables which determine whether or not a facility is built at a certain location, while continuous variables are related to the flows of biomass and energy from one node to another in the network structure. Zamboni et al. (2009b) presents a spatially-explicit MILP model for the integrated management of the key issues affecting corn-based ethanol SCs such as biomass suppliers and production facilities allocation as well as transport logistics. This formulation is based on cost minimization. Akgul et al. (2011) presents an optimization framework to determine the locations and sizes of bioethanol production facilities and the biomass as well as bioethanol flows between regions. Since is a problem of large scale, the authors adopted a neighbourhood flow representation into the mathematical formulation in order to solve the SC network problem.

Even though economic, energetic, environmental and social concerns simultaneously affect the decisions to be made in SCM, most optimization models concentrate on the optimization of economic issues. Marvin et al. (2012) addresses an optimization study focusing on the economic feasibility (net present value) of biomass-to-bioethanol SC in the U.S.A. taking into consideration several types of lignocellulosic biomass the biofuel production. A MILP optimization approach is presented by Leduc et al. (2010) in order to find the cost optimal facility location for lignocellulosic ethanol refineries in Sweden, which is also taken as base formulation by Natarajan et al. (2012) for the methanol and CHP production in Finland. On the other hand, Leão et al. (2011) has developed a model using MP techniques to optimize the structure for supplying oil (considering production, transportation and crushing of oil seeds and transportation of oil) to biodiesel plant. Similarly, Leduc et al. (2009) has used a MILP model to conduct an optimization for the optimal location for Jatropha biodiesel plant analysing various feedstock. Besides that, Akgul et al. (2012b) considered the economic impact in a MILP framework for bioethanol SC network to determine locations and scales of biofuel production facilities, biomass cultivation and biofuel production rates, flow of biomass and biofuel between the components of supply chain, transportation modes of delivery for biomass and biofuel.

It is noteworthy that the influence of the temporal variation is very clear in tactical/operational decision making as well as in the long–term decisions, which are influenced by the temporal variability in the supply of biomass and growing energy demand. Therefore this temporal characteristic arises as multi-period and/or multi-stage MILP in order to optimize the overall system cost along the planning horizon which may be divided in multiple time periods. The consequence is that the decisions regarding to optimal location of the plants and biomass flows are performed in each time period together with the growth in demand, therefore the decision variables (binaries) come to determine whether or not to build a production plant while variables continuous determine the amounts of biomass and biofuel produced. An et al. (2011b) formulates a model dealing with a time-staged, multi-commodity, production/distribution system, prescribing facility locations and capacities, technologies, material flows and the demand profile of fuel by dividing a one-year planning horizon into four quarters in order to maximize the economic performance of a lignocellulosic biofuel SC. Huang et al. (2010) formulated a multi-period optimization model with yearly decisions to determine the location and capacity of the facilities with the possibility of adding capacity expansions onto existing refineries. Another multi-period SC design MILP model (Sharma et al. (2011)) formulated to maximize stakeholder value in the design of a biorefinery and the SC configuration, where the binary variables being used to technology and feedstock selection and decision to expand the capacity of the facilities. Besides that, Dunnett et al. (2008) present a MILP modelling framework with production and logistics features to provide the cost-optimal configurations of the lignocellulosic bioethanol SC considering several technologies, system scale, ethanol demand distribution scenarios and biomass supply. A case of study in Argentina with land usage consideration and crop competition was studied in Andersen et al. (2012) through a MILP multiperiod formulation for a 7-year planning period with monthly decisions for the optimal design and planning of the biodiesel SC. Furthermore, Wang et al. (2012b) presented an energy crop supply chain model to identify the optimal location and capacities for a cogeneration facility, subject to the minimum cost of the overall system.

1.6.1.2 Tactical decision making

Tactical decisions are constrained by the established strategic decisions and cover medium to short term decisions regarding inventory planning, i.e. how much to harvest, and when to harvest and fleet management, i.e. trasport logistics, shipment size, routing, and scheduling. Moreover, in order to integrate the program of action for storage and inventory activities within whole SC operations, Dunnett et al. (2007) used an optimization framework based on MILP formulation focused on the operational processing, harvesting and storage logistical scheduling in order to minimize the total cost of biomass SCs. In another approach conducted by Gunnarsson et al. (2004), a MILP model with time horizon of one year was applied to optimize chipping capacity, storage capacity, demand and transportation costs related to each time period in SC for forest fuel conversion. On the other hand, Flisberg et al. (2012) pointed out that at the operational level only a single system should be used by considering the optimization through a MILP model of inventory planning at terminal to support the choice of chipping technology and location and the route to the heating plants for forest fuel logistics. Similarly, Frombo et al. (2009) developed at this same decisional level a model for the planning of woody biomass logistics for energy production where several thermochemical processes are taken into consideration for the conversion from biomass to electricity, heat, and fuels.

Considering that in the supply network design both strategic and tactical decisions are implicated, multi-period MILP models have been developed in order to to identify size and location of facilities simultaneously with the optimization of inventory planning and/or fleet management. From this perspective, Tembo et al. (2003) proposed a conceptual MILP model for the transportation of lignocellulosic biomass–to–ethanol industry. The model is applied to a case study in U.S.A. in order to determine the tactical decisions about biomass flow and strategic decisions regarding the location and size of conversion facilities endogenously assuming that all investments take place at the beginning of a 15-year cycle. Furthermore, Ekşioğlu et al. (2009b, 2010) show a mathematical formulation for a SC which includes the haversting sites for corn or stover biomass as well as its collection facilities to be shipped to biorefineries passing through blending centers and biofuel demand locations. The optimization procedure aims at minimizing the total cost of the SC involving the network design, modes of transportation, and material flows from feedstock suppliers to end users. In addition, the MILP model presented by Zhu et al. (2011) integrates strategic decisions and tactical decisions on the operation schedule for a switch grass SC prescribing locations of biomass storage and conversion facilities, modes of transportation from farms to refineries, and flows of biomass over multiple time periods.

1.6.1.3 Operational decision making

The decisions in the operational realm are focused on inventory planning, vehicle planning and scheduling to ensure continuous operation of the conversion facilities and other processes in the SC (Shapiro, 2004). Recently, Avami (2013) have developed a MILP model for the biofuel SC in Iran to minimize the total cost of capital and operations. This model provides a regional framework in terms of techno–economic parameters to deeply understand the agricultural, technical, and economic aspects of the SC including resources, production, distribution, and consumer. The decision variables were the technology selection and the potential capacity of each region to cultivate specific biomass. The multi-period MILP optimization model by Van Dyken et al. (2010) is able to economically optimize the operations of the biomass supply system, i.e. transport, storage and pre-treatment, for an entire year allowing the implementation of long-term functions in operational optimization. As key feature, the model includes the CO_2 emissions from various parts of the SC to the cost minimization objective function using a multiplicative factor that represented carbon tax.

1.6.2 Multi–objective Optimization

As mentioned above, a key feature that makes the MILP modelling approach to be an appropriate tool for supporting decision-making is the possibility to have an comprehensive selection upon several alternatives, i.e. to perform multiple criteria optimization.

In fact, most realistic optimization problems require the simultaneous optimization of more than one objective. In these and most other cases, it is unlikely that the different objectives would be optimized by the same variable value choices. Hence, some trade-off between the criteria is needed to ensure a satisfactory solution.

The Multi–objective optimization (MOO) is suitable then for this kind of problems when decision makers are in the need to overcome with a broader picture of the biofuel SC considering not only economic issues but also problems of energy, environmental, and social nature which simultaneously affecting decisions to be taken in SCM (Ulrich and Vasudevan, 2004; Turton et al., 2009). Therefore, the aim is to identify particular solutions representing a trade-off between several objectives (Ehrgott, 2005).

The mathematical representation of a MOO problem is as follows:

$$\begin{aligned} min \quad & \{f_1(x), f_2(x), \ldots, f_P(x)\} \quad (P \geq 2) \\ s.t. \quad & g(x) \leq 0 \\ & h(x) = 0 \end{aligned} \tag{1.2}$$

where $x \in X \subseteq \mathbb{R}^n$, $f : \mathbb{R}^n \longrightarrow \mathbb{R}$, $h : \mathbb{R}^n \longrightarrow \mathbb{R}^l$, $g : \mathbb{R}^n \longrightarrow \mathbb{R}^m$

These solutions are called *efficient* or *Pareto optimal.* A generic pareto front is depicted in the Figure 1.9.

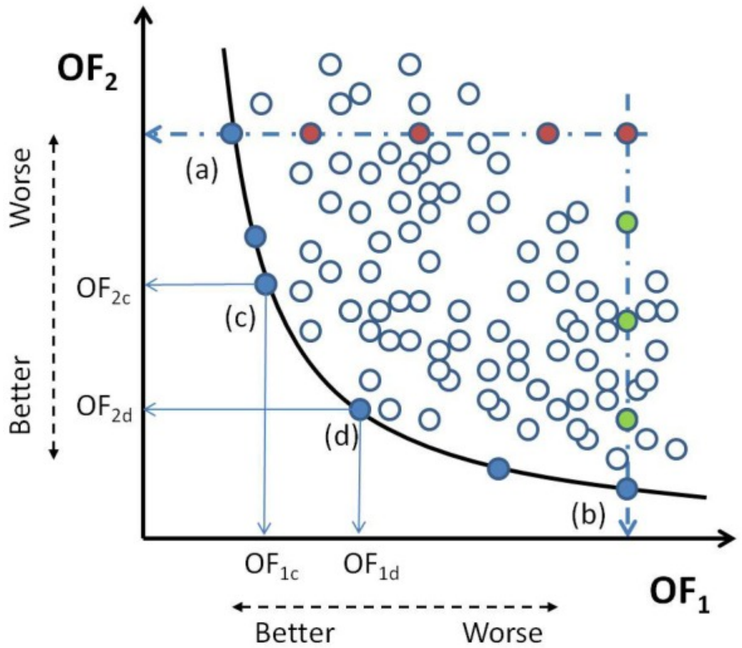


Figure 1.9: *Generic Pareto front. Full blue points indicate members of the pareto set. Point (a) is the optimum for objective function for a given value of (red points). Point (b) minimizes for another value of (compared to green points). For a member of the Pareto set, say (c), any attempt to improve a goal involves worsening the other, point (d) for comparison. Empty blue points are other possible solutions that are worse than those in the Pareto set. (Source: Pozo et al. (2012))*

There are several approaches to obtain Pareto solutions: physical programming method (PP), normal boundary intersection method (NBI), ϵ–constraint method (ϵ–C), normal constraint method (NC), weighted sum method (WS) and the compromise programming method (CP). In practice, they are based on the conversion of the MOO problem into one single objective problem; solving it several times at the same time that each solution represents one feasible point; all the solutions represent the Pareto frontier. Among the available methods, the ϵ–constraint method resulted as the most widely applied in MOO problems due to its aptitude to be implemented into the MP modelling language and to fit with the available solution algorithms (Steuer, 1989).

The MOO has been used to solve SC decision making problems since many of the approaches developed in SCM are modelled as MILP and are solved under one single optimization criterion.The trade–off among multiple objectives must be considered by the decision makers and planner designers. Managing multiple objectives represents one of the most critical problem in SCM; typically, enterprises have different departments taking their own decisions, and in most of the cases they produce contradictory decisions (i.e., marketing and manufacturing departments have different goals and policies). Therefore, the use of MOO techniques become essential in order to improve the decision–making.

The MOO optimization has been successfully applied in several SC industrial problems, such as chemical (Rodera et al., 2002), pharmaceutical (Nicolotti et al., 2011), petrochemical (Zhong and You, 2011), or automotive industries (Cook et al., 2007). Also, there are several works considering MOO approaches solving SCM problems in the bioenergy sector adopting principally the economic, environmental and social aspects. Below is presented the general overview with the highlighted and main optimization models presented in the literature, including MOO of several objectives.

Zamboni et al. (2009a) proposed a general modelling framework to drive the decision–making process to strategically design biofuel SC networks, where the design task was formulated as an MILP problem that considers the simultaneous minimization of the SC operating costs and the environmental impact (measured in terms of greenhouse gas (GHG)). Mele and Kostin (2011) provided a spatially explicit bi–criterion multi–objective mixed integer linear programming (MoMILP) framework where environmental (expressed as Eco–indicator 99 and Global Warming Potential (GWP), metrics) and financial criteria are both addressed in the ethanol production from sugarcane. In Giarola et al. (2011) the strategic design and planning optimization of bioethanol SCs through first and second generation technologies are addressed. A MILP model was proposed in order to optimize both environmental and economical objectives jointly. The formulation serves as a guide for taking decisions and investments through a global approach. Besides, Kim et al. (2011b) presented a MILP model where fuel conversion technologies, facility capacities, biomass supply locations, and the transportation between the different SC nodes are simultaneously selected. They considered distributed and centralized networks and compared them in terms of their profits and robustness, according to demand variations. You and Wang (2011) presented an optimization model to design and plan biomass and liquid fuels SCs based on economic and environmental criteria; this approach was illustrated through a case study for the state of Iowa. A multi-objective optimization model for to optimize a biorefinery was reported by Santibañez-Aguilar et al. (2011); this approach simultaneously maximized the profit while minimizing the environmental impact.

Recently, You et al. (2012) proposed a new approach to optimally plan biofuel SCs integrating the economic objective (i.e. minimising the net present value) with life cycle analysis (LCA) and regional economic input–output (EIO) analysis through a MOO scheme to include an environmental objective measured by life–cycle GHG and a social objective measured by the number of local jobs resulting from the construction and operations of the cellulosic biomass SC. In the same way, Santibañez-Aguilar et al. (2014) have developed a multi–objective, multi-period MILP model based on a state–task network, which seeks to maximize the profit of the SC, while minimizing its environmental impact and maximizing the number of jobs generated by its implementation. The environmental impact was measured by the Eco–indicator 99 according to the LCA technique, and the social objective is quantified by the number of jobs generated.

1.6.3 Environmental Sustainability in Biofuel SC

Nowadays, a proper handling of SCM should be concerned with the sharing of responsibility from various aspects of performance. It has been realized that significant improvements in terms of environmental performance and market competitiveness may be achieved by concentrating efforts from all SC partners. Actually, managerial practice related to environmental issues has expanded from a narrow focus on pollution control within a single site to include a larger set of inter-organizational management decisions, programs, tools, and technologies that prevent pollution before its generation (Klassen and Johnson, 2004). Consequently, the concern to take into account the long-term risks associated with resource depletion, fluctuations in energy costs, product liabilities, and pollution and waste management in the SC has emerged in the last decades (Srivastava, 2007). This implies that sustainable SCM needs to integrate consideration of economical aspects within environmental nature objectives with ongoing SC operations Ratan et al. (2010).

The aforementioned integration may be achieved through the emerging concept regarded as *Green supply chain management (GrSCM)*, defined as the integration of environmental thinking into SCM, including product design, material sourcing and selection, manufacturing/processing equipment selection, delivery of final product to the consumers as well as end of life management of the product after its useful life (Srivastava, 2007). Traditionally, in the process systems engineering (PSE) community the optimization models devised to assist operation and design in the chemical processing industry have focused on finding the solution that maximizes a given economic performance indicator while satisfying a set of operational constraints imposed by the processing technology and the topology of the plant. In recent years, however, there has been a growing awareness of the importance of including environmental and financial aspects in the optimization procedure (Puigjaner and Guillén-Gosálbez, 2008). In fact, there are some successful cases of businesses that have successfully achieved the integration of environmental aspects with SCM which exhibit the potential benefits that can be attained through environmental integration along the SC; the Xerox's Asset Recycle Program which redirects 90% of all materials and components for its photocopiers through re-use, re-manufacturing, and recycling; in this case annual savings are estimated in US $ 300 million (Hart, 2008), while Daimler-Chrysler has deployed a scrap management system which allows for an annual saving of US $ 4.7 million (Klassen and Johnson, 2004).

Given that biofuels are considered as a renewable energy alternative to conventional fossil fuels, the sustainability issues associated with it deserve greater attention to avoid the introduction of adverse effects on the environment. Therefore, in order to reduce these impacts on ecosystem and thereby improve the overall economic profitability of the stakeholders, systematic modelling and optimization frameworks are required to simultaneously assess and identify the sustainable solutions for the design and operation of biofuel SCs. Following this environmental awareness and tightening of environmental policies on biofuels, the study of environmental sustainability has received increasing attention in the past decades. Among the various approaches to assess the environmental impacts (e.g., GHG emissions) the LCA methodology stands out to be the most successful tool for evaluating and analyzing the environmental impacts of product systems (Azapagic, 1999; Azapagic and Clift, 1999). The classical LCA framework is based on stages and processes, which is well regulated by International Standards Organization (ISO) standards and specific methodology guidelines (ISO, 2006).

Hugo and Pistikopoulos (2005) present one of the first works that incorporate LCA into supply chain optimization, Their work address the environmentally conscious process selection problem for the long-range planning and design of chemical SC networks. They present a mathematical programming-based methodology for the explicit inclusion of LCA criteria as part of the strategic investment decisions related to the design and planning of SC networks. By considering the multiple environmental concerns together with the traditional economic criteria, the planning task is formulated as a MoMILP problem. At the strategic level, the methodology addresses strategic decisions involving the selection, allocation and capacity expansion of processing technologies and assignment of transportation links required to satisfy the demands at the markets. At the operational level, it determines optimal production profiles and flows of material between various components within the SC. Meanwhile, Nikolopoulou and Ierapetritou (2012) reviewed studies that developed green supply chain methods, taking environmental and sustainability measures into account. Zamboni et al. (2009a) and Mele et al. (2009) have addressed the optimal planning of supply chains for bioethanol and sugar production with economic and environmental concerns. A bi-criterion MILP model is proposed for the simultaneous minimization of the total cost of a sugar/ethanol production network and its environmental performance over the entire life cycle of the sugar and ethanol. Following the work by Mele et al. (2009), You and Wang (2011) have presented the life cycle optimization of biomass-to-liquids supply chain under the economic and environmental criteria. Their work shows that distributed biomass processing followed by centralized upgrading of intermediates may lead to economically viable and environmentally sustainable biofuels SCs. On the other hand, Čuček et al. (2012) introduced a MOO model that maximized the economic performance of the SC and minimized the environmental and social footprints. On top of the carbon footprint directly generated from the supply chain, they calculated indirect effects caused by product substitutions. The supply chain included the agricultural sector (harvest and storage locations), preprocessing centers, conversion facilities, and distribution sites of fuel products. The MINLP model was solved on two levels, the first to maximize the profit and the second using the multicriteria objective function. In addition, Elia et al. (2011) developed a MILP model that is integrated with LCA for determining an optimal energy-supply network based on hybrid coal, biomass, and natural gas to liquid plants using carbon-based hydrogen production. In addition, the uncertainties in environmental evaluation can have significant influences on the reliability of LCA-based decisions. These uncertainties may stem from the limited knowledge about the physical processes under study and the normative choices regarding scenarios and mathematical models (Huijbregts et al., 2004). Recently, Lam et al. (2013) proposed green strategy for sustainable waste-to-energy supply chain and Ng et al. (2013) synthesized biomass supply network with centralized processing site selection through resources and cost optimization.

1.6.4 Uncertainty in Biofuel SCM

As is well pointed out by Awudu and Zhang (2012), uncertainties impact on the performance of the SC and their effects should be taken into account by decision makers within SCM. The same authors stated as major sources of uncertainty in biofuel SC the following factors: *(1)* raw material supply uncertainty which includes raw material yield, type, quality, quantity, concerns in procurement decisions; *(2)* transportation and logistics uncertainties, which take into consideration the inability to deliver both biomass raw materials and finished products in a timely and cost effective manner (e.g. delays in fleet scheduling, demand and inventory, transportation cost, lack of coordination, delivery constraints, lack of optimized containers due to low yield supply, cost of warehouse and transportation lanes availability); *(3)* production and operation uncertainty issues cause the inability to produce the planned quantity of production; some of these are delays in raw materials acquisition, production yields, machine breakdown, lead time constraints and inventory decisions; *(4)* demand and price uncertainties refer include to the unknown or unpredictable variations in the quantity and timing of demand as experienced in a SC; price uncertainty defines the chance or speculation that price of a product might change. Demand and price uncertainties in biofuel supply chain, include, but do not limited to, raw material cost (e.g. corn prices), crude oil price, tax subsidies, carbon trading, and governmental policies. Incorporating demand and price uncertainties into the decision making process can reduce expectation for profit generation.

In this sense, Sahinidis (2004) establishes that incorporating uncertainty into MP represents a great challenge due to computational requirements needed. The scientific community has long been involved developing PSE tools and a variety of ways to deal with uncertainty in optimization problems. A literature review on this topic reveals that most of the systematic tools currently existing for managing decision–making under uncertainty are: stochastic programming (recourse models, robust stochastic programming and probabilistic models), fuzzy decision–making (flexible and possibilistic programming), and stochastic dynamic programming (Sahinidis, 2004).

The most commonly adopted technique in the literature is the stochastic programming with recourse. In this approach, a solution with the maximum expected performance is obtained by including estimated scenarios in the model; these estimated scenarios are generated by representing uncertain parameters as random variables. The goal is to find a solution that is feasible for all the possible data scenarios and which maximizes the expectation of a performance indicator. The most widely applied stochastic programming models are two-stage programs. In this type of problems, it is relevant to distinguish among two set of decisions variables (main and secondary variables). The first stage decisions must be taken before any uncertain parameter is unveiled. They are also known as “here and now” decisions. The interval of time associated with them is known as the first stage of the stochastic program. The second stage decision are determined after some or all the uncertain data is revealed. On the other hand, the uncertainty might be modelled either by a discrete number of scenarios or by probability distributions. Usually the expectations of second-stage variables (e.g., costs, profits) are included in the objective functions, although, some works properly introduce some kind of variability metrics (Chen et al., 2002; Ahmed et al., 2003) in the model.

The modelling approaches that address the uncertainties that the biofuel industry faces (e.g. biomass supply, biomass yield, biofuel demand and price depend on the market environment, transportation, logistics, production, operation) have attracted attention to the PSE community leading to important insights about system operation and interactions among its components. Cundiff et al. (1997) consider uncertainty in biomass production levels while optimizing the design of storage facilities and arranging transportation issues in the biomass delivery system. This supply uncertainty is assumed to be related to biomass yield due to weather conditions during growing and harvesting seasons. Kim et al. (2011a) incorporated uncertainties into a previous model (Kim et al., 2011b) and the biomass supply, fuel demands, prices, and conversion technologies were modelled in a two-stage mixed-integer stochastic programming model. Similarly, Chen and Fan (2012) implemented a two-stage stochastic programming model to incorporate the uncertainties in fuel demands and feedstock supplies. Furthermore, Walther et al. (2012) have incorporated the technology biofuel production in Northern Germany extending a multi-period, multi-stage MILP into a scenario based planning approach applying different objective functions representing risk attitudes of decision makers. A strategic planning and investment capacity planning problem of an bioethanol SC was developed by Dal-Mas et al. (2011) adding uncertainties in biomass costs and product selling prices in a dynamic MoMILP modelling framework. The uncertainties were accounted for by incorporating the expected net present value (NPV) and conditional value-at-risk (CVaR) into the objective function. Following the same line, Kostin et al. (2012) incorporated uncertainty in the demand to a previous work (Mele and Kostin, 2011) proposing a multi-scenario MILP problem that includes the capacity expansions of the plants and deports over time and the associated planning decisions. In a later work, Giarola et al. (2012) incorporated a carbon-trading scheme into their MoMILP (Giarola et al., 2011) for the selection of the bioethanol conversion technology and capacity planning of a single bioethanol production plant. Uncertainties in the feedstock cost and carbon cost were incorporated via two-stage stochastic programming, and binary variables were used for the facility type and existence of tax in a certain time period. Newly, Giarola et al. (2013) has expanded her model where a multi-criteria decision making tool is proposed to support strategic design and planning on ethanol fuel SC under market uncertainty. The uncertainty arise from feedstock cost and carbon cost within an emission allowances trading scheme is addressed through a multi-scenario two-stage stochastic model. Moreover, in studying the integrated long-term vision for biofuels and their market diffusion, the crucial role of technological learning in determining costs reduction, has been implemented through the experience curve approach so as to link changes in production costs with cumulative production.

1.7 Game Theory in SCM

The last two decades have witnessed a renewed interest by academics and practitioners in the management of supply chains and a new emphasis on the interactions among the decision makers ("players" or "agents") constituting a supply chain. This has resulted in the proliferation of studies dealing with the behaviour of the concerned agents in the analysis of supply chain-related problems. As has been described previously the entire biofuel supply chain is considered as entity centralized system. This could be true in the case that all the stakeholders in the bioenergy system are cooperatives, which happens in the case of every node of the biofuel supply chain (biomass producers, biofuel production facilities and distribution centers) are all acquired by the same organization. However, more often, the parties concerned in the bioenergy system are non-cooperative, thus causing competition in the price and use of materials.

In such scenarios, game theory (GT) is a powerful tool for the study of mathematical models concerning conflict and cooperation between intelligent rational parties in the SC system. In GT, the interactions and competitions between different parties can be modelled as various types of games depending on their behaviours, including cooperative or non-cooperative games. (Dutta, 1999; Myerson, 2013). For the *cooperative* game where the supply chain members may agree to have a contract to coordinate their strategies in order lo improve the global performance of the system as well as their individual profits (all agents share a common objective). For this type of supply chains with cooperation/coordination, channel members may not only achieve supply chain-wide optimization but also they would have no incentives to deviate from the global optimal solution. On the other hand, for the *non-cooperative* game the supply chain members compete to improve their individual performance (each player has an individual objective, which usually will not coincide with the objective of the rest of players) (Cachon and Netessine, 2004). For example, several agents at the same echelon of a supply chain may compete for limited resources or compete for demand from the same group of customers. As a result, various competitive game-related issues arise in the analysis of the supply chains with competition (Cachon and Netessine, 2004).

The application of GT to the economic stability and efficiency of SCs interacting cooperatively or competitively have been discussed by a number of works in a broad range of contexts. Just to list a few examples, Saad et al. (2009) and Vickrey and Koller (2002) discussed the cooperative game of distributed artificial intelligent and multi-agent systems; Zhao et al. (2012) provided an approach in the context of GrSCM using GT to describe strategy selection for environmental risk and carbon emissions reduction; Zamarripa et al. (2012) proposed a GT approach as a decision technique to determine the best SC operating strategy with uncertainty related to the behavior of several SCs competing for the market; Esmaeili et al. (2009) suggested and implemented a modeling framework incorporating elements of competition and cooperation between seller and buyer within the SC. Moreover, de Oliveira Florentino and Pereira Sartori (2003) as well as Nasiri and Zaccour (2009); Sun et al. (2013) proposed the optimization of biomass energy SCs using a GT framework.

Clearly, the biofuel industry, too, is a complex system including many decision makers where GT could be applied to assess complex market dynamics. However, for the realization of this literature survey, hitherto very few works have appeared on the subject. Bai et al. (2012) studied the interactions of competition and cooperation among biofuel supply chain design, agricultural land use and local food market equilibrium implemented through a bi-level non-cooperative game model (the Stackelberg leader-follower game) adopting a modelling approach which involves use of discrete mathematical problem with equilibrium constraints (MPEC) and a mixed integer quadratic programming (MIQP) problem based on Karush-Kuhn-Tucker (KKT) conditions; Wang et al. (2013) considered a framework within a non-cooperative environment between diverse biofuel producers so as to optimize the biofuel SC represented as a MPEC. The representation of the production SC is nonetheless quite simplified, if compared to several works that have appeared over the last years discussing the operational and strategic design of biofuel supply chains, typical through mixed integer linear (or non-linear) programming techniques. Lately, Yue and You (2014b), propose a bi-level MINLP model for the optimal design and planning of non-cooperative supply chains from the manufacturer's perspective. Interactions among the supply chain participants are captured through a single-leader–multiple-follower Stackelberg game under the generalized Nash equilibrium assumption.

Other topics to be analyzed through the use of the GT is how to divide the payoff of collaboration while ensuring that solutions are optimal in terms of sourcing, production, inventory, and distribution policies. The solutions that are obtained from optimization usually exhibit payoff distributions that are not sustainable from the long-term perspective because some of the supply chain players often deem their own share of profit disproportionately small compared to the others. This perception of unfair solutions can result in adversarial attitudes and deteriorating integration of otherwise beneficial supply chain partnerships (Gjerdrum et al., 2001, 2002). Mechanisms that apportion payoffs between supply chain companies must be transparent and clear to enable each company to apprehend the foundation of the profit distribution system. Transfer pricing of the products shipped between the supply chain companies provides a method of distributing the profit received from customers at the downstream nodes of the supply chain (Gjerdrum et al., 2002).

In this point, it is important to note that the SC business analysis through the use of the concepts associated to the GT will commonly lead to negotiation, in terms of prices established for sellers and buyers and profit sharing issues, quantities to be delivered, etc., in order to attain a more comprehensive approach in the SCM.

1.8 Indirect land use change and biofuels

Transport biofuels have occupied a central role within the European Union's renewable energy and climate change mitigation policy portfolio for over a decade, dating back at least to 2003's Biofuels Directive (EC, 2003).

However, over the last years, the image of biofuels have in many places deteriorated considerably, with a diversity of actors questioning their sustainability credentials (Dunlop, 2010; Palmer, 2010). Concerns included the potentially deleterious effects of biofuel production on biodiversity (Danielsen et al., 2009; Howarth and Bringezu, 2008), on water and soil quality (Gerbens-Leenes et al., 2009; Howarth and Bringezu, 2008), on food security (Pimentel et al., 2009; Tilman et al., 2009; Runge and Senauer, 2007), and even on land rights (Franco, 2012; Borras Jr et al., 2011; Anseeuw et al., 2012; Sassen, 2013).

In recent years, arguably the most complex and controversial issue associated with biofuel production have been the land use change issues. There are two types of land use change, direct land use change (dLUC) and indirect land use change (iLUC). These two effects could be induced by an increased demand for biofuels leading to an increase in the crop production, which can only be satisfied by the cultivation of land and/or increasing the productivity of existing crops, thus resulting in a change of land management (Silalertruksa et al., 2009). Initially highlighting the works by Searchinger et al. (2008) and Fargione et al. (2008) the "indirect" process occurs when biofuel production takes place on pre-existing agricultural land, causing farmers to "convert forest and grassland to new cropland to replace the grain that has been diverted to biofuels" (Searchinger et al., 2008). This definition is consistent with that described by Gnansounou et al. (2009), which defines that the iLUC occurs when pressure on agriculture due to the displacement of previous activity or use of the biomass induces land-use changes on other lands in order to maintain previous level of (e.g., food) production. A schematic representation of the iLUC is shown in the Figure 1.10.

(a) (b)

Figure 1.10: *Indirect Land Use Change: (a) When Agricultural activity (Food Production) is displaced by crops for biofuel production, there is the need to produce more food somewhere else; (b) that implies that an additional amount of CO_2 emissions are released into the atmosphere (by changing e.g. forest into agricultural land).*

Complexity surrounding the iLUC issue stems from the diverse range of potentially negative impacts that it might bring about - including not only those listed above but also potentially significant emissions of GHGs, firstly as a "pulse release" owing to landscape conversion (Clift and Mulugetta, 2007), and then subsequently in the form of foregone carbon sequestration. Other authors (Hertel et al., 2010; Searchinger et al., 2008) relate it to the unintended consequence of releasing more carbon emissions due to land use changes around the world induced by the expansion of croplands for ethanol or biodiesel production in response to the increased global demand for biofuels. Due to this change in the carbon stock of the soil and the biomass, indirect land use change has consequences in the GHG balance of a biofuel and when the GHG emissions from iLUCs are taken into account, there is some evidence that the existing technology of biofuels production crop-based can prove to be more detrimental than the conventional fossil fuels (Hertel et al., 2010; Searchinger et al., 2008). Owing to its importance in the policy debate about biofuels, the estimates of the effects caused by iLUCs have been undergoing of considerable debate, which has been strengthened by the uncertainty involved in the estimation (Wang and Haq, 2008; ACE, 2009); on one particularly controversial point is about where iLUC takes place (Hertel et al., 2010).

1.9 Thesis motivation and roadmap

The broad spectrum of issues related to the establishment of biofuel SCs imposes the necessity to adopt more comprehensive approaches to represent and steer a sustainable and rational transition towards alternative fuel production systems.

To this purpose, the Thesis project aims at developing decision supporting tools to steer strategic the transition towards low-carbon biofuels concerning in particular the design of biomass-based bioethanol technologies and their mutual integration within the existing infrastructure. The work focuses on the development of mathematical modelling (an multi-objective mathematical modelling, MoMILP) framework for SC optimization problems to assist decision-making process on biofuels industry at strategic and tactical level. Such tools should be capable of supporting both industrial/financing choices and governmental policies through a quantitative analysis of the "energy problem".
Therefore, in order to tackle and cope the problematic which has been extensively discussed throughout this chapter, the Thesis objectives have been conveniently divided as follows.

① An integrated approach including new alternative technologies (as biogas) together with emissions trading market-based tools is needed. Such approach might play a key role for dealing with the economic and environmental conflicts through multi–objective optimization (MOO) approach, in order to deliver a sustainable transport systems.

② In order to assess the supply chain robustness to changes in price evolution dynamics and mitigate the risk for investors it is necessary to consider a wide analysis of economic details: a methodology to forecast price dynamics of all the commodities related to biofuel production will be discussed and presented.

③ A more comprehensive methodology including Game Theory (GT) concepts through cooperative and competitive behaviour of different agents into the supply chain management will be introduced in order to optimize the design of novel biomass-to-energy supply networks.

The general structure of this thesis has been devised bearing in mind the problematic discussed along this chapter, the Figure 1.11 represents schematically the outline of this project.

Chapter 2 aims at delivering an environmentally conscious decision-making tool for the design of corn grain-based bioethanol production system, considering possibilities of several technologies integration. It is based on a multi-period multi-objective MILP modelling framework for the design and the optimization of bioethanol SCs where economics and environmental sustainability (GHG emissions reductions potential) for first generation ethanol is addressed. The model is capable of assessing the effect of CO_2-equivalent emissions allowances trading and their inherent volatility level to boost investments on sustainable ethanol production. The analysis takes into consideration the set-aside lands, all of them dedicated to energy crops growth in the territory under study.

Chapter 3 aims at delivering the models to predict commodity price evolution dynamics and to extend the price forecasts to all other goods related to bioethanol production. Then, the optimal supply chain is tested under the different evolution paths, to evaluate if it was a robust investment and how the economic performance depended on the commodity prices.

The Chapter 4 assesses the impact on the supply chain design of the recent European Commission proposal to amend the existing Directive. Notably, this proposal significantly impacted the accountability technique for biofuels, therefore important changes in the supply chain design are expected. The changes in the demand for biofuels and in the limits for selected technologies imply a review of the supply chain model. Furthermore, the Chapter discusses the advantages and the drawbacks of the proposed modifications to the existing Directive.

Chapter 5 extends the MILP modelling framework presented in the Chapter 2. Here a multicriteria decision making tool to support strategic design and planning on ethanol fuel including GT features is proposed. The decision-support tool involves multiple cooperative and competitive farmers, biofuel producers, and food and fuel markets in order to address possible business partnership scenarios between feedstock suppliers and biofuel producers. A stochastic formulation will also be implemented to represent the effect of uncertainty on biomass price.

In Chapter 6, a generalization of the Nash concepts to the general multi-enterprise supply chain is developed. A general MILP approach to determine the most appropriate transfer price level between biomass production sites to biofuel production centres is presented.

To close up, the Chapter 7 finally gathers together the main achievements of the research also outlining the main shortfalls and the main objectives to be carried out in the future work.

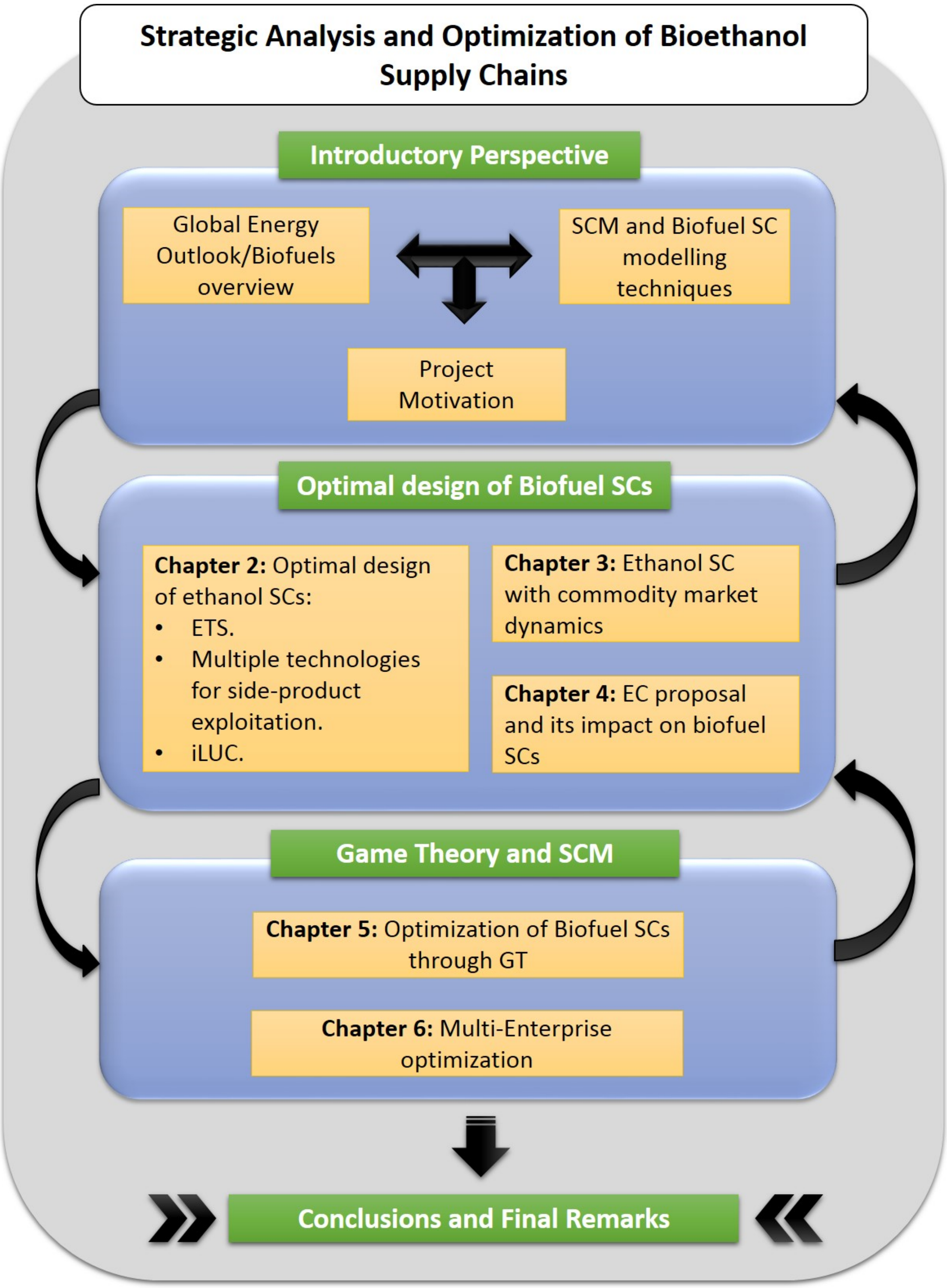


Figure 1.11: *Scheme of the Thesis outline*

CHAPTER 2

Optimal design of ethanol supply chains considering carbon trading effects and multiple technologies for side-product exploitation

THIS chapter[1] addresses the strategic and planning design with dynamic evolution of a bioethanol SC under increasing biofuel demand and GHG emissions savings over the time. An a spatially explicit MoMILP modelling framework is proposed to optimize the SC environmental and financial performances simultaneously. A general description of the biofuels SC design issues is first presented. Next, the mathematical formulation of the model will be outlined. Key features of the proposed framework comprise: *i)* the incorporation of available set-aside rural surfaces for energy crop cultivation; *ii)* the acknowledgement of an economic value to the overall GHG through the introduction of an emission trading system (ETS). Multiple technological options are assessed to exploit the co-product DDGS either as animal fodder (standard usage) or as fuel for heat and power generation or as raw material for biogas production (and hence heat and power). The case study is then introduced testing the model capabilities in terms of the parameters definition and modelling assumptions. Eventually, the results of SC optimization with respect to the MOO strategy are presented followed by a discussion and some final remarks of the main modelling outcomes.

[1]Portions of this chapter have been published in Ortiz-Gutiérrez et al. (2013a,b)

2.1 Motivation

Biofuels still represent one of the most viable options for partial substitution of fossil fuels in transport energy. The European Union (EU) Directives on renewable energy have defined ambitious blending mandates for all the EU Members. The aim is to achieve a 10% energy-based contribution from renewable sources in the transport sector by 2020. Sustainability requirements have been also established and biofuels should allow for a significant GHG emissions with respect to fossil fuels: 35% after 2009, 50% after 2017 and 60% from 2018 onwards (EC, 2009). Bioethanol has been assuming a leading position among biofuels and the earlier impulse came from first generation technologies whose potential environmental drawbacks and social perception have unveiled the need of a more sustainable conversion processing, adding to the foregoing the economics of bioethanol production by first generation technology strongly depends on the feedstocks supply costs (Petrou and Pappis, 2009; Solomon and Johnson, 2009). As widely applied for modern enterprise development, in order to boost the economic and environmental impact of biofuel-based systems, the full management and optimization of the production network along the entire SC, is advocated. In view of the above, there is a need for quantitative design tools assessing both financial and environmental biofuel performance in a holistic way embedding all the production network steps.

This chapter focuses on the on the development of an MoMILP model for bioethanol SC optimization problems by extending the analysis on the available technological options in first-generation ethanol. The purpose is to deliver an environmentally conscious decision-making tool addressing the design and planning of bioethanol production systems to assist the policy-making process on biofuels industry at a strategic and tactical level. The model is based on the approaches commonly applied to the multi-period, multi-echelon and MoMILP steering design and planning tasks under financial and environmental criteria in biofuel production systems (Giarola et al., 2011; Zamboni et al., 2009a), in particular, the possibility to integrate bioethanol plants and anaerobic digestion systems will be considered in this study. Following this rationale, the overall ethanol supply chain has been here optimized in a geographically explicit context by considering multiple technological solutions, including biogas production. According to a MOO approach, both the environmental (based on GHG emission minimization) and economic (based on NPV maximization) performance will be optimized so as to obtain an optimal Pareto curve. Furthermore, as first proposed by Akgul et al. (2012a), the possibility to exploit set-aside land for fuel-dedicated crops is included in the model. Finally, following the approach presented by Giarola et al. (2012) and then extended by Akgul et al. (2012a), carbon trading effects will also be assessed in the optimization framework.

2.2 Assumptions and problem statement

The aim of the work presented in this chapter is the development of a general modelling framework addressing the long-term strategic design and planning of SCs for biofuel systems. The design process is conceived as an optimization problem in which the whole production network is required to comply with the maximization of the financial performance of the business (NPV), and with the minimization of the impact on global warming (in terms of overall GHG emissions) in operating the system.

The problem is formulated as a spatially explicit multi-period and multi-echelon modelling framework devised for the strategic design and investment planning of biofuel supply networks. The biofuel SC under consideration consists of the following nodes: biomass cultivation sites, biomass delivery, fuel production sites and the transport to the demand centres.

The environmental assessment refers to the classical LCA techniques to assess the impact over the biofuel life cycle according to the principles and standards as laid out by the ISO (ISO, 2006) guidelines series, and is implemented following the approach proposed in some previous works (Zamboni et al., 2009a,b). The environmental analysis has been limited to a Well-To-Tank (WTT) approach (CONCAWE, 2008). Therefore, the set of LCA stages s are as follows: biomass production (bp), biomass transport (bt), fuel production (fp) and fuel distribution (fd). The emission credits (ec) in terms of GHG savings (as a result of goods or energy displacement by process side products end-use) are accounted for as a pseudo-life cycle stage. In fact, process by-products can represent valuable products in other markets and reduce the overall supply chain emission bill according to their potentials to displace alternative goods whose production and subsequent impact would therefore be avoided. This approach refers to the allocation method by substitution which assigns to the primary product the total GHG emissions diminished by the emissions avoided as a result of the substitution of alternative goods with by-products (Rickeard et al., 2004). The optimization formulation accounts for this modelling feature by adding to the LCA stages commonly defined for the production system considered (i.e. biomass production, transport, conversion and product delivery), an extra (pseudo) node accounting for an emission discount (or credit) to the total bill due to potentials of market goods replacement with by-products. For instance, considering first generation bioethanol systems based on corn grains, the main by-product is a high-protein meal coming from the solid fraction of the post-process residues (i.e. DDGS). This is a valuable substitute for cattle feed and may also be used as a fuel for CHP generation (Morey et al., 2006).

Accordingly, the set of LCA stages is as follows:

$$s \in S \equiv \{bp, bt, fp, fd, ec\}$$

The model represents a general framework aiming at the optimal design of biofuel system within a MOO formulation, which maximizes the financial profitability of the business while minimizing the GHG emissions. Potential integrations between biogas and bioethanol production networks are investigated in order to assess opportunities for improving economic and environmental performance of the bioenergy system. The influence of an emissions trading scheme is studied through a sensitivity analysis on the cost of the CO_2 emissions allowances traded. Exploitation of set-aside land available is also included in the formulation. Therefore, the key variables to be optimized are:

- geographical location of biomass production sites;
- biomass production for each site;
- supply strategy for biomass to be delivered to production facilities;
- land use allocation to bioenergy purposes, considering the contribution of set-aside terrains;
- bioethanol facilities location, capacity and technology selection, focusing on the potential improvements from the integration between first generation biofuel and anaerobic digestion;

- distribution logistics of biofuel to the demand centres;
- financial performance of the system over the long term;
- system impact on global warming;

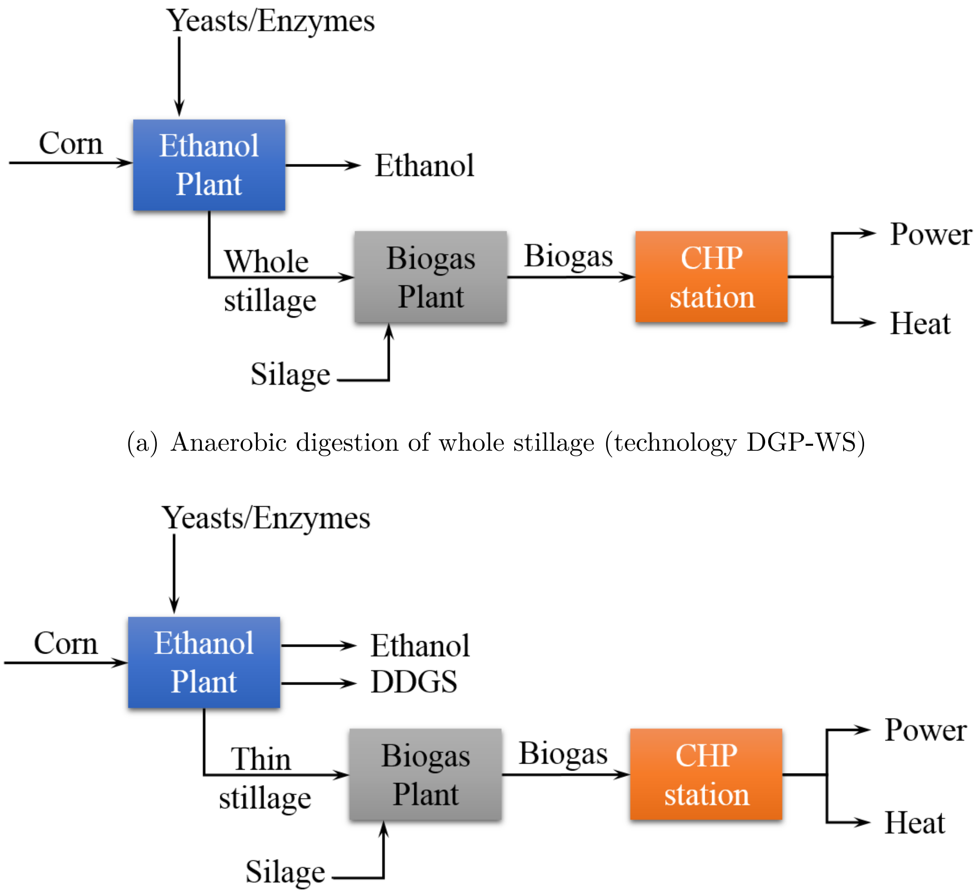
The problem refers to a biofuel SC over a 15-year horizon where has been divided into five time intervals (each three-year long).

2.3 Process configuration

The modelling framework has been conceived considering the first generation technology as a suitable option to convert biomass (corn) into ethanol (a 15% moisture is assumed for corn). A set of alternatives for ethanol production technologies have been investigated. The first option is the DGP, i.e. the standard corn-based ethanol process and is dealt with according to Franceschin et al. (2008), where two instances are analysed according to how power is supplied to the plant: in the first one the co-product DDGS is sold in the cattle feed market thus substituting soy (technology $k = 1$, DGP) and natural gas is used to power the process; in the second case, DDGS is used as fuel and fed to a CHP generation system (technology $k = 2$, DGP-CHP).

In this chapter is add the possibility to exploit the stillage from ethanol distillation to produce biogas. Two process configurations are taken into account. In the first case (Fig. 2.1a), the non-fermentable products obtained from the first stripping column in a typical ethanol production facility (Franceschin et al., 2008; Jacques et al., 2003) known as whole stillage, are directly fed to an anaerobic digester (DGP-WS). Clearly in this case, no DDGS is obtained out of the process. In the second technological option (Fig. 2.1b), the thin stillage resulting from the whole stillage centrifugation (Jacques et al., 2003) is exploited for biogas production (DGP-TS). Note that this last configuration allows for the production of DDGS, too (although in a smaller amount than in the case of DGP technology). In both configurations, biogas is fuelled to a CHP station for heat and power generation.

Finally, it is important to point out that in both technological options with biogas production, some additional feedstock (corn silage) needs feeding to the anaerobic digester to guarantee a regular performance. As suggested by some industrial companies interviewed



(a) Anaerobic digestion of whole stillage (technology DGP-WS)

(b) Anaerobic digestion of thin stillage (technology DGP-TS)

Figure 2.1: *Configurations for the integration of biogas production within an ethanol production facility.*

in this work, a ratio of about 30 tonnes of corn-silage per ton of thin stillage, and of about 2 tonne of corn-silage per tonne of whole stillage are assumed (in both cases, that corresponds to about 0.48 tonne of corn-silage per tonne of corn fed to the plant).

2.3.1 Biogas system

Biogas technology was modelled through a simplified flowsheet accounting for both industrial and literature (Deublein and Steinhauser, 2011) data. A full-load operation of 8150 hours per year is assumed for the biogas plant. It seems reasonable to assume a similar biogas yields on both technological instances and that is equal to 680 Nm^3 of biogas per tonne of total solids (TS). Note that the TS fraction in the whole stillage is 0.235, while in the thin stillage the fraction is 0.016. Biogas composition is set to 53% methane, 46% CO_2

and 1% of inert gas. The overall energy efficiency of the CHP station is set to 90% with an electric efficiency of 40%.

With concern to electricity consumption, the configuration DGP-TS is assumed to have a similar power requirement as the DGP technology (7 MW), whereas power requirement is decreased by 47% for DGP-WS technology (Wooley et al., 1999), because in this configuration there is not DDGS production. Both technologies can produce enough electricity to satisfy the power needs of the conversion plant while providing a power excess which can be sold to the grid, corresponding to a 1.17 kWh per litre of ethanol produced for technology DGP-WS, and 0.72 kWh per litre of ethanol produced for configuration DGP-TS.

The biogas-based cogeneration system is also exploited to produce the steam required by the process: the DGP-TS and DGP-WS configurations are capable of satisfying about 37% and 87%, respectively, of the process steam requirement. The remaining quota is supposed to be compensated for either by using natural gas fed to a steam generation system or by increasing the biogas production capacity by fermenting more silage. Therefore, as summarized in Table 2.1, six technologies are considered: the standard DGP process ($k = 1$), the DGP-CHP process ($k = 2$), the DGP-WS$_{SC}$ process with silage compensation ($k = 3$), the DGP-WS$_{NG}$ process with natural gas compensation ($k = 4$), the DGP-TS$_{SC}$ process with silage compensation ($k = 5$), the DGP-TS$_{NG}$ process with natural gas compensation ($k = 6$).

Table 2.1: *Ethanol technologies: identification and products description of each technology belonging to the set k.*

	Input			Output		
k	Process	Corn	Silage	Ethanol	DDGS	Power
1	DGP	X		X	X	
2	DGP-CHP	X		X		X
3	DGP-WS$_{SC}$	X	X	X		X
4	DGP-WS$_{NG}$	X	X	X		X
5	DGP-WS$_{SC}$	X	X	X	X	X
6	DGP-TS$_{NG}$	X	X	X	X	X

Apart from the biogas produced, anaerobic digestion also produces some digestate that can be used as fertiliser in crop production (Börjesson and Berglund, 2007, 2003; Nielsen et al., 2002). However, the potential (minor) contribution of digestate on the economic assessment of supply chain is not taken into account (however, its environmental impact will be assessed, as discussed in 2.5.1).

2.4 Mathematical formulation

The purpose is to develop a multi-criteria decision analysis tool to guide investments on biofuels SCs at a strategic level. The problem is formulated as a general MoMILP model to promote a sustainable long-term design and planning of ethanol fuel SC. The model is based on the mathematical formulation proposed by Giarola et al. (2011). In a spatially explicit multi-period context, two objective functions are taken into account: the maximization of the NPV [€] and the minimization of total environmental impact ($TGHG$ [kg of CO_2-eq]), which considers the GHG emission rate for each life cycle stage s as well as the effect of emission credits coming from by-products end-use.

2.4.1 Set-aside inclusion

The set-aside land are considerate as additional terrain to the agricultural land normally used for growing crops and with the same agronomic characteristics. However, is taking into account that the reactivation of the culture land after a period of rest time implies in the yield of productivity, which will therefore not be maximum in the first period of use of the land. Therefore it assumes a yield for the first period of reactivation of land equal to 70% of the total productivity of the soils considered. The set-aside areas are considered to be areas destined for energy crops if the model considers it appropriate, or when the use of these surfaces leads to the configuration of great demand for the sector. Set-aside land spatial distribution is defined as in Table 2.2.

However, the data collected outlining the areas (Table 2.2) not intended for cultivation are regionally based and have no special allocations according to the specific topography of the areas considered. The cells in which is subdivided Northern Italy territory are formed from weighted distributions of the provincial area. Consequently, in order to obtain an accurate representation of division of the territory into cells was necessary to adjust the

Table 2.2: *Distribution of set-aside surface distributed in the regions of Italy.*

Region	Set-aside (ha)
Piemonte	15099
Valle d'Aosta	100
Liguria	650
Lombardia	6800
Trentino alto Adige	130
Bolzano	46
Veneto	8600
Friuli Venezia Giulia	5000
Emilia Romagna	17600
Total	54025

provincial data into regional. Accordingly:

$$FL_g = \sum_{r=1}^{n.regions} (YregG_{r,g} \cdot AG_g \cdot YregFL_r), \tag{2.1}$$

where FL_g stands for set-aside land for each cell g; $YregG_{r,g}$ represents a matrix [r x g] for the regions (r) in Table 2.2 with the 59 cells, g, considered as part of the spatial-explicit features of the model; AG_g is the usable area [ha] per cell g; $YregFL_r$ is the specific set-aside surface per hectare per region. The distribution obtained is presented in the following Table 2.3.

The modelling presented here has taken into account the possibility to avail of set-aside lands for corn production is explicitly accounted for. The biomass production $Pb_{g,t}$ [t/time period] in each region g at time period t is described as follows:

$$Pb_{g,t} = Db^T_{g,t} + \sum_l \sum_{g'} (Qb_{(g,l,g',t)} - Qb_{(g',l,g,t)}), \tag{2.2}$$

Note that $Pb_{g,t}$ depends on two contribution: the local demand of biomass, $Db^T_{g,t}$, and flow rate of biomass $Qb_{(g,l,g',t)}$, [t/time period], which is transferred via transport mode l from g and g' at time t (Zamboni et al., 2009b). Biomass production is upper-bounded by the effective regional production capability for ethanol production in cell g (BA_g, [t/time

Table 2.3: *Distribution of set-aside land per cell distributed in North Italy.*

cell (g)	Available Set-aside land (tonne/m)	cell (g)	Available Set-aside land (tonne/m)	cell (g)	Available Set-aside land (tonne/m)
1	9.6	21	1944.1	41	1565.5
2	12.8	22	3395.7	42	1672.9
3	7.7	23	1732.3	43	987.9
4	822.8	24	2237.7	44	1892.3
5	342.4	25	2468.1	45	1469
6	447.5	26	1831	46	814.3
7	516.5	27	1206.1	47	1296
8	11.3	28	1439.5	48	1893.4
9	222.8	29	1405	49	2658.4
10	1633.1	30	1583.9	50	2475
11	3721.5	31	1827.5	51	2108.4
12	1860.7	32	986.9	52	806.6
13	85.7	33	530	53	94
14	1074.1	34	308	54	507.4
15	1623	35	2550.3	55	789.3
16	747	36	1892.3	56	2291.6
17	1556.2	37	1275.8	57	1833.4
18	824.2	38	1495.5	58	1833.4
19	224.1	39	1727.5	59	1925
20	1273.3	40	1907		

period]) and the contribution due to set-aside land ($BAy^{Sa}_{g,t}$, [t/time period]).

$$Pb_{g,t} \leq (BA_g + BAy^{Sa}_{g,t}), \tag{2.3}$$

When set-aside lands are devoted to a non-food crop production destination, they require more intense agricultural practices to remove weeds and start off the cultivation. These lands are characterised by an initial lagging period before crop yield reaches its maximum productivity levels (Timilsina and Shrestha, 2011). This has been modelled accounting for an initial crop yield penalty of 30% during the first period of set-aside land exploitation:

$$BAy_{g,t}^{Sa} = 0.7 \cdot BA_g^{Sa} + Pbcum_{g,t-1}, \tag{2.4}$$

where the term $BAy_{g,t}^{Sa}$ [t/time period], represents a limit for the availability of biomass from set-aside in the region g in the time period t; BA_g^{Sa} [t/time period], corresponds to the theoretical biomass potential (from set-aside) for bioethanol production in the region g, while the term $Pbcum_{g,t-1}$ [t/time period] corresponds to the productivity of biomass accumulated over time and is defined as:

$$Pbcum_{g,t} = Pbcum_{g,t-1} + Pb_{g,t}, \tag{2.5}$$

Also, biomass availability from set-aside land has to compel with the limit of the regional agronomic characteristics, and not to exceed the maximum biomass potential (2.6).

$$BAy_{g,t}^{Sa} \leq BA_g^{Sa}, \tag{2.6}$$

To address the social debate "*biomass for food - biomass for fuels*", a threshold of 14% (Zamboni et al., 2009b) is chosen to define the maximum level of biomass available for ethanol generation over the total crop production, when corn is collected from areas commonly used for food/feed production. No restriction is assumed when the biomass is grown from the set-aside (all corn grown there can be used for ethanol production). In other words, the set-aside areas are assumed to be exclusively dedicated to grow corn for biofuels production.

2.4.2 Carbon trading scheme

The emission allowance trading scheme is dealt with as in Giarola et al. (2012), although that approach has now been extended to a spatially explicit framework. A baseline is set for the overall SC GHG equivalent emissions representing a sustainability requirement for biofuels settled by the legislation, with respect to which tradable permits might be generated (Bojarski et al., 2009; , CGA). It is supposed that any amount of rights can be sold or obtained in the emissions market. Each emission allowance transaction may take place only at the end of each period and is evaluated on the total equivalent CO_2 emission occurring in the SC. Thus, the following relationship holds:

$$TI_t \leq MaxCO2_t + P_t^{all} - S_t^{all}, \tag{2.7}$$

The above equation states that TI_t [kg of CO_2-eq/time period] must be equal to the cap $MaxCO2_t$ [kg of CO_2-eq/time period] plus the extra credits bought to emit P_t^{all}, and minus the sold credits S_t^{all}. The cap $MaxCO2_t$ has been defined as a regulation-based limit on the total emissions from fuel SC, by taking as a reference the EU policy framework. Accordingly:

$$MaxCO2_t = LHV_{EtOH} \sum_k \sum_g (P^T_{"ethanol",k,g,t}) \cdot GHGg \cdot (1 - GHGr_t), \tag{2.8}$$

where LHV_{EtOH} is the ethanol lower heating value, term $P^T_{"ethanol",k,g,t}$ [t/time period] is the total production rate of ethanol produced with the technology k in region g at time t, while $GHGr_t$ represents the GHG emissions savings required by biofuels. $GHGr_t$ is set equal to 35% for the first period, 50% for the second one and 60% for the last 3 periods according to EU regulation. $GHGg$ is the GHG emission factor for the gasoline (85.8 kg of CO_2-eq per GJ) (Woods et al., 2005).

2.5 Case study

The emerging biomass-based ethanol production in Northern Italy during the period from 2012 to 2026 is assessed as a real world case study to illustrate the applicability and capabilities of the proposed approach in steering the strategic design and planning of biofuels supply networks. Spatially explicit-related features (i.e. cultivated areas distribution, cellular crop yields, emissions and production cost, network logistics for trucks, rail and barges, location of ethanol demand centres) are described as in Zamboni et al. (2009b). The ethanol demand varies over time through the effect of the legislation and it is defined as in Giarola et al. (2011). It is worth noting that in addition to existing cultivated terrains, this work addresses the inclusion of the set-aside land to investigate its potential to help the deployment of a corn-based ethanol production in a sustainable way. Set-aside land spatial distribution is defined as in Table 2.4.

Table 2.4: *Distribution of set-aside surface distributed in the regions of Italy.*

Region	Set-aside (ha)
Piemonte	15099
Valle d'Aosta	100
Liguria	650
Lombardia	6800
Trentino alto Adige	130
Bolzano	46
Veneto	8600
Friuli Venezia Giulia	5000
Emilia Romagna	17600
Total	54025

The SC analysis and LCA approaches proposed by Zamboni et al. (2009b,a) for bioethanol production have been adopted to evaluate the specific modelling parameters (i.e. transportation costs and GHG emissions, standard corn-based ethanol production capital and operational costs). Market prices for ethanol, DDGS and power are fixed equal to 710 €/t_{EtOH}, 300 €/t_{DDGS} and 180 €/MWh (considering current subsidies for green credits), respectively. Corn price is set to 162 €/t, which represents a 10 years average value in Italy.

2.5.1 Emision credits

The emissions credits are assigned when conventional products are replaced with biomass-derived by-products, i.e. the DDGS and electric energy (Zamboni et al., 2009a). In addition to that, it is assumed that the credits to be applied for the fertilisation effects of the digestate amount to 97.78 kg of CO_2 per tonne of biomass (Meyer-Aurich et al., 2012). The set of parameters regarding to the emission credits, fec_k, are reported in Table 2.5.

2.6 Results and discussion

The problem was solved by means of the CPLEX solver in the General Algebraic Modelling System (GAMS)® modelling tool (Rosenthal, 2010). In this work, the set of Pareto

Table 2.5: *fec_k credits for avoided emissions of conversion technology k.*

k	fec_k (kg CO2-eq/t$_{EtOH}$)
1	342.2
2	1427.4
3	1694.8
4	1482.2
5	1803.2
6	769.1

solutions of the MOO problem was obtained by means of the ϵ-constraint method (Ehrgott, 2005), according to which an auxiliary scalar optimization problem is formulated by transforming one of the objective functions into additional constraints. The Pareto curve can be found by solving the scalar problem with an appropriate choice of the epsilon parameter. The resulting MILP problem has about 208809 continuous variables and 8500 discrete variables and the all set of Pareto optimal designs are generated in about 5 hours.

In the subsequent discussion, a first part is dedicated to the presentation of the strategic investment decisions in accordance with the framework of simultaneous optimization of GHG emissions savings and economic profitability. A second part explains how the results would change, if a trading scheme were implemented, assuming a GHG emission baseline according to the EU reduction targets (EC, 2009).

2.6.1 Multi-Objective optimization

The results trend produces a Pareto curve (Figure 2.2) revealing the conflict between environmental and economic performance in dealing with biofuels production.

For instance, the economic optimum (point A in Figure 2.2) entails a marginal NPV of 1.19 €$/GJ_{EtOH}$ against a global environmental impact of 91.7 kg CO_2 equiv.$/GJ_{EtOH}$. The SC configuration would involve the settlement of ethanol plants either exploiting a standard DGP process ($k = 1$) or relying on an alternative thin stillage valorisation route and on natural gas supplement for energy needs (DGP-TS$_{NG}$, $k = 6$). Thus, ethanol production combined with anaerobic digestion of thin stillage would lead to a profitable business,

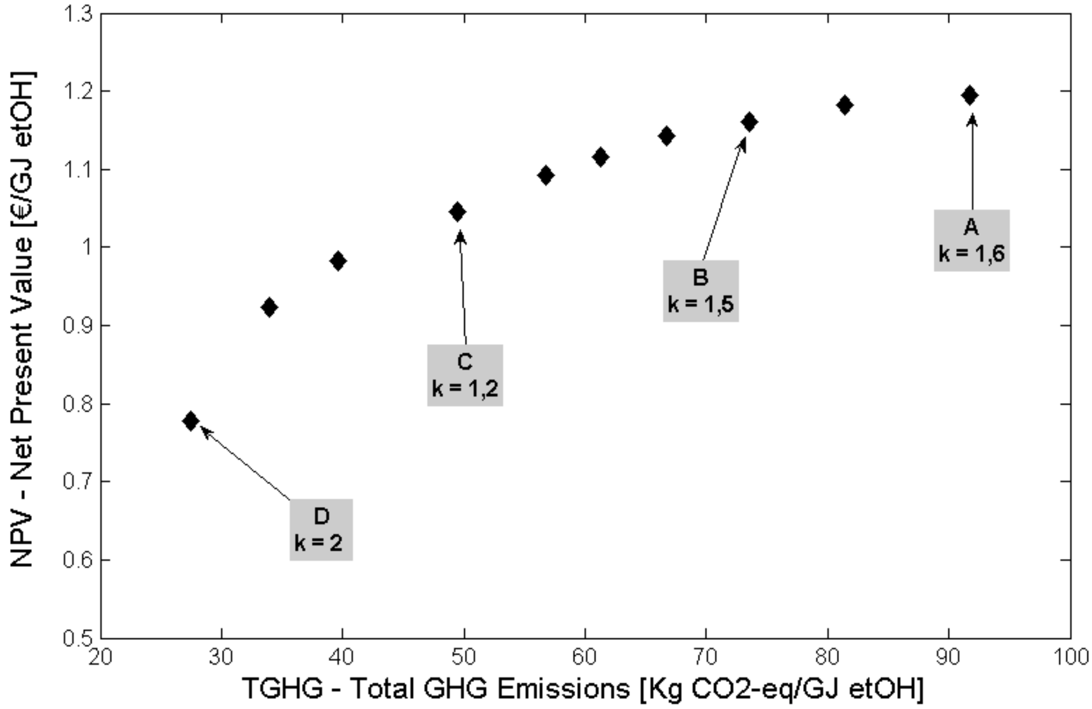


Figure 2.2: *Pareto set of optimal solutions: simultaneous optimization under NPV maximization and GHG emissions minimisation criteria (k = production technology).*

although quite sensitive to incentives on electricity production. However, the additional supply of natural gas is detrimental to the environmental performance of first generation technologies, which are acknowledged a 10% GHG emission reduction compared to fossils (Zamboni et al., 2009b).

The integration of the standard first generation ethanol process ($k = 1$) with the technology DGP-TS$_{SC}$ ($k = 5$) (point B in Figure 2.2) would improve the environmental performance of the system. The substitution of natural gas with corn silage to environmental impact is reduced down to 73.5 kg CO_2 equiv.$/GJ_{EtOH}$ but it is still inadequate to achieve the GHG emission reduction targets. The economic performance is still good with a marginal NPV of 1.16 €$/GJ_{EtOH}$.

Moving down towards better performance in terms of environmental impact mitigation a suitable SC configuration is represented by the Pareto non-inferior point C in Figure 2.2, where processes operating with a traditional DGP technology ($k = 1$) are exploited along with processes where the whole DDGS is devoted to power generation (DGP-CHP, $k = 2$). The overall GHG emissions are about 42% lower with respect to the gasoline pathway, thus getting closer to meet the EU environmental targets. The marginal NPV is about 1.05

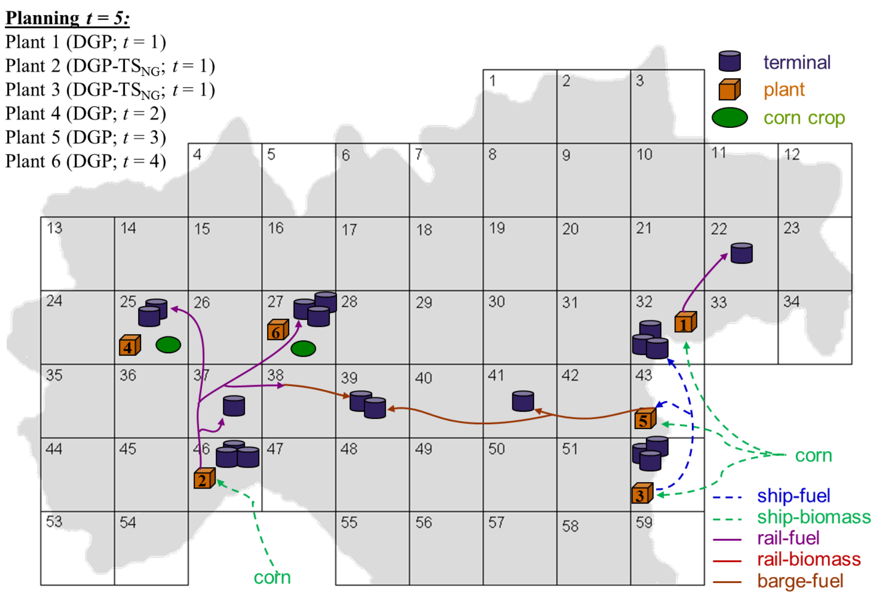
€$/GJ_{EtOH}$.

The best performing supply design in terms of the environmental performance is obtained by point D in Figure 2.2 based on the technology DGP-CHP ($k = 2$). This solution reduces the environmental impact down to 27.5 kg CO_2 equiv.$/GJ_{EtOH}$ while maintaining a good economic performance (NPV = 0.78 €$/GJ_{EtOH}$). The mitigation effects on GWP, now accounting for about 68% of GHG reduction, would be sufficient to meet both the 2017 and the 2020 targets (set to 50% and 60%, respectively).

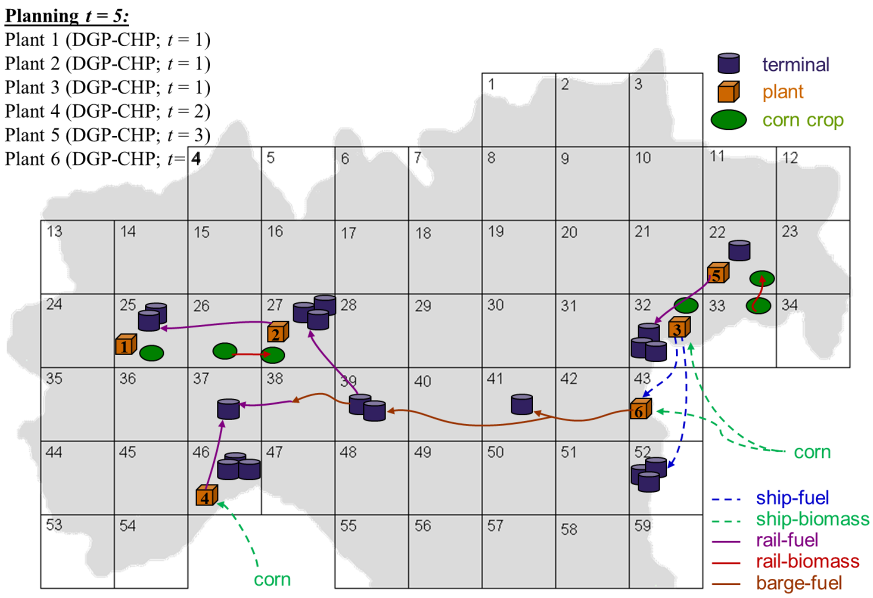
As is clear from the above, the environmental benefits which might derive from the integration between biogas and ethanol production could generate more sustainable first generation biofuel SC only when the input of fossil energy is reduced (as in the technology DGP-TS_{SC}, $k = 5$). Also, the full compliance of the EU GHG emission reduction targets would require a large fossil energy displacement, achievable when all the DDGS is devoted to bioenergy production (as with the technology DGP-CHP, $k = 2$).

Figure 2.3 illustrates the design and planning strategy including the detailed transport system of the optimal solutions for the economic and environmental performance at the end of the time horizon.

The SC configuration for the economic optimum (Figure 2.3a) would involve the establishment of six production plants. In the first time period ($t = 1$), the SC configuration involves the establishment of three ethanol production facilities relying on imported corn grain. A first plant, based on the traditional DGP-based technology, with a capacity of 110 kt/year, is settled close to the Venice harbour ($g = 32$). A second facility, operating with technology DGP-TS_{NG} (with natural gas compensation) ($k = 6$) at a nominal production capacity of about 250 kt/year is located in the port of Genoa ($g = 46$). A third facility planned to be exploiting a technology DGP-TS_{NG} (k = 6) is set up in the industrial area of Ravenna (g = 52) with a nominal production capacity of 200 kt/year. In the second time period ($t = 2$), a DGP-based facility ($k = 1$) with a capacity of 110 kt/year is located within the industrial area of in Turin ($g = 25$), supplied with locally grown biomass. In the third time period ($k = 3$), another ethanol production plant operating with a standard DGP technology ($k = 1$) and a nominal capacity of 110 kt/year, is located in the industrial area of Porto Viro ($g = 43$), taking advantage of the proximity to the coast from which biomass is imported. Finally, in the fourth period ($t = 4$), a DGP-based facility ($k = 1$) is



(a)



(b)

Figure 2.3: *Design and planning strategy at time period $t = 5$ for both economic (a) and environmental (b) optimal solution.*

planned to be placed near Milan ($g = 27$) with a nominal capacity of about 185 kt/year. Note that in this optimal configuration the biomass is mainly imported from abroad (69%).

The optimal environmental configuration (Figure 2.3b) proposes the establishment of six plants, all based on DGP-CHP technology ($k = 2$), the majority of which are planned to be put in operation in the first time period ($t = 1$). Three of them have a nominal production capacity of about 110 kt/yr, while the remaining plants are established with medium-sized capacity of about 210 kt/yr. The ethanol SC configuration does not differ much from the economic optimum described above in what concerns the facility positions. All production sites match previous locations, but no plant is expected close to Porto Viro ($g = 52$); a DGP-CHP facility settled northwards ($g = 22$) using homegrown biomass is preferred instead. As is clear from Figure 2.3b, the overall environmental performance takes advantage of a net cut of biomass import along with larger credits coming from avoided emissions due to DDGS burning and its conversion into energy, thus displacing significant fossil fuels. In terms of the transport system in both cases, water ways (barge and ships) wherever viable are preferred, otherwise railways are chosen to deliver both biomass and products.

Due to its high fragmentation, overall scarce availability and more expensive exploitation than cultivated rural areas, contribution of set-aside land is never a relevant one (6% of the cultivated land for the economic optimum; 4% in the environmental optimum).

2.6.2 Carbon trading scheme

The trade mechanism of carbon allowances (ETS), provides for the opportunity to sell or purchase permits to emit CO_2. Note that with the current value of the European Unit Allowance (EUA), i.e. the price of CO_2 (approximately 5 €/t, according with the average in the first two months of the 2013 (EEX, 2013)), the ETS does not impact on the selection of the optimal technologies along the Pareto curve, i.e. the best economic performance still involve both standard DGP production plants ($k = 1$) as well as DGP-TS_{NG} (with natural gas compensation) ($k = 6$), whereas the environmental optimum adopts the DGP-CHP technology ($k = 2$). In other words, the effects of ETS are not such to affect the overall economic performance significantly, however, the environmental performance of the economic is slightly improved with a reduction on the GHG emissions from 91.7 down to 86.8 kg CO_2 equiv./GJ_{EtOH}. The Figure 2.4 illustrates the behaviour of the two extreme optimal points in the ETS framework.

The actual SC emissions are compared with the cap imposed along the time horizon thus originating a need (or a benefit) to buy (or to sell) permits to emit. In particular, when applied to the economic optimum of the ethanol SC, the mechanism of trading carbon, offers

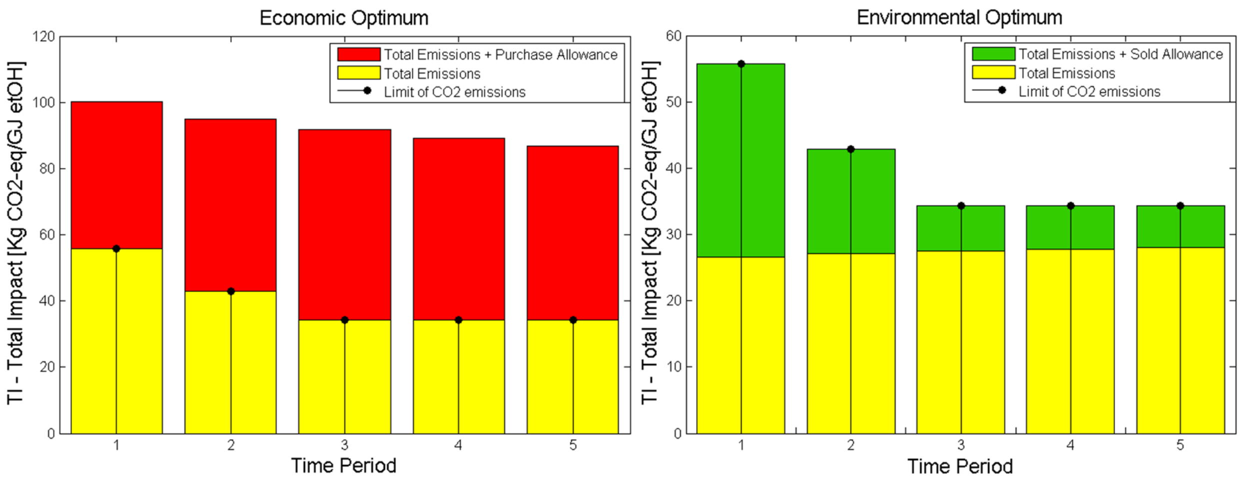


Figure 2.4: *Emissions in the SC and allowance trading in the various time periods for both economic and environmental solutions.*

the opportunity to purchase quantities of CO_2 to compensate for the excess of CO_2 emitted (Table 2.6).

Table 2.6: *Purchased-specific emissions (P_t^{all}) in each time period, t, for the economic optimum configuration.*

Time period	TI_t (kg CO2-eq/GJ_{EtOH})	P_t^{all} (kg CO2-eq/GJ_{EtOH})
1	100.22	44.45
2	95.04	52.14
3	91.73	57.41
4	89.08	54.76
5	86.75	52.43

Conversely, the optimal environmental configuration is characterised by low levels of emissions, which allows selling CO_2 emission quotas (Table 2.7).

A sensitivity analysis was carried out by varying the selling price of EUA, according to the recent historic fluctuations (Mizrach, 2012), in order to quantify the profit due to CO_2 quotas sold or purchased. Results are summarised in Table 2.8.

Note that in the range 10-25 €$/t_{CO2}$ there is a technological change in the economic optimum and the technological option devoting the whole DDGS production to energy valorisation (technology DGP-CHP, $k = 2$) is preferred to the combined generation of a quota of DDGS and energy from biogas (technology DGP-TS_{NG}, $k = 6$) as more credits are

Table 2.7: *Sold-specific emissions (S_t^{all}) in each time period, t, for the environmental optimum configuration.*

Time period	TI_t (kg CO2-eq/GJ$_{EtOH}$)	S_t^{all} (kg CO2-eq/GJ$_{EtOH}$)
1	26.62	29.15
2	27.15	15.75
3	27.52	6.80
4	27.82	6.50
5	28.08	6.24

Table 2.8: *Sensitivity analysis on the value of the NPV at different prices of EUA.*

EUA (€/t$_{CO2}$)	5	10	15	20	25	No ETS
NPV_{econ} (€/GJ$_{EtOH}$)	1.14	1.10	1.07	1.05	1.03	1.19
Technology (k)	1,6	1	1	1	1,2	1,6
NPV_{env} (€/GJ$_{EtOH}$)	0.79	0.81	0.83	0.85	0.86	0.78
Technology (k)	2	2	2	2	2	2

gained from avoided emissions. On the other hand, quite obviously there is no change in the environmental optimum, although a higher EUA improves the overall profitability. In fact, we verified that a EUA worth about 100€is needed to make the environmental optimum also the economic one, i.e. to catch up with the NPV of the best economic solution.

2.7 Final remarks

In this chapter a spatially explicit and multi-period MoMILP modelling framework for the design and planning of feasible and sustainable multi-echelon corn-based ethanol SCs has been presented and discussed. Results demonstrate that producing biogas through the anaerobic digestion of solid residues after biomass conversion could ensure a viable trade-off between economic and environmental performance. The effect of carbon trading scheme on ethanol SC development has been assessed. At the current CO_2 price, this contribution would hardly promote environmental performance improvement.

However, as the emission trading market is expected to grow in the long term, a sensitivity analysis has been performed on the permit price showing some benefits on the promotion of more sustainable technologies. At a CO_2 allowance price of 25 €$/t_{CO2}$, the overall profitability of the economic optimum would be reduced by about 13%, while the economic performance of the environmental optimum would be enhanced by about 10%.

Moreover, some stakeholders have concerns that the use of crops for biofuels could displace existing agricultural production. This could cause the expansion of crop land to replace those crops that had been used for biofuels instead of other uses, such as food or animal feed. This potential impact, known as iLUC, which has been widely discussed in Section 1.8, could ultimately result in new GHG emissions due this change on land activity. The issue in question is introduced into the modelling framework presented in this Chapter, both results and discussion are presented in the Appendix A.

CHAPTER 3

Strategic Design of Bioethanol SCs Including Commodity Market Dynamics

In this chapter[2], the limiting assumption of keeping constant the price/cost of raw materials, products, and utilities is relaxed. The economic assessment is based on the forecasted price dynamics of the commodities related to ethanol production. Specifically, three price-forecast models are introduced and tuned according to the Italian context. The robustness of the SC with respect to changes in price evolution is assessed to mitigate the risk for investors. Finally, different strategies to keep the SC operative are discussed, and their impact on final customers and Italian taxpayers is detailed. This chapter analyzes the establishment of a corn-based bioethanol SC in northern Italy through a MILP modelling framework, which allows its financial performance to be evaluated by optimizing the spatially explicit layout in terms of production technologies, biomass production sites, and the transport network.

3.1 Motivation

Since the economic performance of a production system depends on the prices of its raw materials and sold products, a key aspect, in the economic analysis of the bioethanol SC in northern Italy is forecasting the future prices of corn, ethanol and other related products

[2]Portions of this chapter have been published in Mazzetto et al. (2013)

over a rather long period. Previous works that assessed the economic performance of the bioethanol supply chain either considered the prices to be constant (Zamboni et al., 2009b) or, more realistically, used a stochastic approach to cope with the commodity price or demand uncertainty (Dal-Mas et al., 2011; Kostin et al., 2012). However, even the stochastic approach is not able to grasp the inherent trends in commodity prices and the complicated links in the biofuel market.

Clearly, both commodity and fuel prices are affected by a number of issues, including both market dynamics and regional policies. For instance, the volatility in the price of agricultural products is related to weather effects, stock levels, energy prices, increasing demand, and trade regulations (FAO/OECD, 2011). In this chapter, price prediction models were based on previous historical fluctuations and on the correlation of corn and fuel-grade ethanol quotations with crude oil prices. In fact, the price of a grain commodity can be affected by the price of oil on both the supply and the demand sides. On the supply side, an increase in the crude oil price pushes crop production costs up as a result of higher costs of fertilizers, fuel, and transportation (Chen et al., 2010b). On the demand side, grain commodities are linked to the crude oil price through the grains demand for biofuels and through other macroeconomic issues. In addition, on the demand side, biofuels can be regarded as either substitutes or complementary goods of fossil fuels (Marzoughi and Kennedy, 2012). In the first case, biofuels can substitute for fossil fuels at a percentage that is determined only by economic factors (eventually lower and upper boundaries can be set for technological issues), whereas in the second case their share in the final fuel is fixed even in case where blending is not economically convenient. The law of supply and demand determines that in the former case, as fossil fuels prices increase, the demand for biofuels also increases, because it becomes increasingly convenient to blend them with fossil fuels. Consequently, the price of biofuels increases (along with the price of raw materials). In the second case, biofuels are considered as complementary goods to fossil fuels (as is typical in Europe), and if the price of fossil fuels increases, then fuel demand decreases according to supply and demand equilibrium. As a result, demand for biofuels also decreases, since their share in the final fuel is fixed (Yano et al., 2010). In such an entangled situation, key information for an investor is an assessment of the robustness of the supply chain layout with respect to changes in price evolution dynamics in order to mitigate investment risk.

In view of the above, the objective proposed for this chapter is to propose three price prediction models for both corn and ethanol and to assess how the results of a SC economic optimization based on a MILP model would be affected by price dynamics. First of all different models for predicting price evolution dynamics are presented and discussed, and then a SC design model is applied and optimized to assess the resulting structure and economic performance. Finally, the effect on Italian taxpayers and fuel consumers is critically evaluated. Northern Italy is chosen as geographical case study.

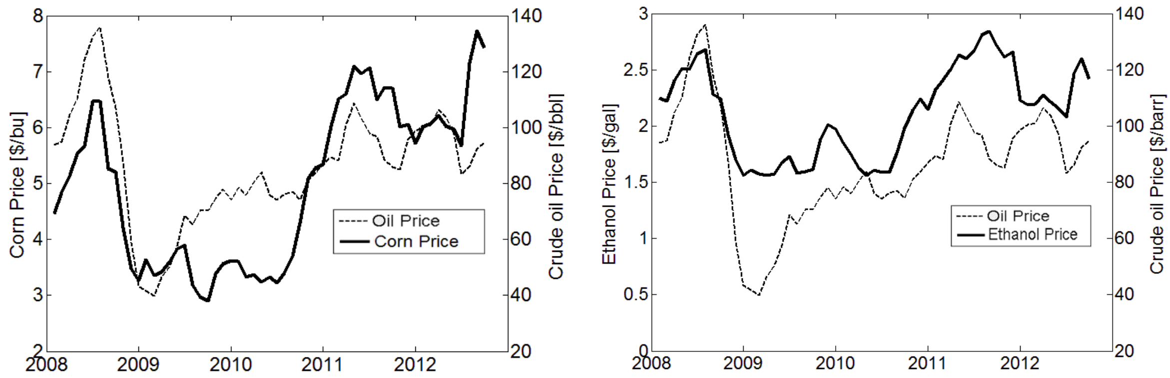
3.2 Commodity price forescast models

The objective is to forecast corn and ethanol prices in the medium to long term. The time horizon considered here was a 15-year period (i.e., 2013-2027), which we assumed to be a reasonable period where first-generation technologies would still be the dominant ones. Furthermore, 15 years can be assumed to be the average operating lifetime of an ethanol plant (Solomon et al., 2007).

3.2.1 Autoregressive Distributed Lag Model

A widely used model to express the linkage of a commodity price to the price of a reference good is the autoregressive distributed lag (ADL) model (Stock and Watson, 2003; Huang and Jane, 2009; Pinto et al., 2011). This technique permits the functional time dependence of the price of a commodity to be identified from its previous values and those of the reference component (Ghaffari and Zare, 2009). This method was recently employed (Manca et al., 2011; Manca, 2012) to estimate future prices of toluene and benzene as the raw material and final product, respectively, of a hydrodealkylation plant.

In the present case, the ADL model was used to link the corn and ethanol prices with the price of crude oil, which was used as the reference component. In fact, it is known that corn and ethanol prices are affected by a number of other variables, but they either are relatively constant on a multiyear basis in developed countries (e.g., feedstock yield, corn demand for food purposes) or can be indirectly related to crude oil demand. Historical data on corn, ethanol, and crude oil prices were obtained from the U.S. market, where corn-based ethanol production is more mature. Data from 2008 were used in order to buffer the lag



(a) (b)

Figure 3.1: *Dynamics of crude oil price since January 2008 compared with (a) corn and (b) fuel-grade ethanol quotations in the same period. All of the goods are expressed in U.S. units [dollars per barrel of crude oil, dollars per bushel of corn (25.4 kg), and dollars per gallon (3.78 L) of ethanol]. The graphs represent monthly average prices, as elaborated by Hofstrand (2012).*

time between the approval of the Energy Policy Act and the large-scale use of bioethanol as a fuel. WTI-Oklahoma quotations were used for crude oil prices, while corn prices were Iowa average values and ethanol prices were averaged from the U.S. market (Hofstrand, 2012). The linear dependence between each commodity price-time series and the crude oil one was quantified using the Pearson correlation coefficient (Stock and Watson, 2003) between the variables (there is a perfect correlation if the Pearson correlation coefficient is 1 and a perfect anticorrelation if its value is -1).

The correlation coefficients between corn and oil prices and between ethanol and oil prices were investigated at different lag periods. For both commodities, the highest correlation coefficient was found in the case of the no-lag-time series, thus indicating an immediate response of both corn and ethanol prices to the price of oil. Notably, the Pearson coefficient between the corn and crude oil prices without a lag time was 0.69, and the ethanol-oil one was 0.76. Such values demonstrate that there is a significant correlation between the two commodities and oil, as is also illustrated in Figure 3.1*a,b*. The correlation coefficients were quite significant also when the lag time was set to 1 month (0.64 for corn and 0.70 for ethanol), and therefore, the effect of the price of crude oil in the previous period was included in the model, too. Furthermore, since the current commodity price is highly self-correlated with the price in the previous period, such a correlation was also included in the ADL model. Thus, the generic model $ADL(p,q)$, where $p = 1$ is the delay of the dependent variable and

Table 3.1: *Parameters of the corn and of the ethanol price forecast functions 3.1 and 3.2 according to the ADL model.*

Parameter	A_C	B_C	C_C	D_C	A_E	B_E	C_E	D_E
Value	-0.1317	0.0467	-0.0448	1.001	0.0109	0.0155	-0.0156	1.001

$q = 1$ is the delay of the independent variable, is expressed for the two commodities as:

$$CornPrice_t = A_C + B_C \cdot OilPrice_t + C_C \cdot OilPrice_{t-1} + D_C \cdot CornPrice_{t-1}, \quad (3.1)$$

$$EthanolPrice_t = A_E + B_E \cdot OilPrice_t + C_E \cdot OilPrice_{t-1} + D_E \cdot EthanolPrice_{t-1}, \quad (3.2)$$

where $CornPrice_t$ is the price of corn [$/bu] at time t, $EthanolPrice_t$ is the price of fuel-grade ethanol [$/gal] at time t, $CornPrice_t$ is the quotation of oil [$/bbl] at time t. The values of the parameters A_C [$/bu], B_C [bbl/bu], C_C [bbl/bu], D_C, A_E [$/gal], B_E [bbl/gal], C_E [bbl/gal] and D_E (Table 3.1) were estimated with a MATLAB minimization routine through a regression on data from January 2008 to December 2011 in order to test it for predictive purposes on 2012 data (i.e., the so-called validation set). The coefficients of determination (R^2) of the obtained functions were 0.72 and 0.59 for the prices of corn and ethanol, respectively, thus showing that the ethanol price has a behavior that is less consistently related to oil (however, the errors never exceeded 50 $c\$/gal$).

Once the relationships for corn and ethanol prices had been determined, it was necessary to predict the future oil price in order to use the ADL model for forecasting purposes. The principle adopted here was the same as in the works based on analysis of oil price "shocks" (i.e., relative variations) (Manca et al., 2011; Manca, 2012). In fact, it was verified that oil price shocks were independent of the previous variations (the lagged Pearson correlation coefficient was always below 0.25) and that they were distributed according to a normal distribution, as illustrated in Figure 3.2.

In view of the above, it made sense to simulate oil price shocks as a Markov process (Manca, 2013b), that is, a stochastic discrete-time process in which the transition probability to a new state of the system is determined only by the previous state and not by the way

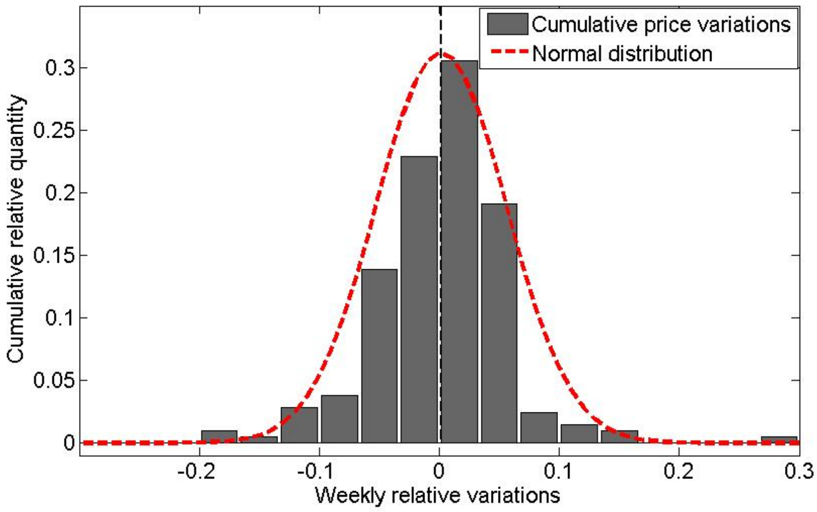


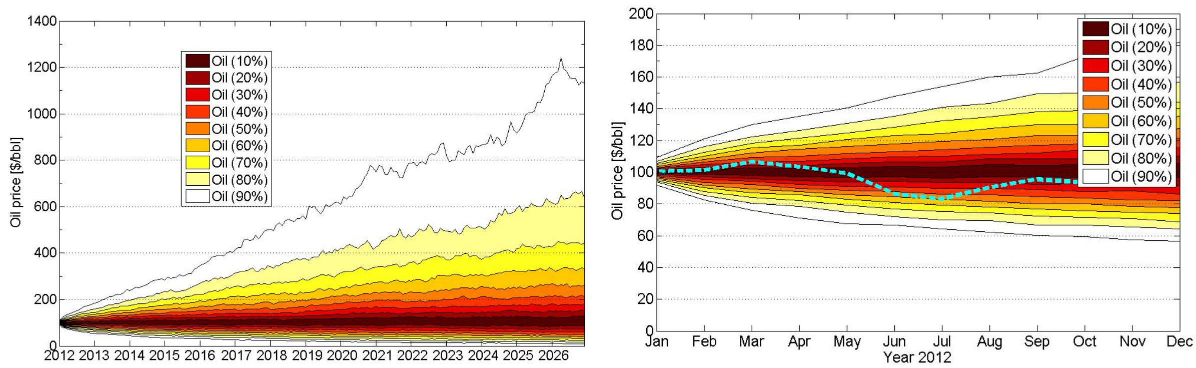
Figure 3.2: *Cumulative oil price "shocks" and comparison with a normal distribution with the same mean and standard deviation as the "shocks"*

that state was reached (Häggström, 2002). The proposed relation is the following one:

$$OilPrice_t = OilPrice_{t-1} \cdot (1 + \mu + \sigma \cdot \zeta), \tag{3.3}$$

where ζ is a function whose output is a random number with mean 0 and standard deviation 1, while μ and σ are the mean and the standard deviation, respectively, of the distribution that describes the crude oil price shocks. Their values were estimated to be $\mu = 0.0015$ (therefore, increasing relative variations are more frequent than decreasing ones) and $\sigma = 0.0541$. A map representing the probability of future oil prices was obtained by running 2000 simulations. Cumulative probability areas were then plotted in a "fan chart" also known as a "river of blood" (Figure 3.3) (Stock and Watson, 2003). The most probable regions of the graph (i.e., the darkest ones in the figure) showed good accordance with the 2012 data (Figure 3.3b), thus confirming the quality of the simulation; in fact, little cumulative distribution was needed to include the model predictions.

The forecasted prices for corn and ethanol according to the ADL model were calculated using equations 3.1 and 3.2 by assuming for the oil price a trend lying within the most probable region as forecasted by the stochastic approach for crude oil prices. The quotations obtained with the intermediate scenario are reported in Table 3.2. The estimated prices for 2012 showed a small underestimation for ethanol forecasts (-1.8% of the real price) and more significant errors for corn ones (-8.6%).



(a) (b)

Figure 3.3: *(a) Cumulative probability regions of future crude oil prices and (b) comparison with actual 2012 prices.*

Table 3.2: *Forecasted corn and ethanol prices using the* $ADL(1,1)$ *model under intermediate oil price scenario.*

Forecasted good	2013-2015	2016-2018	2019-2021	2022-2024	2025-2027
Corn price [$/bu]	8.78	11.35	14.24	17.04	20.09
Ethanol price [$/gal]	2.43	2.60	2.77	2.85	3.01

3.2.2 Fully Stochastic Model

The stochastic technique used to draw scenarios for crude oil prices can be applied to the commodity prices under investigation once it is proven that their behaviors can be described as Markov processes. In fact, it was verified that the weekly relative variations of the prices of both commodities since 2008 were limited within a narrow range (±10% level, except in a couple of cases) and that there was no trend in the shocks, as illustrated for corn prices in Figure 3.4a. The correlation coefficient between the commodity price variations and their lagged series (i.e., lagged autocorrelation) was minimal, as shown for corn prices in Figure 3.4b.

In both cases, it was possible to describe the cumulative relative price variations through a normal distribution, having the same mean and standard variation of the data. Finally, the relative variations of prices of both commodities can be set as a Markov process and their price evolution scenarios can be obtained through the same stochastic technique used for crude oil price. Consequently, forecasts of corn and ethanol prices have been drawn from

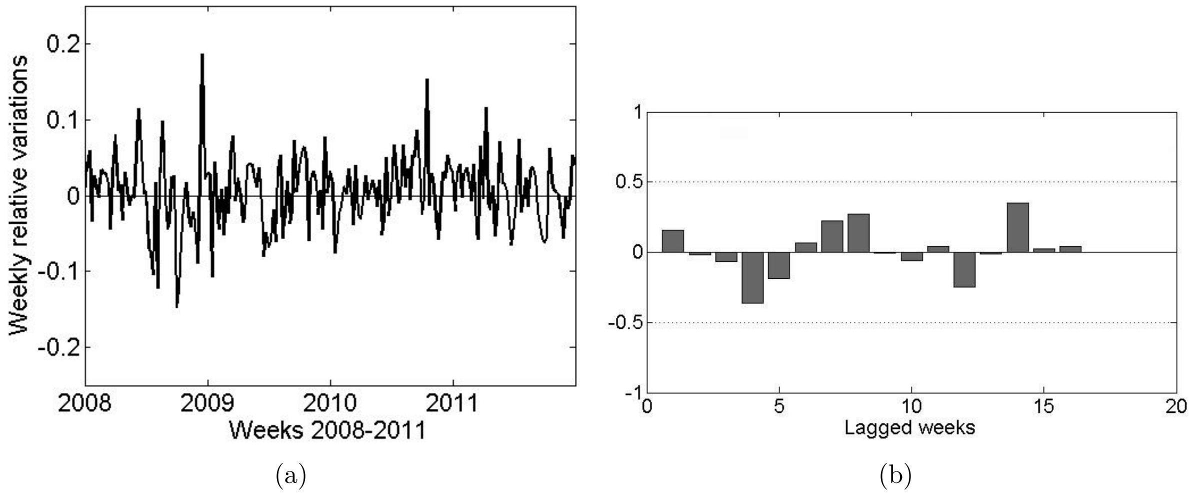


Figure 3.4: *(a) Weekly relative variations in corn prices over the period 2008-2011 and (b) lagged autocorrelation of the corn price relative variations at different lag times.*

Table 3.3: *Parameters of the corn and of the ethanol price forecast functions 3.4 and 3.5 according to the fully stochastic model.*

Parameter	μ_C	σ_C	μ_E	σ_E
Value	0.0027	0.0467	0.00037	0.0369

the reconstructed Markov process, as defined by the following equations:

$$CornPrice_t = CornPrice_{t-1} \cdot (1 + \mu_C + \sigma_C \cdot \zeta), \tag{3.4}$$

$$EthanolPrice_t = EthanolPrice_{t-1} \cdot (1 + \mu_E + \sigma_E \cdot \zeta), \tag{3.5}$$

The parameter values are reported in Table 3.3.

The probability regions were obtained through 2000 simulations for each commodity. Figure 3.5 illustrates the corn case. Similar results were obtained for ethanol. It can be noticed that in both cases the actual data from 2008 to 2012 fall within the 90% cumulative probability region and show a good fit with the most probable area of the graph. If the most probable region is considered as the most reliable one for future average quotations of the commodities, its average value can be chosen to predict the prices of both corn and ethanol. These values are reported in Table 3.4. This model also underestimated the 2012 prices

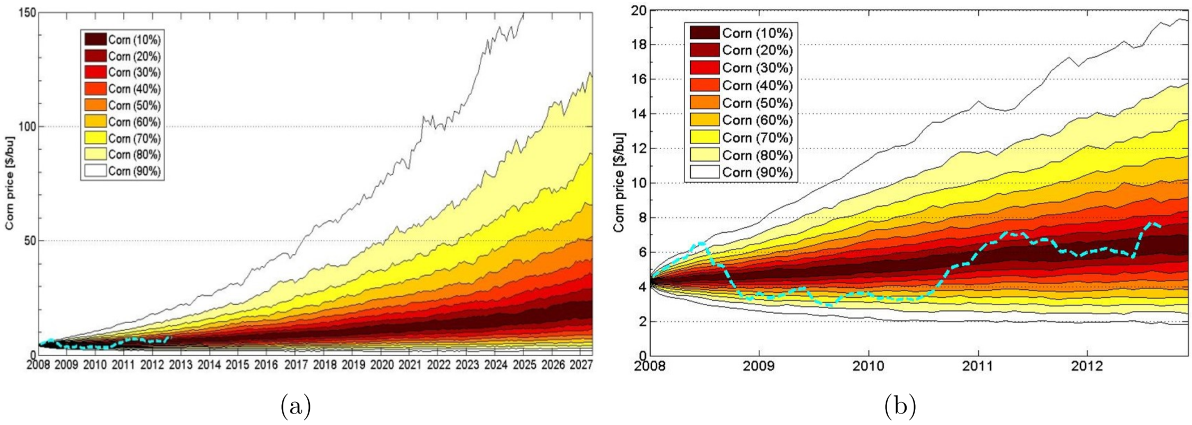


Figure 3.5: *(a) Probability regions for corn price and (b) comparison with actual 2008-2012 prices (represented by the dashed light blue line).*

Table 3.4: *Corn and ethanol prices forecasted using the fully stochastic model.*

Forecasted good	2013-2015	2016-2018	2019-2021	2022-2024	2025-2027
Corn price [$/bu]	6.65	8.25	10.50	13.09	16.30
Ethanol price [$/gal]	2.07	1.97	1.87	1.77	1.70

(the errors for the 2012 average quotations were -9.7% for corn and -6.3% for fuel-grade ethanol).

It is worth noting that corn prices are expected to grow significantly over next years, as shown by the trend of the most probable region in Figure 3.5a, while the average quotation of ethanol is expected to decrease in the future. This is not unexpected and is related to Ito's integral calculus, which extends the concept of integration to stochastic processes (Itô et al., 1944). Notably, according to Ito's lemma, the mean of stochastic processes generated by a distribution of mean μ corresponds to an equation of mean $\mu - \sigma^2/2$, where σ is the standard deviation of the generator distribution. In the case of ethanol price variations, the value of $\mu - \sigma^2/2$ is negative, since $\mu_E = 0.00037$ and $\sigma_E = 0.0369$. Therefore, the resulting decrease of the most probable region is caused by the high standard deviation and the low mean of the ethanol price shocks, and its trend is due to an endogenous characteristic of stochastic processes.

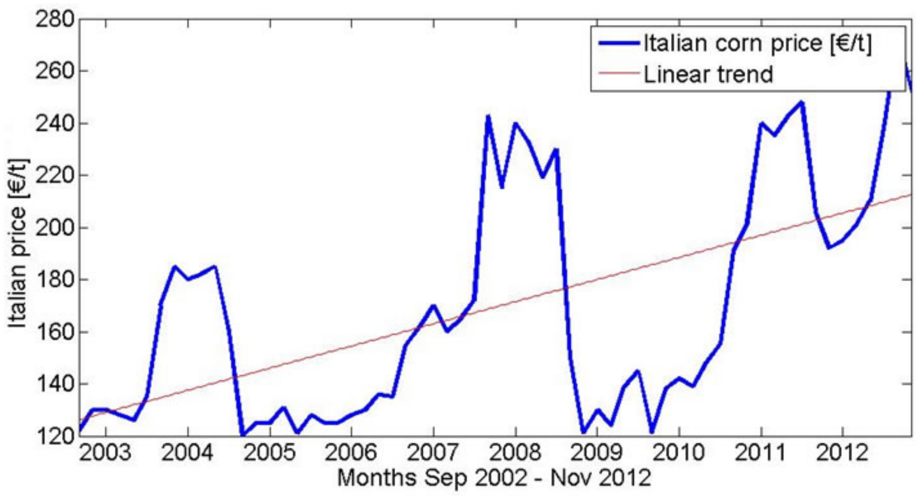


Figure 3.6: *Italian corn prices over the past decade compared with a linear trend.*

3.2.3 Time series decomposition model

Corn and ethanol prices showed an increasing trend with many peaks and troughs in recent years, as shown by the behavior of corn prices in Italy over the past decade (Figure 3.6, where the corn quotations at the *Borsa Granaria* in Milan (Associazione Granaria di Milano, 2014) were used).

One of the most used techniques to evaluate the composite behavior of a time series is the time series decomposition (TSD) method (Zarnowitz and Ozyildirim, 2006), which evaluates a time series as the product of a trend function and a periodic function, with the residuals considered as a random contribution. Suitable models to describe the two commodities prices are as follows:

$$CornPrice_t = (q_{CC} + m_{CC} \cdot t)\left[A_{CC} + B_{CC} \cdot sin\left(\frac{2\pi \cdot t}{T_{CC}} + \phi_{CC}\right)\right], \tag{3.6}$$

$$EthanolPrice_t = (q_{EE} + m_{EE} \cdot t)\left[A_{EE} + B_{EE} \cdot sin\left(\frac{2\pi \cdot t}{T_{EE}} + \phi_{EE}\right)\right], \tag{3.7}$$

where m_{CC} [\$/(bu·months)] and q_{CC} [\$/bu] are the parameters of the linear component of the corn price function and q_{EE} [\$/gal] and m_{EE} [\$/(gal·months)] of the ethanol one, while A_{CC} [-] B_{CC} [-], T_{CC} [months] and ϕ_{CC} [-] are required to define the periodical component of the corn price function, and similarly A_{EE} [-], B_{EE} [-], T_{EE} [months] and ϕ_{EE} [-] for the ethanol price function. The fits of the two models with actual data were rather good:

Table 3.5: *Parameters of the corn and ethanol price forecast functions (3.6) and (3.7) according to the Time Series Decomposition model.*

Parameter	Value	Parameter	Value
q_{CC}	3.5874	q_{EE}	1.8674
m_{CC}	0.0486	m_{EE}	0.0086
A_{CC}	0.9562	A_{EE}	0.9728
B_{CC}	0.3057	B_{EE}	0.2135
T_{CC}	41.703	T_{EE}	41.692
ϕ_{CC}	1.0926	ϕ_{EE}	1.2616

Table 3.6: *Forecast corn and ethanol prices using the Time Series Decomposition model.*

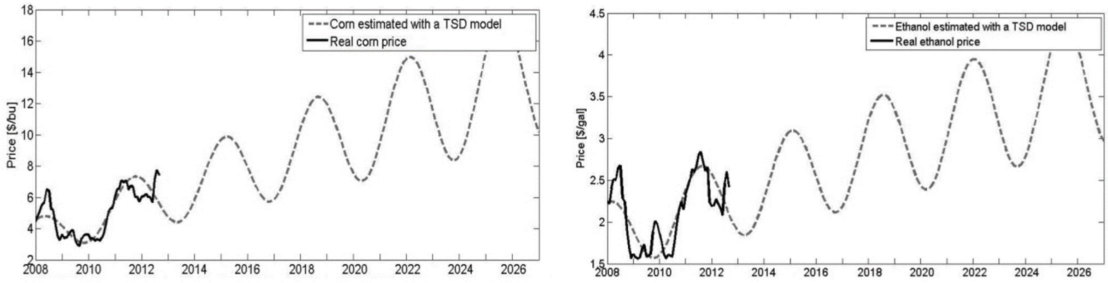
Forecast good	2013−2015	2016−2018	2019−2021	2022−2024	2025−2027
Corn price [$/t]	6.21	7.83	9.77	11.91	13.87
Ethanol price [$/gal]	2.30	2.59	2.95	3.35	3.71

for instance, the coefficient of determination of the corn price model with data from 2005 to 2011 was 0.82. As in the other cases, the parameters of the equations (Table 3.5) were calculated using U.S. data from 2008 to 2011.

It is interesting to notice that the periodicities of the two commodities are the same ($T_{CC} \approx T_{EE}$) and that they are almost synchronized ($\phi_{CC} \approx \phi_{EE}$). This may be linked to the fact that the corn and ethanol price series are highly correlated. The model predictions are illustrated graphically in Figure 3.7, and the average quotations per period are reported in Table 3.6. This model showed the best predictions of the 2012 prices; in fact, it slightly underestimated the actual 2012 corn prices (-3.3%) and gave a very good fit to the ethanol quotations (+0.4%).

3.2.4 Adapting the price forecast to the Italian context

The models introduced in the previous sections were used to provide the supply chain simulations with realistic commodities prices for the whole operative life of the supply chain. The model parameters were tuned on U.S. data because of their extensiveness and completeness. A price adaptation to the Italian context was thus needed. The straightforward conversion of historical prices from American units to European ones gives



(a) (b)

Figure 3.7: *Comparisons of (a) corn and (b) ethanol prices calculated using the TSD model (dashed) with actual quotations (solid).*

rise to some observations. In fact, an analysis of Italian and U.S. corn and ethanol prices over the last years showed that the Italian corn price and its dynamics have been basically equivalent to the U.S. ones (Itô et al., 1944; Ferrazzi, 2008) while ethanol prices have on average been 15% higher than the corresponding U.S. values converted to euros (ICIS, 2012). This difference can be explained by an analysis of the international markets of the two commodities. The world corn export market is concentrated within a few countries, with the U.S. as the main actor (Abbassian, 2008). As is usually the case, in this situation an international reference corn price is set, and that is the Chicago trade price (ERS, 2012). As a result, U.S. prices can be reasonably applied to all net-importer countries, including Italy (Assosementi, 2012). On the other hand, there is no free world-scale market for ethanol, since the commodity is subjected to many import restrictions, such as quotas and import duties (Akkerhuis, 2010; Kfouri, 2011; EIA, 2012).

In view of the above, for our simulation concerning the Northern Italian context, we chose to use the price predicted by the models in the case of corn and the model price increased by 15% in the case of ethanol. The forecasted corn prices (€/t) and ethanol prices (€/kg) for each time period considered in the simulated case study are summarized in Table 3.7.

3.2.5 Comparison of forecasted prices with real data

In the previous paragraphs, the prices obtained with the different forecasting techniques were compared with actual 2012 average data. A possible way to compare the forecasted prices on a long-term horizon is to consider the equivalent yearly growth rate of each commodity

Table 3.7: *Average corn and ethanol prices by period according to different models.*

Model	2013−2015	2016−2018	2019−2021	2022−2024	2025−2027
			Corn prices [€/t]		
ADL	257	332	416	498	587
Stochastic	194	241	307	383	477
TSD	181	229	286	348	406
			Ethanol prices [€/kg]		
ADL	6.69	7.15	7.60	7.83	8.27
Stochastic	5.69	5.42	5.14	4.87	4.67
TSD	6.32	7.12	8.11	9.21	10.20

Table 3.8: *Historical compound annual growth rates (CAGRs) of the commodity prices and CAGRs for 2013-2027 as predicted by the models.*

	Corn (%)	Ethanol (%)
Historical [3]	+12.2	+6.0
ADL	+7.8	+1.7
Stochastic	+8.1	-1.5
TSD	+7.8	+3.3

as predicted by the models for the future periods and to compare it with its historic value. This rate is commonly called the compound annual growth rate (CAGR) (Investopedia, 2013), and it is currently used to compare investments. Notably, 2011 average corn price is 280% of the 2002 average price, corresponding to a CAGR of 12.2%, while the increase in the price of fuel-grade ethanol is equivalent to a CAGR of 6.0% since 2005. Table 8 reports the CAGRs predicted by the models and compares them to the historical values.

In general, it appears that all of the models might underestimate the price increases for both commodities. In fact, this may turn out to be a sensible prediction, since the end of U.S. subsidies and the decrease in the profitability of corn ethanol plants (IEA, 2012) will halt an important demand factor for the corn market and also for the ethanol one (although

[3]The corn CAGR was calculated using 2002-2011 data and the ethanol CAGR using 2005-2011 data

biofuel policies in the EU and China, which seem likely to support the ethanol market, may partly compensate for this). Furthermore, it seems more sensible to expect a higher increase in corn price because of the continuous pressure on stocks and the surge in the demand as animal fodder (Food and Institute, 2011). The data confirm that the TSD model may provide the best predictions, since the forecasted CAGRs are about 60% of the historical ones. On the other hand, the fully stochastic model showed the highest underestimations of commodities prices and predicts the ethanol price to decrease by 1.5% per year, which seems to be far from reality.

3.2.6 Bioethanol byproduct prices

Two important byproducts are related to the ethanol production process based on corn: DDGS and electricity. DDGS is used as animal fodder with nutritional properties similar to soybean (Tonsor, 2006), and it is obtained from the classic DGP, on which most operating plants are based, in about same quantity as ethanol. Although DDGS is only marginally present in the Italian market (Flake, 2012), the DDGS price evolution in the U.S. after the large-scale establishment of the bioethanol supply chain shows that after the approval of the Act it aligned to the price evolution for corn, fluctuating between 75% and 110% of the corn price (Hofstrand, 2012). It appears reasonable to assume similar dynamics of the DDGS price for the Italian market. Therefore, the DDGS price was set at 90% of the corn price.

Electricity can be produced in CHP modules from DDGS combustion or biogas production (Martin et al., 2012), and its excess is sold to the grid. Electricity produced by renewable biomass can benefit from governmental subsidies. A new incentive scheme has been adopted in Italy for plants producing "green" electricity (GovIta, 2012) that has modified the market dynamics, thus making it a difficult task to forecast future electricity subsidies reliably. However, according to experts, subsidies will decrease in the mid-term by around 15% (ELEMENS, 2012) compared to current standards. For this reason, the subsidy level was set to the current value (200 €/MWh) for the period 2013-2015 and then reduced by 15% and kept constant until 2024; in the last period (2025-2027), subsidies were assumed to diminish by an additional 15%.

3.3 Bioethanol Supply Chain design model

The problem addressed in this chapter deals with the strategic design and planning of a general biofuel SC over a 15-year horizon. The optimization problem involves the maximization of the NPV of the whole SC during its entire operative life. The strategic decisions in designing a biofuel production network deal with the geographical location of biomass cultivation sites, logistical definition of the transport system, and supply chain node locations, while planning decisions regard the capacity assignment of production facilities and the demand satisfaction along the periods, as defined by European Directive 2009/28 (EC, 2009).

The demand scenario is assumed that gasoline and diesel should separately reach the targets set by the directive starting from negligible ethanol production in Italy in 2012 (Flach et al., 2011). Therefore, it was supposed that the ethanol blending rate in 2013 should be the one fixed by the directive as the starting point in 2010 (i.e., 5.75% on an energy basis). Consequently, the increasing trend in the substitution quota was extended until 2027 in order to anticipate further regulations and to take into account the starting delay in achieving the targets. The overall time horizon was divided into three-year periods in order to reduce the computational burden. Accordingly, each blending percentage is an average value over each period. The commodity price forecast was represented using piecewise constant values over each time period.

The biofuels supply chain design problem can be formulated as follows. The input data include the following:

i) geographical distribution of demand centers;

ii) fuel demand over the entire time horizon;

iii) geographical availability of biomass;

iv) biofuel market characteristics in terms of commodity prices, as predicted by the price forecast models;

v) capital and operating costs for biofuel production facilities;

vi) transport logistics (modes, capacities, distances, availability, and costs).

Given these inputs, the objective is to determine the optimal system configuration that maximizes the financial profitability of the supply chain. Therefore, the key variables to be optimized are the following:

i) geographical location of biomass production sites;

ii) biomass production for each site;

iii) supply strategy for biomass to be delivered to production facilities;

iv) location and scale of biofuel production facilities;

v) distribution processes for biofuel to be sent to blending terminals;

vi) supply chain economic performance.

This problem is formulated as a MILP modelling framework in order to capture the behavior of the entire supply chain, and a spatially explicit approach was adopted to consider the strict dependence on geographical features characterizing biofuel systems. The mathematical formulation is based on the modelling approaches adopted in the strategic design of a multi-echelon SC encompassing features to address the siting of spatially explicit facilities and capacity planning for strategic fuel systems, just as has been previously presented in Chapter 2. On the other hand, regarding to the bioethanol production technologies are considered for this analysis the same that have been taken into account in Chapter 2 and are described in Table 2.1.

3.4 Results and discussion

3.4.1 Optimal SC layout

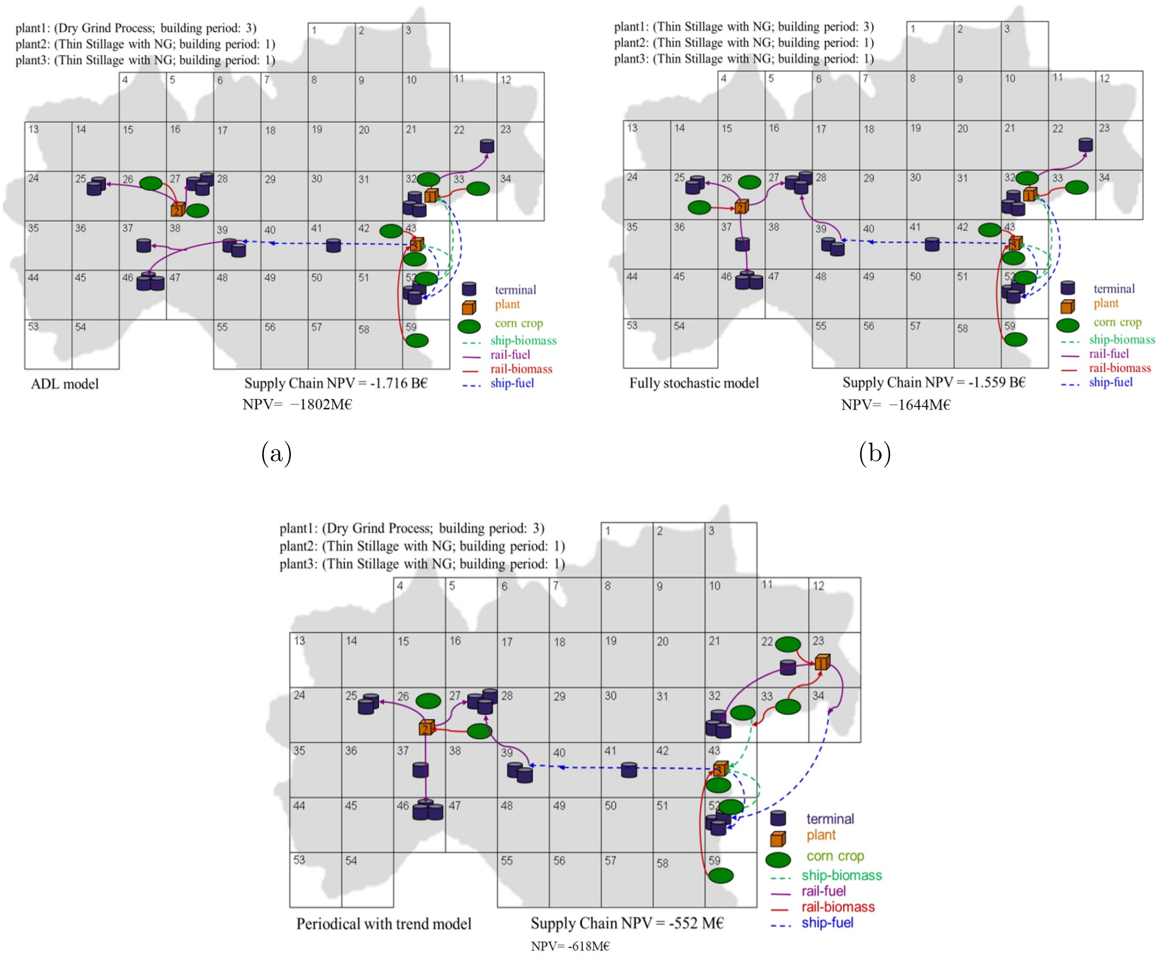
The main objective of this chapter is to compare the optimal SC layout under different price evolution models in order to assess the robustness of the design to changes in price dynamics.

A first important result of the simulations is that the supply chain NPV was always negative, independent of the forecast model being adopted, thus indicating that bioethanol production is not a profitable business at the predicted price levels and under the currently demanded quantities. On the other hand, the optimal supply chain proved to be very robust to changes in the price evolution dynamics.

As illustrated in Figure 3.8, in all cases three production plants are proposed to satisfy the bioethanol demand: two bigger ones, which should reach a production rate of 350 kt/y of ethanol, and a smaller one to be built between 2019 and 2021, which should reach a production rate of 265 kt/y of ethanol. Clearly, the effect of scale economy for capital investment is a general requirement. The preferred technologies are the ones that take advantage of DDGS sales (i.e., standard DGP technology and DGP with biogas production from thin stillage). The reason relates to the assumption that the price of DDGS is linked to that of corn, whereas revenues from sales of electricity are supposed to decrease because of diminishing incentives on renewable energy production. In all of the simulations, two production facilities are located in northeast Italy and the third in northwest Italy (between Milan and Turin). The transportation network is similar in all the cases, with the Po River serving as an important axis for the western demand centers. The crop cultivation areas are also very similar in all the simulations, with biomass growing near the production plants.

These results were obtained under the hypothesis that Italian and imported corn prices are the same. However, it was proven that if imported corn is cheaper than autochthonous corn, the production plants tend to be located close to the main hubs (i.e., around the Venice and Genoa harbors). Notably, if imported corn is more than 12 €/t cheaper than Italian corn, no internally grown corn is used by the bioethanol supply chain.

We also estimated the break-even prices of corn and ethanol, that is, the maximum corn price allowing for a profitable supply chain for a given ethanol price (for the optimal supply chain configuration described in Figure 3.8): the break-even line in Figure 3.9 represents the calculated zero-profit loci and separates profitable from non-profitable regions. Figure 3.9 also shows the supply chain performance for the case where the mean corn and ethanol prices for each year since 2005 were used to estimate the system profitability. It is interesting to notice that after 2007 (corresponding also to the period where massive ethanol production was established in the U.S.), the profitability has decreased significantly. In fact, it appears that since 2011 the supply chain has been unprofitable. This situation was confirmed by the U.S. ethanol industry, where many activities reported losses in 2012 because of the end of government subsidies (IEA, 2012; NACS, 2012). Similar studies were conducted in the U.S. and showed good accordance with these results (BioPact, 2007; Tyner, 2008).



(c)

Figure 3.8: *Optimal supply chain design at the final period (2025-2027) according to the three price prediction models: (a) ADL model, (b) fully stochastic model, and (c) TSD model. In each panel, the description of the preferred plant technologies and the resulting NPV are reported.*

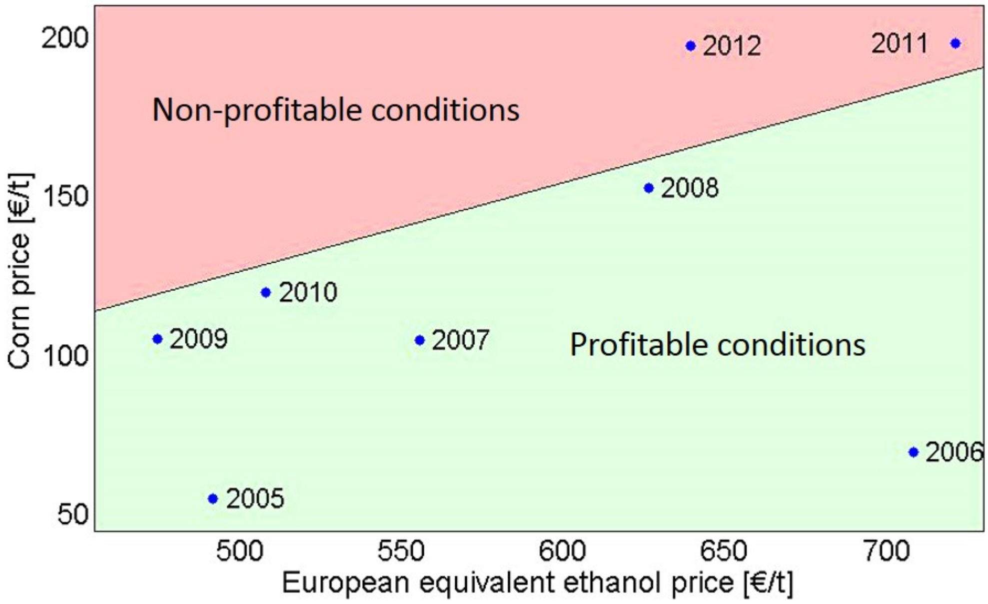


Figure 3.9: *Profitable and non-profitable conditions for the supply chain for given corn and ethanol prices. The break-even line separates the two regions. The average European corn and ethanol prices are projected on the plane for years 2005-2012.*

3.4.2 Impact on fuel consumers and taxpayers

To comply with the European legislation under the assumption that ethanol will not be imported from abroad (which would be rather contradictory with respect to many political objectives underlying the directive), an ethanol supply chain should be established in the European Union. However, since this is likely to be unprofitable, losses should either be transferred to final customers or recompensed by governmental subsidies (as was done in the U.S. until 2011). The required subsidies are shown in Table 3.9, along with the overall amount computed in current terms (i.e., discounted at the 15-year Italian government bond rate, which was 4.70% in February 2013).

Table 3.9: *Required subsidies (in M€) under the different price evolution dynamics forecasted by the models.*

Model	2013-2015	2016-2018	2019-2021	2022-2024	2025-2027	Total equivalent in current terms [4] [M€]
ADL	574	511	1027	1565	2249	4130
Stochastic	472	384	966	1478	2350	3870
TSD	333	18	164	381	632	1089

[4] Discounted at the 15-year Italian bond rate.

Table 3.10: *Ethanol cost per liter of blended fuel, supply chain losses repayments and total fuel price in the next periods according to different price paths forecasted by the models.*

Model	Quantity	2013-2015	2016-2018	2019-2021	2022-2024	2025-2027
ADL	Ethanol cost (c€/L)	8.77	10.95	13.26	15.19	17.62
	Losses repayments(c€/L)	2.32	2.03	4.02	6.04	8.56
	Total fuel price (€/L)	1.74	1.74	1.75	1.77	1.80
Stochastic	Ethanol cost (c€/L)	7.46	8.29	8.96	9.44	9.95
	Losses repayments(c€/L)	1.91	1.53	3.79	5.71	8.95
	Total fuel price (€/L)	1.73	1.70	1.71	1.71	1.73
TSD	Ethanol cost (c€/L)	8.29	10.90	14.14	17.86	21.72
	Losses repayments(c€/L)	1.35	0.07	0.64	1.47	2.41
	Total fuel price (€/L)	1.73	1.72	1.73	1.75	1.78

The per-liter equivalent of these subsidies is similar to the U.S. subsidy (which was fixed at 51 c$/gal, i.e., 10.5 c€/L) only in the first period and then increases up to 2-7 times this value depending on the price evolution dynamics. If losses are to be repaid by fuel consumers, the blended fuel price would be composed of the following:

i) the gasoline price plus taxes weighted on the volume fraction of gasoline;

ii) the ethanol price plus the value-added tax (21% in Italy) and the per-liter loss repayment.

If the gasoline price [5] is assumed to remain constant at the 2012 average Italian price (MSE, 2013) (i.e., 1.785 €/L), the fuel prices calculated using the different price forecast models are reported in Table 3.10.

It has to be remembered that the blended fuel has an inferior lower heating value (LHV) than normal gasoline because the ethanol LHV is about two-thirds that of gasoline (the blending quotas in the five periods considered in this study were 6.3, 7.5, 8.7, 9.8, and 10.9% on energy basis, respectively). Nevertheless, ethanol has a higher octane rating (research octane number = 113), and thus, the loss in heating value can be partly counterbalanced by the increase in engine performance. However, since this increase in engine performance is difficult to calculate, it was decided to take a conservative point of view and ignore this performance effect. Table 3.11 reports the calculated blended fuel price differences

[5] The gasoline price was considered to be constant at 1.785 €/L

Table 3.11: *Price difference between the blended fuel and gasoline at equivalent mileage under different price evolution dynamics.*

Model	2013-2015	2016-2018	2019-2021	2022-2024	2025-2027
ADL	+0.4%	+0.4%	+1.9%	+3.3%	+5.3%
Stochastic	-0.6%	-1.4%	-0.7%	-0.3%	+1.0%
TSD	-0.5%	-0.7%	+0.5%	+2.2%	+4.1%

with gasoline at equivalent mileage, considering only the decrease in LHV, as previously explained. It can be noticed that the differences with the gasoline price are very small at the beginning and then increase with the increase in the ethanol-blending quota, which determines a decrease in the fuel LHV.

3.5 Concluding remarks

The approach presented in this chapter is focused on the economic optimization of a bioethanol SC in nothern Italy by using variable commodity prices as predicted by three price evolution models based on historical data. These models provided a more detailed description of the ethanol supply chain as far as the economic assessment of this feasibility study is concerned and allowed the gap between real price/cost dynamics and constant values of raw materials, products, and utilities (e.g., fuel substitutes, complementary goods, fodder) to be covered.

The resulting SC spatial layout and its economic performance were proposed and discussed. The bioethanol SC is not expected to have a positive economic performance, since the net present value is estimated to be negative whatever the commodity price evolution, but the optimal bioethanol supply chain layout was proved to be robust to changes in price evolution dynamics.

CHAPTER 4

Impact on the optimal design of bioethanol SCs by a new European Commission proposal

THE European Commission recently proposed to review the existing 2009/28/EC Directive on biofuels, in order to increase their environmental sustainability and to decrease the recourse to alimentary biomasses. In this chapter[6] the impact of this proposal on the emerging bioethanol production system in northern Italy is evaluated and compared with the current European Directive. The impact of the proposed policy is also assessed in terms of greenhouse gas emissions and fuel security. Eventually, the effects on fuel consumers and taxpayers are taken into account.

4.1 Motivation

Biofuels are acknowledged to have a positive effect in terms of energy security, because they decrease the dependence on fossils of oil-importing countries (RFA, 2012). Currently most used biofuels based on crops growing in a temperate climate (i.e. corn-based ethanol and rapeseed-based biodiesel) may deliver only limited environmental benefits (Farrell et al., 2006) and may lead to severe ethical issues because of the arising competition between food and fuels (Tenenbaum, 2008; Gomiero et al., 2010).

Recently, the European Commission (EC) proposed a revision of the existing Directive

[6]Portions of this chapter have been published in Mazzetto et al. (2015)

(2009/28/EC) that regulates the production of biofuels in the European Union and aims at reaching a quota of 10% biofuels in the transport sector and on energy basis by 2020, in order to promote more sustainable biofuels, both on the environmental and the ethical points of view, while maintaining their role in terms of energy security. In particular, there is a will to "limit the contribution that conventional biofuels make towards attainment of the targets in the Renewable Energy Directive [and to] encourage a greater market penetration of advanced biofuels by allowing such fuels to contribute more to the targets in the Renewable Energy Directive than conventional biofuels" (EurLex 52012PC0595, 2012).

Thus, the EC proposal aims at promoting second-generation biofuel technologies that do not use food-competitive raw materials capable of achieving higher GHG emission savings and higher energy efficiency compared to first-generation technologies (Wang et al., 2012a). The measures suggested by the EC do not include any financial incentive, but propose to limit the allowed production of first-generation biofuels by creating a new accountability technique to reach the European biofuel production objectives. In fact, first-generation biofuels shall not exceed 50% of total biofuel production and a new categorization of biomasses used for biofuel production is introduced (EurLex 52012PC0595, 2012):

a) bioethanol produced from technologies involving a food-competitive feedstock is accounted "as is" in terms of energy content for the satisfaction of European targets;

b) bioethanol produced from technologies involving second-generation feedstock from a dedicated culture is accounted twice in terms of energy content with reference to European targets;

c) bioethanol produced from technologies involving second-generation feedstock from waste materials is accounted four times in terms of energy content with reference to European targets.

This chapter discusses briefly how the new proposal would affect the configuration of a biofuel (ethanol) production system on a medium term horizon, and demonstrates how process systems engineering techniques and methods can be utilized advantageously to assess the effect of policy proposals and directives in a quantitative way. The optimization of the supply chain layout in northern Italy is taken as a case study. The impact on taxpayers and consumers is also evaluated and compared with the one that would be determined by the current demand scenario.

Three types of plant technologies, corresponding to the three biomass categories in the EC proposal (EurLex 52012PC0595, 2012), are included in the model:

i) Standard DGP: feedstock is corn grain (*category (a)*); products are ethanol and DDGS (Kwiatkowski et al., 2006; Franceschin et al., 2008);

ii) Dilute acid prehydrolysis (DAP-I): feedstock is miscanthus (*category (b)*); products are ethanol and electricity (Giarola et al., 2012);

iii) DAP-II: feedstock is corn stover (*category (c)*); products are ethanol and electricity (Giarola et al., 2012).

Corn grain, miscanthus, and corn stover have been selected respectively for the three plant technologies since they play a major role in the panorama of bioethanol production within the northern Italy domain.

The evolution of feedstock prices is a key issue in the performance assessment of biofuel supply chains. Some literature studies proposed a stochastic approach to take into account the uncertainty of commodity prices in biorefinery design (e.g., Dal-Mas et al. (2011); Kostin et al. (2012); Gebreslassie et al. (2012); Giarola et al. (2013)). Here, the approach proposed in the Chapter 3 will be followed and feedstock and products prices are estimated according to some forecast models based on historical data.

4.2 Prediction of commodity prices dynamics

Since the economic performance of a production system depends heavily on the prices of raw materials, utilities, and final products (Manca, 2013a,b), a key aspect in the economic analysis of the bioethanol supply chain in northern Italy is the estimation of the future prices of such goods. Several works studied the relationships between the prices of commodities used for first-generation biofuels (Yano et al., 2010; Chen et al., 2010a; Marzoughi and Kennedy, 2012). Here we adopt a time series decomposition approach (Zarnowitz and Ozyildirim, 2006), which proved to have a very good fit with the historical data (Chapter 3). The same approach was adopted to forecast the ethanol price, which appears to exhibit a similar trend.

The model slightly underestimates real 2012 corn prices (-3.3%) while it has a very good fit on ethanol quotations(+0.4%). The predicted prices for the whole supply chain life-time

Table 4.1: *Forecast corn and ethanol prices using the Time Series Decomposition model.*

Forecast good	2013 − 2015	2016 − 2018	2019 − 2021	2022 − 2024	2025 − 2027
Corn price [€/t]	181	229	286	348	406
Ethanol price [€/kg]	6.32	7.12	8.11	9.21	10.20

Table 4.2: *Forecast miscanthus and corn stover prices by period.*

Forecast good	2013 − 2015	2016 − 2018	2019 − 2021	2022 − 2024	2025 − 2027
Miscanthus price [€/t]	50.50	54.10	58.50	63.20	68.40
Stover price [€/t]	40	40	35	35	35

are reported in Table 4.1.

In order to assess the effect of the EC proposal, second-generation technologies from dedicated second-generation feedstock and waste material also need to be included in the supply chain model. Miscanthus and corn stover were selected respectively as the most promising energy crop and waste material for bioethanol production. The choice is based on the work developed by Giarola et al. (2012), and on the fact that their cultivation in northern Italy is also recommended by some technical reports (Veneto-Agricoltura, 2010).

With concern to miscanthus, no well-established market exists, but rhizome producers (Terravesta, 2012), institutional sources (Veneto-Agricoltura, 2010; Teagasc-AFBI, 2010), and biomass experts (Hasings, A., Sunnenberg, G., Lovett, A., Finch, J., Wang, S., Hillier, J., Smith, P., 2011) agree that miscanthus can be currently sold at about 50 €/t. Medium-term price forecasts are difficult, but a recent study in the UK reported that the breakeven cost of generic energy crops is expected to increase by about +25% by 2020 (Panoutsou, C., Castillo, 2011). A detailed analysis of the production costs (Veneto-Agricoltura, 2010) shows that 50% of the costs are related to yearly expenses, which are mostly due to fertilization (13%), harvest (26%), and transport inside the farm (61%) and which are essentially related to manpower and oil. If such costs are assumed to grow according to the Italian inflation rate, we obtain a long-term increase, which is consistent with the prediction of Panoutsou, C., Castillo (2011). Thus, the approach was applied to forecast future miscanthus prices as shown in Table 4.2.

Corn stover is currently priced at about 35 €/t (Euroforaggi, 2012; Camera di

Commercio di Forlì-Cesena, 2013). Quite recently, the American Department of Energy (Perlack, 2011) proposed a corn stover supply curve trend until 2030 (Figure 4.1) based on US data: it is shown that the supply curve may change in time since an increasing demand will also determine an increase in the corn stover availability. These curves were scaled to the Italian context according to local corn productions (IndexMundi, 2013). It can be inferred that the maximum feasible stover supply (indicated by the change in the slope of the supply curve) is reached if an additional demand of two million dry tons is assumed. Even if the whole bioethanol production in northern Italy were based on corn stover plants, the maximum demand would not exceed 1.7 million dry tons with a price increase of about 12 €/t.

The Figure 4.1 shows that such a stover demand would cause a significant price increase in 2012. However, the shift in time of the supply curve shows that the demand would have a negligible effect on 2022 stover price and would not cause any price shock on 2030 prices. Therefore, if part of the Italian bioethanol production were satisfied by corn stover, its price would suddenly rise as soon as the supply chain is established,but then increasing supply would compensate for the price shock. This price behavior is summarized in Table 4.2.

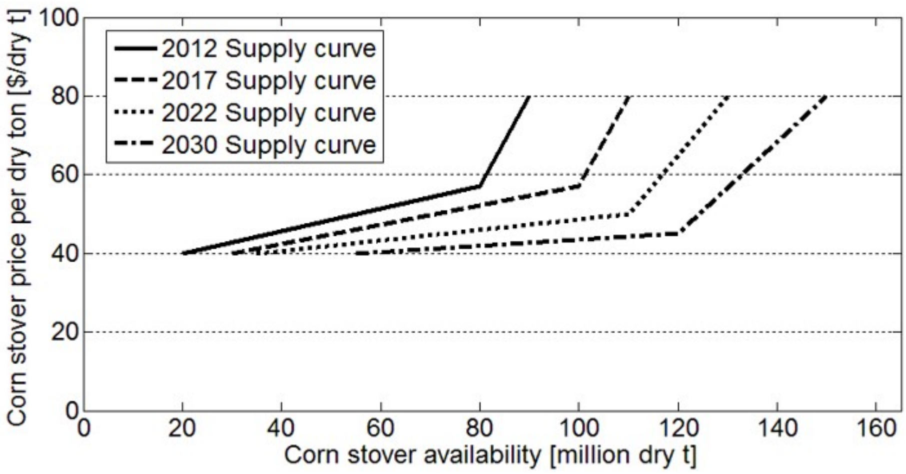


Figure 4.1: *Trend of the corn stover supply curve until 2030 in the U.S.A. (adapted from Perlack (2011)).*

4.2.1 Prediction of side-products prices

Two important side-products are related to the ethanol production processes. The DDGS and electricity (Kwiatkowski et al., 2006; Balat et al., 2008; Piccolo and Bezzo, 2009).

Table 4.3: *Forecast prices of by-products by time period.*

Forecast good	2013 − 2015	2016 − 2018	2019 − 2021	2022 − 2024	2025 − 2027
DDGS price [€/t]	163	206	257	313	365
electricity price [€/MWh]	200	170	170	170	150

DDGS are used as animal fodder with nutritional properties similar to soybean (Tonsor, 2006) and are obtained from the corn-based DGP technology. In the United States, after the big-scale establishment of the bioethanol supply chain, the DDGS price aligned to the corn one and fluctuated between 75% and 110% of the corn price (Hofstrand, 2012). Therefore, it seems reasonable to set the DDGS price as 90% of the corn price also for the Italian context. Electricity can be produced in combined heat and power modules from combustion of solid wastes from the lignocellulosic biomass (Piccolo and Bezzo, 2009). The electric energy produced by renewable biomasses can benefit from governmental subsidies, whose grant system is currently under renewal (DM 6/7/2012). Nonetheless, experts agree that in midterm subsidies will lower by around 15% compared to current level (ELEMENS, 2012), and it seems reasonable that this reduction will be confirmed on a ten-year horizon. Table 4.3 summarizes the forecast prices of by-products.

4.3 Problem formulation

This chapter deals with the strategic design of the economically optimal bioethanol supply chain over a 15-year horizon.This is achieved by maximizing the NPV of the whole SC during its operative life in a spatially explicit configuration where northern Italy is discretized into 59 grid cells plus one representing the raw material imports. The mathematical formulation in terms of a MILP framework is based on the work of Giarola et al. (2011). The supply chain layout is obtained by optimizing:

i) geographical location of biomass production sites;

ii) biomass production for each site;

iii) supply strategy for biomass to be delivered to production facilities;

iv) biofuel production facilities location and scale;

v) distribution processes for biofuel to be sent to blending terminals in order to maximize the supply chain NPV.

The environmental impact of the supply chain in terms of GHG emission is estimated as in Zamboni et al. (2009a) according to Houghton et al. (2001) directives, by assessing the impact of LCA stages, i.e. biomass growth, biomass pre-treatment, biomass transport, fuel production and fuel distribution. A WTT approach is assumed. In addition, emission credits (i.e. GHG emission savings as a result of goods or energy displacement by process by-products end-use) are accounted for. The GHG impact on global warming is captured by a whole set of burdens (CO_2, CH_4, N_2O). They have been grouped together in a single indicator representing the carbon dioxide equivalent emissions (CO_2-eq) as derived through the concept of 100-year global warming potentials.

Ethanol demand is forecast assuming that gasoline and diesel should reach the targets set by the Directive separately,starting from a negligible ethanol production in Italy in 2012 (USDA Foreign Agricultural Service, 2011). Therefore, it is sup-posed that the ethanol blending rate in 2013 is the one fixed by the Directive as the starting point in 2010, i.e. 5.75% on energy basis. Consequently, the increasing trend in the substitution quota is extended until 2027 in order to anticipate further regulations and to take into account the starting delay in achieving the targets (11.5% on energy basis from 2023).

Since the technologies discussed in this framework exhibit significant differences in their maturity, it was assumed to limit the maximum capacity of second-generation production plants to 110 kt/y (representing the size of largest planned conversion facilities). Conversely corn-based plants were assumed to reach a production capacity up to 350 kt/y (which is about the size of largest existing plants.

4.4 Results

The supply chain model has been optimized taking into account the existing EU regulation (*Scenario I*) and the new EC proposal (*Scenario II*). It is assumed that production targets (calculated as is or as per the EC proposal) need to be satisfied.

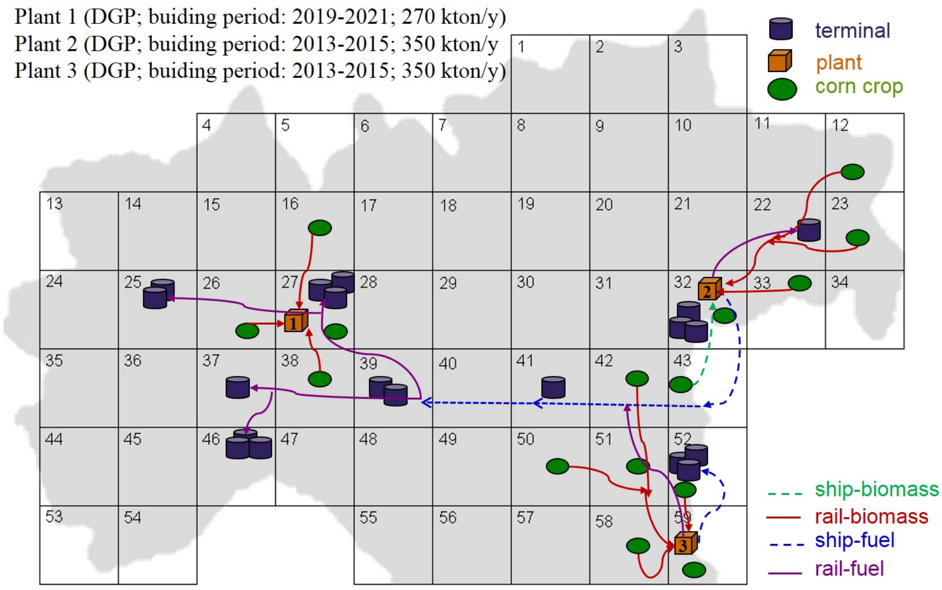
The new proposal has a strong influence on the profitability of the supply chain, since economic losses are reduced by 27% compared to the optimal supply chain defined by the

Table 4.4: *Production fulfillments of the current ethanol demand (referring to the existing Directive) in case the EC proposal were put into effect*

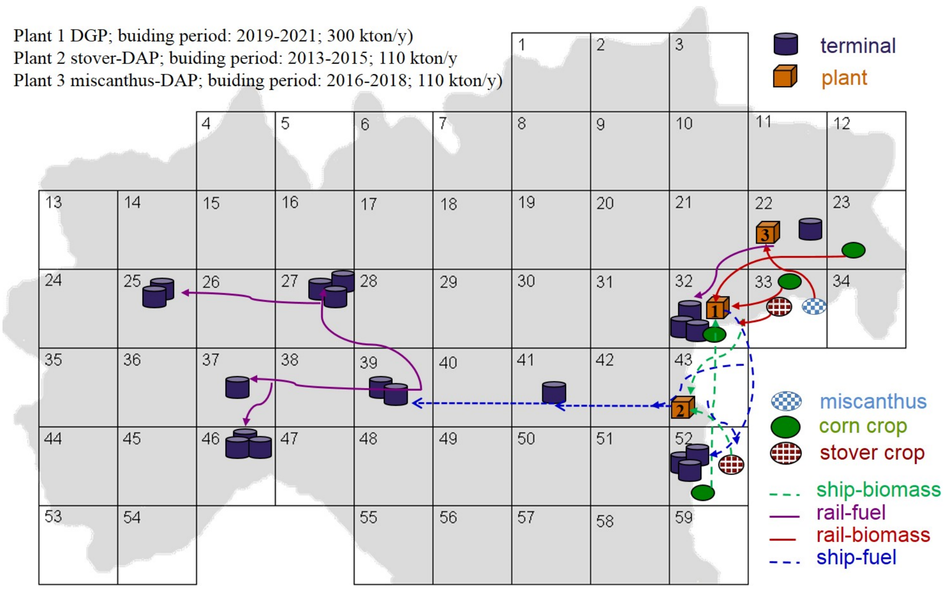
	2013 − 2015	2016 − 2018	2019 − 2021	2022 − 2024	2025 − 2027
Demand fulfillment (%)	42	38	44	50	55

existing legislation. In fact, although a negative NPV is still obtained (-594 M€), the economic losses are significantly lower than the ones obtained with current configuration (815 M€). This is simply achieved by producing less ethanol, thanks to the multiplicative effect assigned to second generation ethanol. According to Scenario I, at the end of time horizon, the 970 kt/y ethanol production would be satisfied by first generation DGP technology, whereas the new EC proposal would lead to a reduced capacity of 520 kt/y satisfied by both first and second generation technologies. Notably, the ethanol production in the simulation of the EC proposal would not comply with the production targets of the current directive as the new multiplicative factors allow producing less ethanol and still "satisfy" the targets. In other words, in case of a non-profitable business (as this one), the EC proposal would allow producing less (and therefore losing less money). Table 4.4 shows the actual ethanol production (represented as percentage) with respect to target quotas.

As illustrated in Figure 4.2, both scenarios determine the eventual establishment of three plants. The effect of current policies is represented in Figure 4.2a, while Figure 4.2b shows the final supply chain layout of Scenario II. In the latter case (Figure 2b), two 110 kt/y second generation plants (i.e. stover-based and miscanthus-based), and a 300 kt/y first generation DGP plant would be required, while in Scenario I (Figure 4.2a) three DGP plants would be built, two of them producing 350 kt/y and the remainder 270 kt/y. As intended, a result of the EC Proposal appears to be that of promoting second generation technologies. The reduction of the ethanol content in the blended fuel does not reduce its overall sustainability. Scenario II determines that the ethanol-related CO2-emissions are halved (36.9 kg CO_2-eq/GJ of ethanol) with respect to *Scenario I* (73.2 kg CO_2-eq/GJ of ethanol). However, the lower production determines that less bioethanol is blended with gasoline. As a consequence, the emissions of the blended fuel are reduced by about 3% only (81.1 kg CO_2-eq/GJ fuel with the EC Proposal *vs.* 82.7 kg CO_2-eq/GJ fuel with the current regulation). In other words, although the EC proposal appears to promote second generation technologies, its impact on fuel GHG emissions is hardly significant and obviously it deteriorates the security for transport energy since a lower amount of alternative fuels would be produced.



(a)



(b)

Figure 4.2: *Optimal supply chain layout under the existing Directive (*Scenario I*) at the end of the time horizon (time period 2025-2027), (a); Optimal supply chain layout with the EC proposal (*Scenario II*) at the end of the time horizon, (b).*

In order to verify that the resulting scenarios are not affected by the price prediction models, the optimization problem has been studied also considering fixed feedstock and ethanol prices. The prices were set as the average real quotations of the commodities in

Table 4.5: *Bioethanol supply chain losses per time period and over the whole horizon in current terms. For* scenario II*, in periods 2019-2021, 2022-2024, and 2025-2027 the 0 value denotes that there are no losses (in fact, the supply chain is profitable)*

	2013-2015	2016-2018	2019-2021	2022-2024	2025-2027	Total equivalent in current terms[7] [M€]
SC losses in *Scenario I* [M€]	379	211	359	506	706	1507
SC losses in *Scenario II* [M€]	506	198	0	0	0	670

the last three years (182 €/t for corn, 5.75 €/kg for ethanol, 50 €/t for miscanthus and 35 €/t for corn stover). The resulting supply chain was nearly identical in terms of adopted technologies and general layout as the ones at variable prices, which is very encouraging about the robustness of the supply chain design, because it proves that the results are not dependent on the chosen price prediction model. The main differences concerned the estimated profitability of the supply chain. In case of *Scenario I* a 5% increase in the NPV is obtained, simply because there is not a significant increase in the corn price as on the contrary predicted by the forecast model. Conversely, the NPV of *Scenario II* deteriorates by about 18% with respect to the case where price dynamics is accounted for (mainly because the predicted growth in ethanol price is not considered), but still outperforms *Scenario I.*

4.4.1 Impact on consumers and taxpayers

Since the ethanol supply chain is predicted to be unprofitable, losses should be either transferred to final customers or compensated for by governmental subsidies (as was done in the United States until 2011). If the latter case is assumed, Table 4.5 shows the calculated governmental subsidies per period and their equivalent amount in current terms. The comparison with subsidies that should be granted with the current legislation shows that a reduction by 56% would be obtained thanks to the recent EC proposal. Table 4.5 also shows a potential benefit of the EC proposal. Although quantitative results depend on models for price forecast, it appears that in Scenario II, subsidies would be needed in the initial operation period only (i.e. for about 5 years), when losses occur. Conversely, in the current state of things (Scenario I) government intervention seems necessary along the entire business activity.

If losses were repaid by fuel consumers, the blended fuel price would be composed of:

[7]Discounted at the 15-year Italian bond rate.

Table 4.6: *Expected total fuel prices and fuel prices at equivalent mileage in the case with or without EC proposal (Gasoline price assumed to be constant at 1.785 €/L)*

	2013-2015	2016-2018	2019-2021	2022-2024	2025-2027
Total fuel price with the EC proposal [€/L]	1.77	1.76	1.75	1.76	1.77
Total fuel price with current regulation [€/L]	1.73	1.72	1.74	1.76	1.78
Total fuel price difference	+2.4%	+2.0%	+0.7%	0.0%	-0.9%
Total fuel price at equivalent mileage with the EC proposal [€/L]	1.80	1.79	1.79	1.80	1.82
Total fuel price at equivalent mileage with current regulation [€/L]	1.78	1.78	1.80	1.83	1.86
Total fuel price at equivalent mileage difference	+1.1%	+0.5%	-0.7%	-1.5%	-2.3%

i) Gasoline price plus taxes weighted on the volume fraction of gasoline;

ii) Ethanol price plus VAT (22% in Italy) and the per liter losses repayment.

If the gasoline price is assumed to remain constant at the 2012 average Italian price (1.785 €/L according to Ministero dello sviluppo Economico (2013), the fuel prices with the EC proposal would be more expensive at the beginning (because of the very high capital costs of second generation plants), but then they would be cheaper by about 1% compared with the ones obtained with current legislation.

Nevertheless, it is worth remembering that the blended fuel has a LHV that is inferior to that of normal gasoline, since ethanol LHV is about 65% of the gasoline one. Table 4.6 reports the comparison both on the "pump price" and at equivalent mileage, which is most meaningful. It can be seen that the EC proposal would guarantee after 2019 a cheaper fuel up to 2.3%.

4.5 Final remarks

A recent European Commission proposal on the promotion of the use of energy from renewable sources, which amends both Directives 98/70/EC and 2009/28/EC, has been critically analyzed with concern to its effects on the design of bioethanol supply chains. The economic optimization based on a MILP model of the supply chain showed that the proposal can promote the establishment of a bioethanol supply chain, where lignocellulosic biomasses are extensively used in the production processes. However, since a possible consequence would be a lower ethanol production, the advantages in terms of reduction of GHG emissions would be hardly significant and there would be deterioration in energy security for transport. On the other hand, probable economic losses would be less aggravating, and accordingly the burden either on final fuel consumers or on governmental incentives would decrease. The approach is considered as innovative and of critical importance to limit the use of alimentary competitive feedstock, thus giving a concrete contribution to the debate on biofuels ethics. Nevertheless, the energy security principles on which the biofuels production is based cannot be altered; therefore, it can be advisable to maintain the maximum production quota for first generation biofuels, and to decrease the multiplying coefficients for advanced biofuels. This solution would also allow increasing the environmental benefits of the European Commission proposal, since a larger share of the blended fuel would be composed of low-pollutant fuels. While this option could engender worse economic configurations of the supply chain than those based on the current values, it is possible to arrange the multiplying coefficients of second generation technologies so that the new supply chain would still be more profitable than the one based on current legislation. In fact, the coefficient values can be chosen in a number of ways, since there are no constraints on either of them. In this perspective, the European Parliament has recently subscribed a call on the Commission (Europarl, 2013) to amend the factors in the original proposal, thus asking for a modification of the accountability technique to reach the European biofuel production objectives as required by the legislative procedure (EurLex C 115/47, 2008). Notably in the proposed amendment, the Parliament appears to endorse bioethanol production from dedicated cultures (where a x2 accountability method would be maintained), whereas waste materials such as straw (or corn stover) would be somewhat penalized being accounted just once as occurs for first generation technologies. A high multiplicative factor (x4) would be retained only for highly advanced (and not quite mature) technologies such as algae-based fuel production systems. Our interpretation is that, according to the EU Parliament, promotion policies should be directed either towards the more mature second generation technologies, which are based on dedicated cultures and have already demonstrated a high capacity potential (e.g., Biochemtex (2013)), or towards high-risk ground breaking processing technologies.

CHAPTER 5

Optimization of Biofuel SCs through a Game Theory approach

THE novel optimization framework presented in this chapter proposes the incorporation of a GT approach within a MILP modelling framework devised to optimize the design and planning of biomass-based fuel SCs behaving under conditions of cooperation and competition in order to address possible business relationship situations among feedstock providers and biofuel producers. On the other hand, the approach developed intends to bridge the gap between game theory and the comprehensive approaches for the strategic design of complex biofuels SC. The chapter is organized as follows. After a general description of SC planning and design problem and the GT as optimization tool, the mathematical formulation of the model will be outlined. The case study is then introduced by testing the model capabilities in terms of the parameters definition and modelling assumptions. Eventually, the results of diverse scenarios within the MILP optimization framework are presented followed by a discussion of the main modelling outcomes. Some final remarks will conclude the chapter.

5.1 Motivation

As has been extensively discussed previously, in the last decade has existed a large expansion in the use of biofuels, especially corn-based bioethanol, into the transport sector as alternative substitutes to current oil-dominated fuels. However, this expansion has also been diverting a large amount of agricultural crops, thus affecting farm land allocation, feedstock market equilibrium, and agricultural economic development in local areas. This situation has led to a new outlet for agricultural commodities resulting in an open competition between food use or energy dedicated crop, with a resulting increase in food prices (HLPE, 2013).

On the other hand the problem of decision making connected to the operational management of the SC such as raw materials acquisition in diverse markets, product allocation to different plants and their distribution to different customers has attracted significant scientific interest (Guillén-Gosálbez and Grossmann, 2009) over recent years, becoming increasingly complex when it is required to coordinately consider multiple criteria in the analysis and optimisation of the fuel supply chain (Akgul et al., 2011; Zamboni et al., 2009a). This situation is further complicated when other sources of uncertainty need considering. One uncertainty factor, which has been little discussed in the literature, is concerned with the presence of alternative supply chains capable of competing or cooperating with each other on a common stage.

In fact, GT approaches have been widely used as a mathematical and logical tools to study the interactions between the "players" or "agents" who are involved in the business (Von Neumann and Morgenstern, 1944). The central purpose of GT in SCM problems is to help decision makers to identify the most probable choices and strategic interactions among players (Cachon and Netessine, 2004). Two opposite types of game are typically considered: the cooperative game where all players share a common objective, and the competitive game where each player has an individual objective, which usually does not coincide with the objectives of other players (Aumann and Peleg, 1960; Nagarajan and Sošić, 2008; Nash, 1951). In the latter case, the Nash solution strategy aims at identifying the Nash equilibrium (NE) point, i.e. the situation in which no player has nothing to gain by changing his own strategy unilaterally, if the other players keep their own strategy unchanged (Nash, 1951). A basic assumption is that the players act or process their information at the same instant, while having knowledge of others performance functions beforehand.

Thus, the objective of this chapter is to start bridging the gap between GT and more comprehensive approaches for the strategic design of complex biofuels SCs. Taking as reference the work performed by Zamarripa et al. (2012), a decision-support tool will be proposed, involving multiple cooperative and competitive farmers, biofuel producers, and food and fuel markets in order to address possible business partnership scenarios between feedstock suppliers and biofuel producers. A stochastic formulation will also be implemented and discussed to represent the effect of uncertainty on biomass price. The use of the proposed system is illustrated through a demonstrative case study representing a bioethanol production in Northern Italy.

5.2 Assumptions and Methods

The design process is conceived as an optimization problem dealing with the maximization of the financial performance of the actors in a cooperative environment or conversely in a competitive one. The model is formulated as MILP modelling framework which embodies game-theoretic features for both game models in order to assess the behavior of the SCs under the proposed scenarios.

5.2.1 Game Formulation and Basic Assumptions

The game situation can be defined through three key elements: *i)* the farmers as biomass/crop suppliers, *ii)* the biofuel producers, and *iii)* the local food markets (Figure 5.1). Under this framework, corn is taken as the reference raw material for both biorefineries and the food markets.

Two players (hereinafter referred as *P1* and *P2*) will be considered in this chapter. They represent a spatially distributed substructure (i.e. farmer consortium) who provides resources (corn) bioethanol or food production in a geographical region. These players are conformed by three corn production sites each: P1 is composed by the farmers located in [g = 26, 39, 41] while P2 is made up by the farmers in the regions [g = 31, 33, 43], in where both cooperative and competitive game models have been developed to address possible business partnership scenarios between feedstock suppliers and biofuel producers.

Biorefineries are described as dry-grind first generation technologies capable of meeting the ethanol demand as defined by European Directive 2009/28 (EC, 2009) over a 15-year time horizon, which has been divided into five time intervals of each three-year long in order to reduce the computational burden. The SC model is as in Giarola et al. (2011). The food

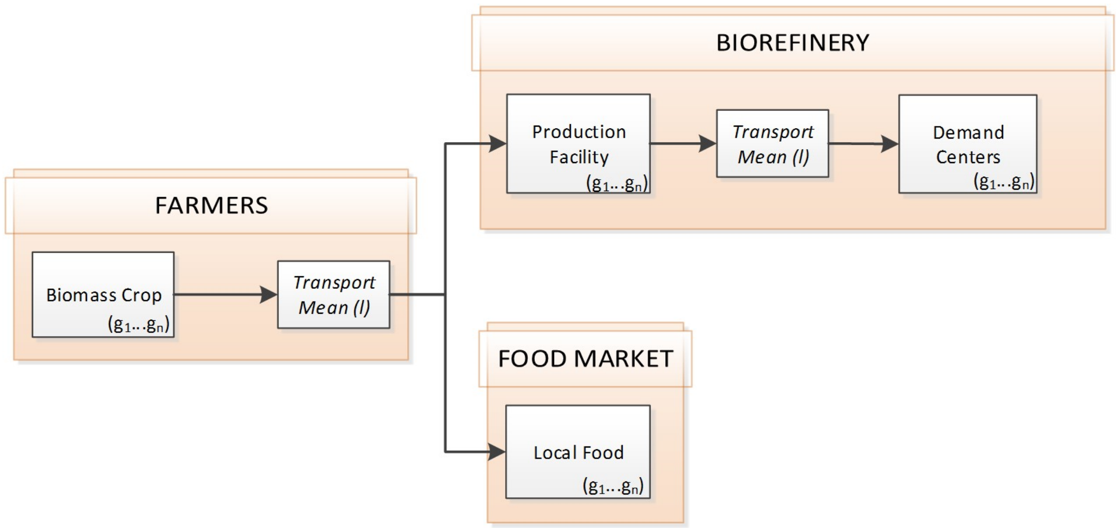


Figure 5.1: *Biofuels network supply chain where g and l stand for an element in the spatial grid and a generic transport mean, respectively.*

market substructure is described through thirteen local terminals spatially distributed in the territory. Each terminal is characterized by a constant corn demand of 17 kTonnes per year.

Thus, the optimization problem discussed here can be stated as follows. Given the following inputs:

i) geographical distribution of biomass demand centers for both markets

ii) fixed location of biomass production sites (players)

iii) fuel and food demand over the entire time horizon

iv) biofuel market characteristics in terms of prices distribution

v) biomass geographical availability

vi) biomass market stochastic behaviour

vii) biofuel production facilities capital and operating costs

viii) transport logistics (modes, capacities, distances, availability, and costs)

The objective is to provide the optimal system configuration in terms of profitability of the biomass suppliers (i.e. players) including as a key feature a game-theoretic approach where the players involved are capable of competing or cooperating with each other on a common stage. Therefore, the key variables to be optimized in order to determine the best operating strategy in terms of financial performance of the system over the long term for the players are:

i) biofuel production facilities location and scale

ii) biomass supply strategy to be shipped to the refineries and food markets

iii) biomass production for each site

Northern Italy is considered as a geographical landmark for biofuel production.

5.2.2 Mathematical Features

The mathematical formulation was based on the modeling approaches adopted in the strategic design of a multi-echelon SCs as a MILP problem encompassing features to address the siting of spatially explicit facilities and capacity planning for strategic fuel systems (Sahinidis et al., 1989; Tsiakis et al., 2001). The basis of this formulation is based on the work by Giarola et al. (2011). It also embodies different features to address both cooperative or competitive environments focusing on fuel systems design at the strategic level (Zamarripa et al., 2012; Bai et al., 2012).

5.2.2.1 Cooperative scenario

A cooperative game approach is considered to determine the total maximum profit of the farmers if they work cooperatively. In a cooperative scenario, stakeholders are assumed to collaborate and to look for trade-off solutions for the common financial benefit.

Such cooperation is thus described through the optimization of the overall profit TFP [€]. Accordingly:

$$TFP = \sum_{g} \sum_{t} Fin_{(g,t)} - TOC_{(g,t)}, \tag{5.1}$$

where $TOC_{(g,t)}$ [€/time period] stands for the total operating cost (production and transportation of the biomass) for each player in g at time period t, $Fin_{(g,t)}$ [€/time period] represents the incomes from corn selling of the players in g for each time period t. These incomes are evaluated by multiplying the total biomass rate produced by the player in region g at time t, $TPb_{(g,t)}$ [t/time period] by the corresponding biomass selling cost (set to 170 €/tonne representing a 10 years average value in Italy) $USC_{(g)}$ [€/t]:

$$Fin_{(g,t)} = TPb_{(g,t)} \cdot USC(g), \tag{5.2}$$

the total operating costs for both players, $TOC_{(g,t)}$, are evaluated by summing up the feedstock production cost, $FPC_{(g,t)}$ [€/time period], and the transportation costs, $FTC_{(g,t)}$ [€/time period], for each player:

$$TOC_{(g,t)} = FPC_{(g,t)} + FTC_{(g,t)}, \tag{5.3}$$

where the feedstock production cost, $FPC_{(g,t)}$ [€/ha], takes into account a constant cost of 65 € as a function of the cultivated area through time t, according to MAFRI (2013); $FTC_{(g,t)}$ stands for the transportation costs [€/time period] is evaluated as in Giarola et al. (2011).

5.2.2.2 Competitive scenario

The application of a scenario under competitive conditions is based on the simulation of the results obtained by a set of players pursuing different strategies to get their maximum individual benefit. Therefore, to enter into this game modality the two players P1 and P2 as biomass suppliers behaving competitively should deal one against the other in order to satisfy the customer (ethanol producer), establishing a competitive strategy to offer the raw material to the customer through the application of price discounts on biomass so as to exclude the competitor and maximize the individual benefit.

In order to represent this behaviour the non zero-sum game is proposed, since the single player will not try to maintain the overall benefit of the system . This approach is implemented through the computation of a payoff matrix, which is made up by the different potential strategies of the players and shows the behaviour for each action of the player against the actions of its competitors (Zamarripa et al., 2012). The following equation is introduced in order to represent the competitive behaviour through biomass price discount offered by each player. Accordingly:

$$RBE = \sum_{g} \sum_{t} USC_{(g)} \cdot TPb_{(g,t)} \cdot \beta_{(g)} + TOC_{(g,t)}, \tag{5.4}$$

where RBE [€] represents the trade-off between the expenses of the ethanol producer and the economic performance of the farmers and $\beta_{(g)}$ represents an applicable discount rate offered by every player. So when each player tries to maximize its individual profit at same time the customer tries to purchase the corn from the cheaper offerer and thus the GT approach will have a sense of competition.

The solution approach is the same as the one adopted by Zamarripa et al. (2012). A payoff matrix collecting information from multiple competing SCs (players) is used to assess how the competitive behaviour affects the decision of the stakeholders. This matrix is obtained through the execution of the MILP model for every combination of the five scenarios (strategies) considered for each player, starting from the base price settled-up in 170 € per tonne reaching a 40% discount on the price of biomass, thus representing a matrix of [5 x 5]. The solution comes from the concept of NE (Nash, 1951, 1950), which states that each predicted strategy must be the best response of each player with respect to the strategies of the other players, supposing that the players are rational and choose their strategies independently.

5.3 Case study

Under the scheme presented before, the system behaviour is tested in a case study based on a previous modelling framework representing the dynamic evolution of a bioethanol supply chain under increasing biofuel demand (Giarola et al., 2011).

First we will discuss the results in a cooperation scheme where players sell biomass at a fixed price. Then, a non-cooperative case will be analyzed, where agents (i.e. the farmers) try to maximize their profit while competing to supply biomass for biofuel production. Finally, a stochastic optimization approach will be introduce to assess the effect of uncertainty on the biomass selling cost in a cooperative scenario.

The problem was solved by means of the CPLEX solver in the GAMS® modelling tool (Rosenthal, 2010).

5.3.1 Economic performance under cooperation scheme

The outcomes in this first part represent the cooperative behaviour of the farmers, who are divided in two instances: in the former the economic optimal solution assumes that farmers only have to supply a food market; the latter illustrates the optimal solution in economic terms for the farmers considering both fuel and food crops supply.

The results of the first instance foresees a positive outlook for the players with an economic optimum profit of 58.89 M€/yr. Figure 5.2a illustrates the design and planning strategy including the detailed transport system of the optimal solution for the economic performance of the farmers at the end of the time horizon. As can be observed in Figure 5.2a, the supply of food-crops to the market is well distributed. Player P1 is mainly benefited in terms of lower cost of transportation in order to provide the biomass due to her/his great geographical location in the northern territory of Italy. It should be noted that in general farmers exploit geographical location to minimize costs and improve the common economic profits.

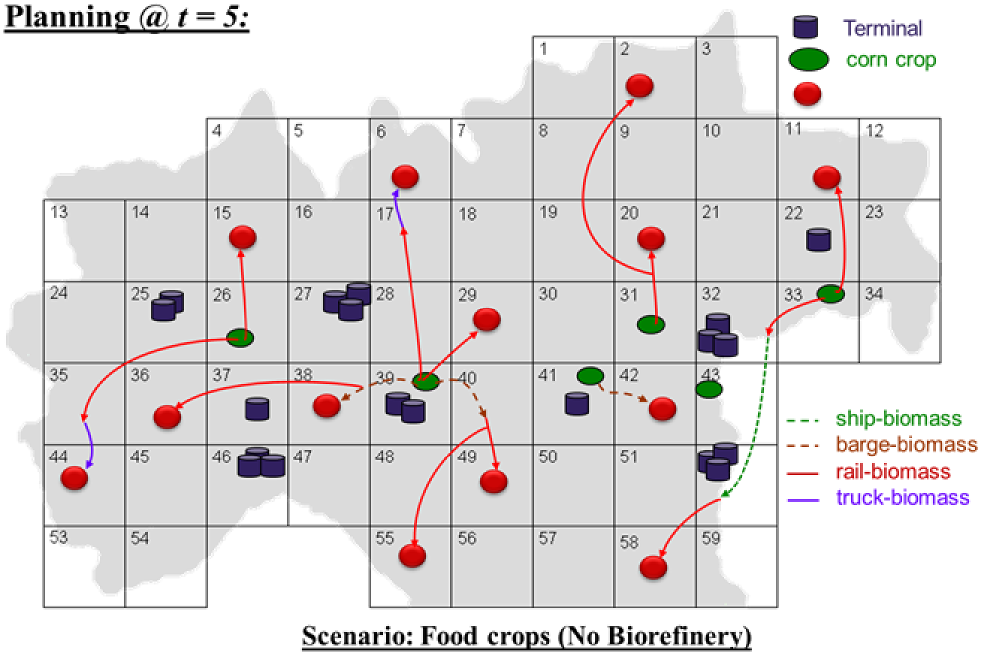
The second instance introduces the effect of bioethanol producers determining an extra demand. The optimum solution for this case involves a TFP of 493.35 M€/year and it is worth mentioning that at this stage the greatest profits of the players come from the sale of fuel crops representing 90% of total profit. Figure 5.2b captures the final design, which includes the siting of biorefineries. The optimal solution involves the establishment of four bioethanol production plants with medium-sized capacity of about 125 kTonne/year whose location is typically very close to the feedstock production site. This configuration allows a balanced supply of biomass between the players. Although corn producers appear to make money, the outcome for bioethanol producers is not a positive one (NPV = -0.008 €/GJ_{EtOH}).

In fact, the entire system could be improved if an effective pricing mechanism were designed for the industry to drive the stakeholders towards a favorable economic situation for both biorefineries and the farmer as supplier of corn. Therefore, with the purpose to represent a more realistic behavior between the interest parties, in the following section a sensitivity analysis on the corn price is presented.

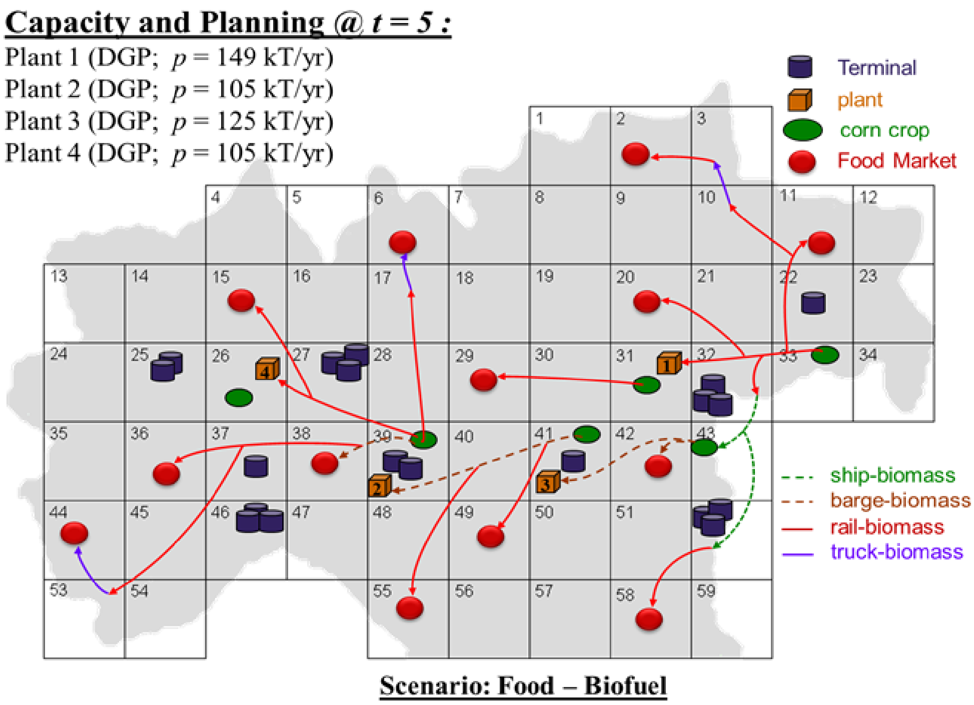
5.3.1.1 Sensitivity analysis on biomass price

A sensitivity analysis on corn price for both corn for food and corn for biofuel production in order to identify the economic behavior of the farmers as well as the biorefineries. The emerging profits of the farmers grouped in the players involved are presented in Figure 5.3 .

Farmers do not make any profit if the corn price is below 100 €/tonne. An intermediate situation is illustrated in Figure 5.3, where a corn price of 130 €/tonne is considered.



(a)



(b)

Figure 5.2: *Design and planning strategy at time period $t = 5$ for the optimal solutions for food crop (a) and food-fuel crop (b) supply.*

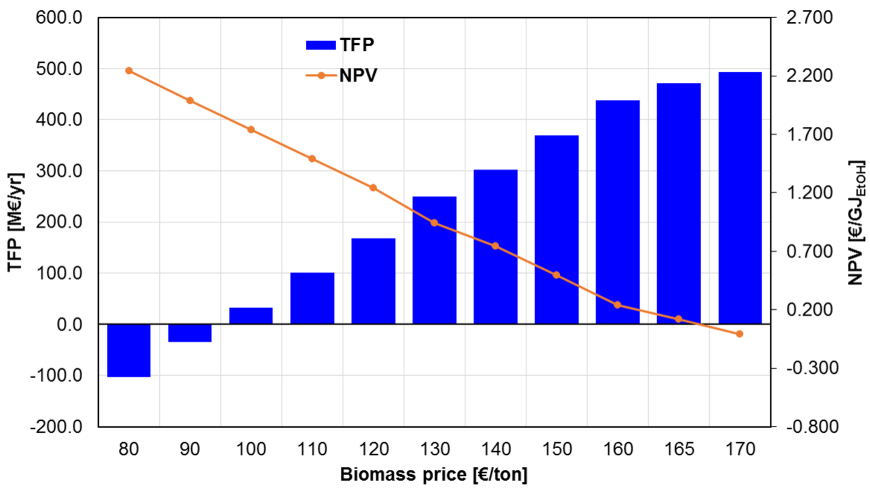


Figure 5.3: *Effect on farmers' TFP and biorefinery NPV of biomass price variation.*

From the results emerges that the economic performance of the bioethanol SC increases from almost zero (-0.008 €/GJ$_{EtOH}$) to 0.941 €/GJ$_{EtOH}$ leading to a slight change in the configuration of the location of the plants to be established, as is shown in the Figure 5.4. However, the panorama faced by the farmers also changes, since their profits due to the sale of corn dedicated for the biorefineries fall drastically by nearly 49% (446 M€/yr to 234 M€/yr); the opposite occurs with the profits from the sale of corn to the food market growing by about 10% (48 M€/yr to 52 M€/yr).

5.3.2 Economic performance under competition scheme

In the competitive case, the model needs accounting for the customer preferences, which have been modelled in terms of customer costs. This is expressed as reduction of the buyers expenses (RBE) through the adoption of a feasible strategy based on biomass price discount. The result is the payoff matrix illustrated in Figure 5.5 and showing the effect of a player action against the actions of its competitors.

The NE point is an almost obvious outcome since it occurs when there is no discount on biomass price. However it should be noted that this solution will be the worst decision for the customer (biorefinery) since the NPV is almost zero (-0.008 €/GJ$_{EtOH}$) as occurs in the cases previously presented. If we assume that the biofuel producer may prefer a specific provider of biomass (either of the two players involved), in the case the preference is with P1, the NE point would be when the P1 offers the corn with 0% of discount (170 €/tonne)

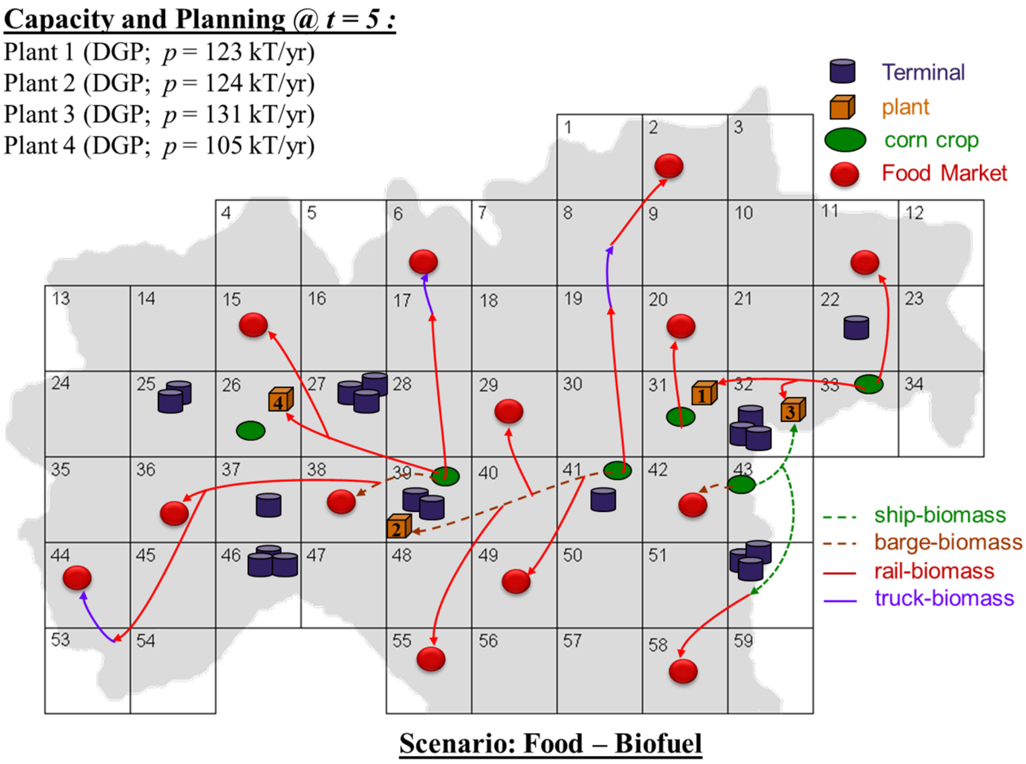


Figure 5.4: *Design and planning strategy at time period $t = 5$ for the optimal solution (average price).*

and the P2 with the highest discount of 40% (102 €/tonne). The opposite result is obtained is the preferred player is P2, i.e. the NE point represents a scenario where P2 does not offer any discount, while P1 offers maximum discount (Table 5.1).

Possibly, the most important benefit of this kind of studies relies in the possibility to use the overall information computed during the optimization procedure to negotiate agreements with the customer and/or the competing partners, and thus be able to create an environment of economic benefit ("*win-win*") to all parties concerned.

Table 5.1: *Optimum solutions for each player in the competitive case.*

	P1 (leading supplier)	P2	P1	P2 (leading supplier)
Strategies (Discount %)	0	40	40	0
TFP (M€/yr)	74.76	2.52	6.96	128.52
NPV (€/GJ$_{EtOH}$)	1.354		1.252	

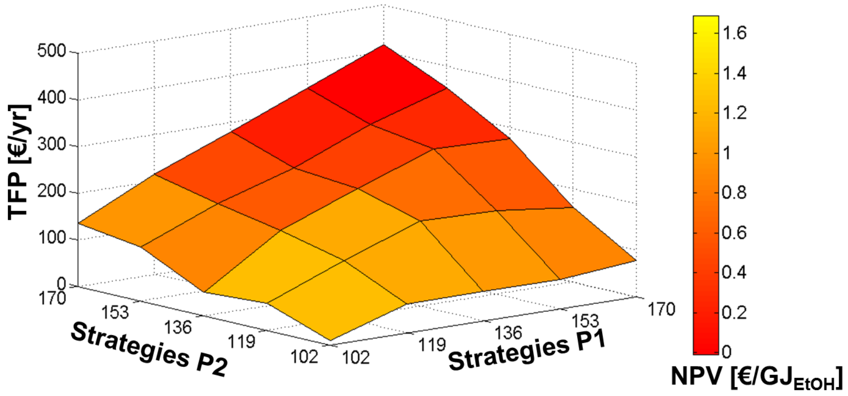


Figure 5.5: *Graphic surface representing the payoff matrix for the competitive case.*

5.4 Stochastic approach for cooperative configuration

This section discusses the effect of uncertainty on biomass purchase costs. The stochastic optimization is based on a set of possible scenarios over the time horizon. The analysis of historical data concerning the biomass purchase cost in Italy for the time period 2004–2014 (Associazione Granaria di Milano, 2014) is shown in the Figure 5.6.

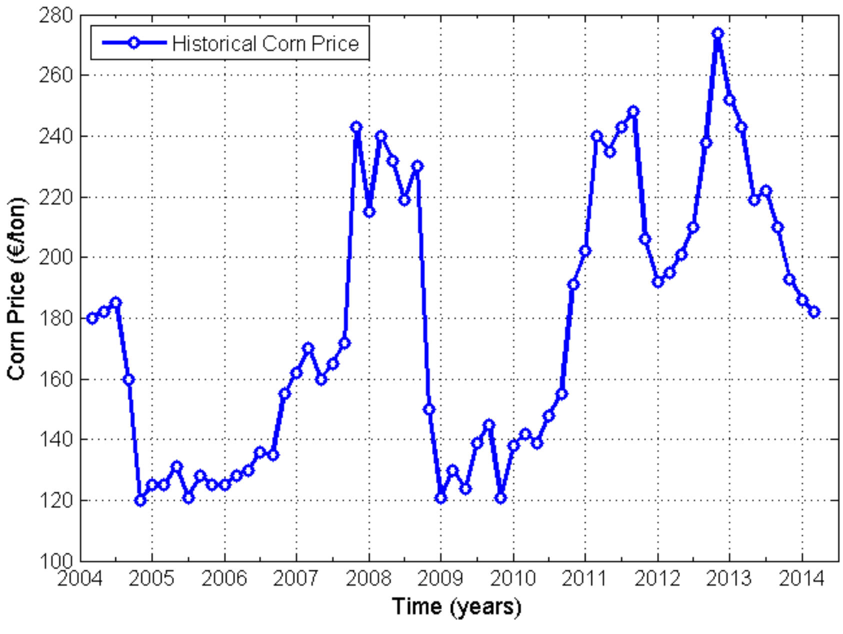


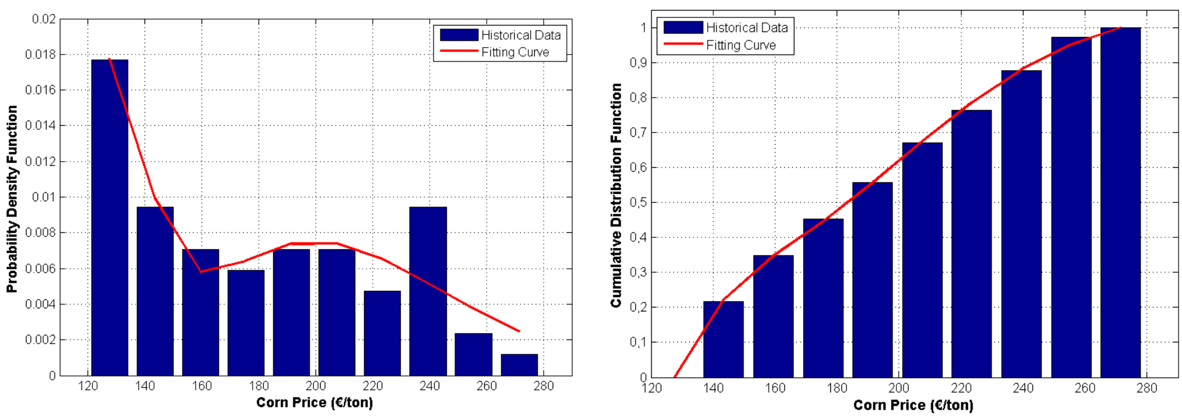
Figure 5.6: *Evolution of the Italian corn price between the 2004 - 2014 in €/tonne, and the average value in these 10 years.*

The fitting of the histogram in order to find the best curve approximating the probability density, was not able to perform with symmetric functions, such as, the normal distribution.

The probability density function (PDF) cannot be described through simple functions. As in Dal-Mas et al. (2011), we used the probability function represented as the sum of two gamma (Γ) distributions defined by the price of corn (USC €/tonne). Six ϕ parameter are used for regression and fit the data. The final function is as follows:

$$pdf(USC) = \phi_{(5)} \cdot \Gamma[UPC, \phi_{(1)}, \phi_{(2)}] + \phi_{(6)} \cdot \Gamma[UPC, \phi_{(3)}, \phi_{(4)}]$$
$$\Phi = [75.1206 \quad 1.6701 \quad 22.3362 \quad 9.3620 \quad 34.6479 \quad 45.7758] \tag{5.5}$$

The normalized histogram is presented in the Figure 5.7a where historical data are compared with fitting curve resulted of the PDF. Figure 5.7b shows the normalized and cumulative histogram of the data and of the integral function of the PDF.



(a) (b)

Figure 5.7: *Normalized (a) and cumulative (b) histogram of historical data (discretized) and the integral function of the probability density function*

For the simulations that will be carried out subsequently under conditions of uncertainty regarding the acquisition price of the raw material, it has been necessary to take into account a discretization of the thirty-two intervals of the historical data in order to avoid high computation times to solve every scenario. This discretization has been performed in 10 fractions, which, by integrating equation 5.5 between the extreme values, it was possible to associate the corresponding probability of occurrence given in Table 5.2. In this way, the uncertainty has been calculated and the same will be applied to each scenario proposed.

The objective function to be maximized is the expected revenue of the farmers ($eTFP$)

Table 5.2: *Discretization intervals for corn price and the associated probability.*

Scenario	Corn Price (€/tonne)	P(USC)
1	UPC $\leq$ 135	0.2459
2	136 $\leq$ UPC $\leq$ 151	0.1311
3	152 $\leq$ UPC $\leq$ 167	0.0984
4	168 $\leq$ UPC $\leq$ 183	0.0820
5	184 $\leq$ UPC $\leq$ 199	0.0984
6	200 $\leq$ UPC $\leq$ 215	0.0984
7	216 $\leq$ UPC $\leq$ 231	0.0656
8	232 $\leq$ UPC $\leq$ 247	0.1311
9	248 $\leq$ UPC $\leq$ 263	0.0328
10	UPC $\geq$ 264	0.0164

as stated by the following equation:

$$eTFP = \sum_{sc} TFP_{sc} \cdot \pi_{sc}, \tag{5.6}$$

where TFP_{sc} [€] represents the total profit of the farmers under scenario sc, whose occurrence probability is expressed as π_{sc}. The stochastic optimization produces the profits of the farmers presented in the Table 5.3 for each scenario.

Table 5.3: *Farmer Revenues with the associated probability.*

Scenario	Farmer Revenues (€/month)	Medium Scenario Probabilites (%)
1	17.98	24.6
2	27.00	13.1
3	36.02	9.8
4	45.03	8.2
5	54.05	9.8
6	63.07	9.8
7	72.09	6.6
8	81.11	13.1
9	90.13	3.3
10	99.14	1.6

From Table 5.3 it should be noted that for the first scenario corresponds to the highest probability of occurrence (almost 25%). This is a simulation with corn price below 135 €/tonne and representing the possibility of a good economic performance for both farmers and biorefineries. On the other hand, from Figure 5.8 it can be noted that from the fourth scenario onwards the biorefinery is in an unfavourable financial situation. However, it is worth observing that the probability of occurrence of such scenarios is considerably low, in other words, the procurement price of biomass must be greater than 170 €/tonne to place the biorefinery in a risky economical situation.

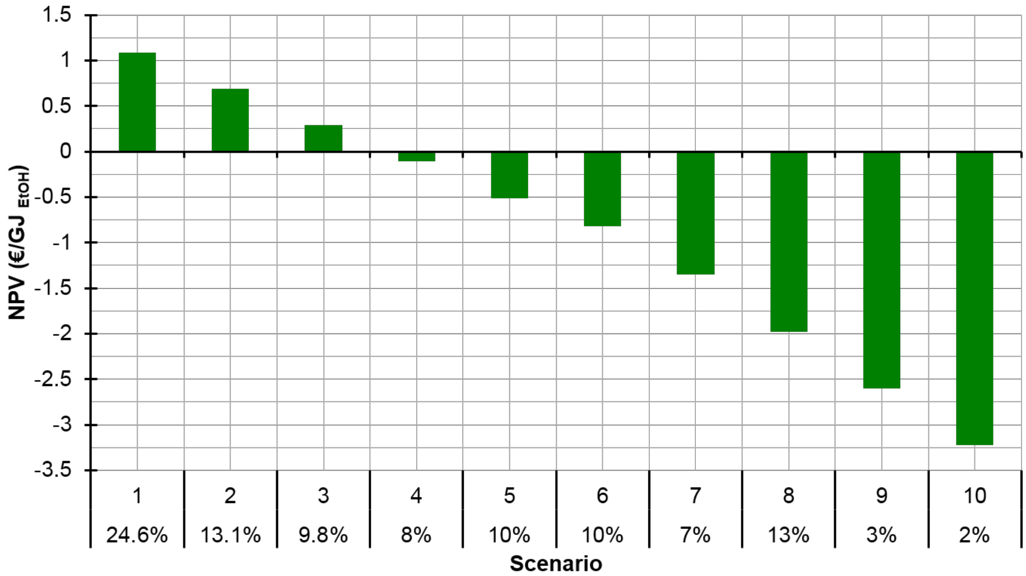


Figure 5.8: *Net present values (€/GJ_{EtOH}) for each of the 10 scenarios with the occurrence probability.*

5.5 Final Remarks

In this chapter a MILP modelling framework including as a key feature a game-theoretic approach for the design and planning of feasible biofuels SCs has been presented and discussed. The cooperative and non-cooperative problems have been assessed through the GT as optimization based decision support system.

Results demonstrate that the integration of GT as decision technique can open a new pathway in order to introduce more realistic approach to the SC planning problems. In accordance with the scenarios considered the results suggest that under certain conditions the best possible outcome for the biofuel industry in the cooperation mode is worse than the one that could be achieved through competition of the biomass providers whereas farmers would take advantage from a cooperative situation.

However, this cooperative behaviour determines a new issue, i.e. the proper allocation of the profits in a fair fashion among the stakeholders in the supply chain. This is addressed and discussed in the next chapter.

CHAPTER 6

An approach to optimize multi-enterprise biofuel SCs including Nash equilibrium models

THE main goal proposed in this chapter[8] is to model and optimize multi-enterprise biofuel supply chains in order to obtain a comprehensive approach of such complex systems. A solution model for fair profit distribution between two supply chain participants through a generalization of the Nash concepts is applied. A game-theoretical Nash-type model approach within a general MILP framework to optimize the most appropriate transfer price level for the biomass transferred between production sites to biofuel producers is presented. In order to demonstrate the capabilities of the proposed model a dynamic evolution of a bioethanol SC driven by the fulfilment of an increasing biofuel demand in Northern Italy is considered.

6.1 Motivation

An increasing concern in the SCM is the determination of policies aiming to improve the performance of the whole system while preserving an adequate retribution for each partaker. A simple as well as direct approach to enhance the performance of a multi-enterprise SC is to maximize the summed enterprise profits of the entire supply chain subject to various network constraints. When the overall system is optimized in this fashion there is no

[8]Portions of this chapter have been published in Ortiz-Gutiérrez et al. (2015)

automatic mechanism to allow profits to be *fairly* apportioned among participants. Solutions to this class of problems usually exhibit quite uneven profit distributions and are therefore impractical. They do however give an indication of the best possible total profit attainable in the SC as well as an indication of the best activities to carry out.

Although a certain level of cooperation can be achieved among participants within the supply chain, efficient policies and mechanisms are needed to maximize the overall performance of the supply chain and simultaneously ensure adequate rewards for each participant. It should be emphasised that the companies involved in the supply chain are in business only to create as much value for themselves as possible. The underlying assumption is the surrounding business environment is suitable for long-term partnerships and that the power relations between the companies can somehow be quantified in terms of minimum acceptable profit levels. These levels are clearly dependent on the customer market for the products manufactured in the supply chain as well as the vertical inter-company power relations in the supply chain. It should be added that these power relations maybe affected by the existence of external competitors.

In recent years GT approaches have been widely used as mathematical and and logical tools to study the interactions between the "players" or "agents" who are involved in the business (Von Neumann and Morgenstern, 1944). However, the integration of profit allocation mechanisms with the optimization of operational decisions along a SC might require sophisticated solution algorithms (Aplak and Sogut, 2013; Hennet and Arda, 2008; Zhang and Liu, 2013). Gjerdrum et al. (2002) proposed a MINLP model based on the game-theory Nash bargaining solution approach for a two-enterprise SCs and formulated a spatial branch-and-bound solution algorithm. There has been a general lack of focus on the multi-enterprise SC optimisation for biofuel systems. Only recently, Yue and You (2014a) applied the game-theory as solution approach through revenue sharing policy to the arbitrary allocation of the total profit and to align the interests of individual participants in a non-cooperative biofuel SC.

Besides the problem in decision making, the energy production from biomass has become increasingly important, both for energy security and climate change concerns (Höök and Tang, 2013). Therefore, rather than focusing the framework on general supply chain networks, the approach presented in this chapter will have as focal point biofuel supply chains. Corn-based biofuels are considered as part of the solution to increasing concerns about climate change, energy security, and our heavy dependence on petroleum-derived liquid transportation fuels. Since the economics of first generation bioethanol strongly depends on the feed stocks supply costs, the presence of suitable market mechanisms for a fair profit allocation among the main partakers involved, i.e. feedstock suppliers and biofuel producers, is crucial.

Therefore, following this rationale, this chapter aims at incorporating a game-theoretical Nash-type model approach within a MILP framework in order to optimize a fair profit distribution between members of multi-enterprise SCs. The modelling framework proposed in Giarola et al. (2011) was extended to include GT principles and study the effects on the dynamic evolution of a bioethanol SC driven by the fulfilment of an increasing biofuel demand (Giarola et al., 2011). Model decision variables included the biomass production per site and its supply strategy, the location and capacity of biorefineries as well as the transport logistic of the product. The price transfer policy, an efficient method to create a fair, optimized profit distribution in the biofuel SC using the GT, was used as powerful tool in the decision making. Corn represented also the major variable in this optimization problem in order to maximise the financial performance of the actors involved over the time horizon. The proposed method was applied to the design of a corn-based bioethanol SC network in Northern Italy.

6.2 Problem Description

The emerging biomass-based ethanol production in Northern Italy was assessed as a real world case study to illustrate the applicability and capabilities of the proposed approach in steering the strategic design and planning of systems such as biofuels supply networks. All the assumptions concerning the case study formulation (i.e. territory discretization, logistics, biomass availability, biomass and energy market characteristics as well as technology definition) are as in the Chapter 2. Here, we will mainly focus on the changes applied to both the mathematical formulation and the case study in order to include a GT analysis.

The design process was conceived as an optimization problem for two-enterprise bioethanol SCs. One enterprise was devoted to growth and sale of biomass to a biorefinery (the second enterprise) in order to produce bioethanol and byproducts for their onward sale to external customers (see Figure 6.1).

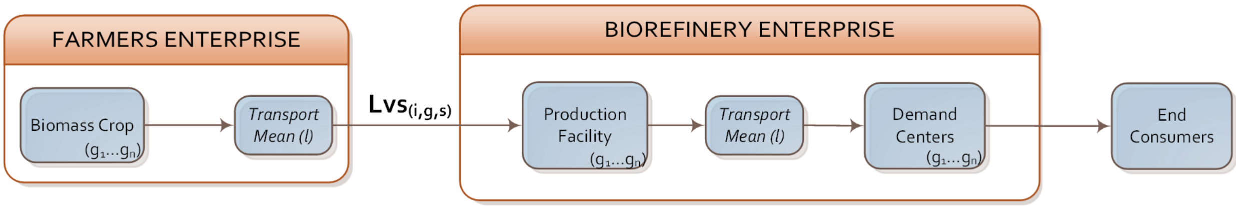


Figure 6.1: *Two-enterprise description.*

The system is capable of meeting the bioethanol demand as defined by European Directive 2009/28 (EC, 2009). The overall timeframe of 15-years was divided into five time intervals (t) of each three-year long in order to reduce the computational burden. Northern Italy was discretized into 59 square cells, considering an additional one for biomass import. The biorefinery was described using three alternative corn-based bioethanol production technologies: *(i)* dry-grind process (DGP), which is the standard corn-based ethanol process; *(ii)* DGP-CHP plants, where the DGP byproducts are burnt to cogenerate electricity and heat; and *(iii)* the fermentation of the thin stillage (considering natural gas supplement for energy needs) enabling production of both electricity and DDGS (DGP-TS_{NG}).

Table 6.1: *Corn price levels.*

Level (S)	Price (€/tonne)
1	100
2	145
3	175

Three price levels have been taken into consideration for the corn purchased from the local market within a range of 100-175 €/ton (according to table 6.1), which is aligned to market price variation in the last decade. Biomass imported from foreign suppliers was supplied at a constant price of 110 €/ton. Price levels were not fixed to a certain amount of biomass supplied by farmers.

6.3 Mathematical Features

The mathematical formulation was based on the modelling approaches adopted in the strategic design of a multi-echelon supply chains as a MILP problem encompassing features to address the siting of spatially explicit facilities and capacity planning for strategic fuel systems. In this chapter have taken as a reference work by Gjerdrum et al. (2001) also following the Nash approach for the equilibrium model as follows.

6.3.1 Nash based approach

The approach presented here uses a game theory feature called the Nash model (Nash, 1950). This is built on four axioms that a rational bargaining solution should obey. These are characterized by *Pareto optimality*, *symmetry*, *scale invariance*, and *independence of irrelevant alternatives* (Conley and Wilkie, 1996). The solution delivers an optimal fair split of payoff to each of the rational players in a game, and the Nash approach is therefore a suitable method to solve the particular type of problems under consideration.

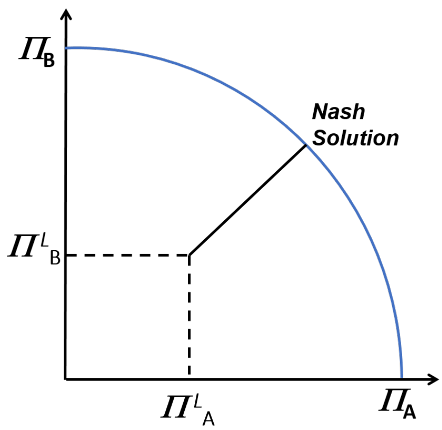


Figure 6.2: *Geometric description of Nash solution.*

If the *status quo* point (also referred to as the conflict point) of a game is (x_0, y_0), then the Nash solution is (x, y), $x \geq x_0$ and $y \geq y_0$, which maximizes $(x - x_0) \cdot (y - y_0)$. Based on the assumption of a symmetric game where neither player has a competitive bargaining advantage (i.e. a posteriori to the determination of the *status quo* point), neither of the supply chain partners will have any reason to grant the other partner better terms than the latter is prepared to grant him. The symmetric game will thus have a symmetric solution. Both players will agree on a solution that allocates payoffs equitably between them subject to the *status quo* point. The figure 6.2 illustrates the bargaining positions of the different players based on their original agreements, which in this case is the minimum acceptable profit levels, (Π_A^L and Π_B^L), that according to the generalized Nash-Harsanyi extension (Harsanyi, 1997) to the Nash solution, proposes that each member has a lower profit requirement point. The figure also shows the outcome of the game, the Nash solution. The solution according to Nash is the point, (Π_A, Π_B) with $\Pi_A \geq \Pi_A^L$ and $\Pi_B \geq \Pi_B^L$ which maximizes the product $(\Pi_A - \Pi_A^L) \cdot (\Pi_B - \Pi_B^L)$. The Nash solution can be regarded as a negotiation process where the *status quo* is a point where the bargaining will end up if no cooperation is to be had.

The threat strategies leading to the choice of a *status quo* point imply that there is a separate game of choosing the optimal *status quo* point for each player when regarding power relations and negotiation capabilities. The Nash solution has been criticized for disadvantaging players with a low value *status quo* point, but the *status quo* point is representing the structural advantage in the game of one player in favour of the other player.

6.3.2 Two-enterprise model

According to Gjerdrum et al. (2001) approach and adopting our case for the two enterprises before declared as {*Farmers, Biorefinery*}, where the lower profit levels for each firm, $\Pi_{farmers}$ and $\Pi_{biorefinery}$, are calculated as single optimization problem for each biomass transfer price (s), in order to find the solution that according to Nash is the point, $(\Pi_{farmers}, \Pi_{biorefinery})$ with $\Pi_{farmers} \geq \Pi_{farmers}^L$ and $\Pi_{biorefinery} \geq \Pi_{biorefinery}^L$ which maximizes the product $(\Pi_{farmers} - \Pi_{farmers}^L) \cdot (\Pi_{biorefinery} - \Pi_{biorefinery}^L)$ declared here as our Nash-type objective function, Φ, for a two-echelon SC. Accordingly:

$$\Phi = (\Pi_{farmers} - \Pi_{farmers}^L) \cdot (\Pi_{biorefinery} - \Pi_{biorefinery}^L) \tag{6.1}$$

where Π represents the profit of each enterprise (i.e. farmer, biorefinery) which is subject to meet a minimum profit requirement (Π^L) as stated below.

$$\Pi_{farmers} \geq \Pi_{farmers}^L \tag{6.2}$$

$$\Pi_{biorefinery} \geq \Pi_{biorefinery}^L \tag{6.3}$$

The equation presented in 6.1, produces non-linearities in the formulation; consequently a separable programming approach is applied utilizing logarithmic differentiation and approximations of the variables of the objective function resulting in a model of the MILP form:

$$\hat{\Phi} = \sum_{s}^{n} \lambda_{f(s)} ln(\Pi_{farmers(s)} - \Pi_{farmers}^{L}) + \sum_{s}^{n} \lambda_{b(s)} ln(\Pi_{biorefinery(s)} - \Pi_{biorefinery}^{L}) \tag{6.4}$$

$$\sum_{s}^{n} \lambda_{f(s)} \Pi_{farmers(s)} + \sum_{s}^{n} \lambda_{b(s)} \Pi_{biorefinery(s)} = \Pi_{farmers(s)} + \Pi_{biorefinery(s)} \tag{6.5}$$

$$\sum_{s}^{n} \lambda_{f(s)} = 1 \tag{6.6}$$

$$\sum_{s}^{n} \lambda_{b(s)} = 1 \tag{6.7}$$

$$\lambda_{f(s)} \geq 0 \tag{6.8}$$

$$\lambda_{b(s)} \geq 0 \tag{6.9}$$

The equation 6.4 represents the new objective function ($\hat{\Phi}$) where the enterprise profits were approximated as piecewise linear functions using $s \in S = [1, n]$ transfer price levels and introducing the continuous variables $\lambda_{f(s)}$ and $\lambda_{b(s)}$ for farmers and the biorefinery, respectively. While the equation 6.5 is the convexity requirement, the equations 6.6, 6.7 and 6.8, 6.9 guarantee that two adjacent nodes take non zero values, using n grid points.

The overall profit of biomass growers (TFP [€]) was calculated as follows:

$$\Pi_{farmers} = -TFP \tag{6.10}$$

$$TFP = \sum_{i} \sum_{g} \sum_{t} FR_{(i,g,t)} \cdot \epsilon_{CF(t)} \tag{6.11}$$

$$FR_{(i,g,t)} = Pb_{(i,g,t)} * Pr_{(g,t)} - TOC_{(i,g,t)} \tag{6.12}$$

$$Pb_{(i,g,t)} \geq Pb_{(i,g,t-1)} \tag{6.13}$$

where $\epsilon_{CF(t)}$ is discount factor related to time period t specific for $FR_{(i,g,t)}$ representing the incomes from biomass sale, which is evaluated by multiplying the total biomass rate produced by the player in region g at time t, $Pb_{(i,g,t)}$ [t/time period] by the corresponding variable, $Pr_{(g,t)}$ as the biomass selling price. Besides, the equation 6.13 constraints the farmers to long-term contracts with the biorefinery. However, the last two terms in the equation 6.12 produce a non-linear element; thus, the following linearization based on Gjerdrum et al. (2001) has been applied. First of all, we introduced a linearized variable of the amount of biomass depending of certain levels of price to be chosen. Accordingly:

$$Pbl_{(i,g,s,t)} \leq binl_{(g,s,t)} \cdot Lvs_{(i,g,s)} \tag{6.14}$$

where the S segment for prices for each price level, described as $Lvs_{(i,g,s)}$, the term $binl_{(g,s,t)}$ stands for the linearized quantity, $Pbl_{(i,g,s,t)}$, of biomass i from the farmer in g at time t of the s available price levels. The $binl_{(g,s,t)}$ is a binary variable which takes the value 1 if the s^{th} price level is chosen for the farmer in g at time period t, and 0 otherwise. Accordingly, the term presented below is used instead of the non-linear term $(Pb_{(i,g,t)} \cdot Pr_{(g,t)})$ in the equation 6.12:

$$\sum_s Pbl_{(i,g,s,t)} \cdot Lvs_{(i,g,s)} \tag{6.15}$$

The following two constraints:

$$\sum_s \sum_t binl_{(g,s,t)} \leq 1 \tag{6.16}$$

$$\sum_s Pbl_{(i,g,s,t)} \geq 0 \tag{6.17}$$

ensure that only one of the S price levels available is chosen at time period t for the biomass growers in g. Furthermore, the linearized term cannot take negative values.

Therefore, the equation 6.12 is replaced by the following:

$$FR_{(i,g,t)} = \sum_{s} Pbl_{(i,g,s,t)} \cdot Lvs_{(i,g,s)} - TOC_{(i,g,t)} \tag{6.18}$$

which is evaluated by multiplying the linearized quantity, $Pbl_{(i,g,s,t)}$, of biomass i from the farmer in cell g at time t of the s available levels by the corresponding variable for biomass selling prices for each level ($Lvs_{(i,g,s,cl)}$); $TOC_{(i,g,t)}$ stands for the farmers total operating cost and accounts for biomass i production and transport cost at time period t.

The mathematical model describing the biorefinery company was based on the work by Giarola et al. (2011) to which we refer for the mathematical details. The overall profit of the biorefinery represented as the NPV was calculated by summing up the discounted annual cash flows [CF_t (€/period)] for each period t minus the capital investment [TCI_t (€)] for establishing or enlarging a production facility.

$$\Pi_{biorefinery} = -NPV \tag{6.19}$$

$$NPV = \sum_{t} (CF_t \cdot dfCF_t - TCI_t \cdot dfTCI_t) \tag{6.20}$$

where $dfCF_t$ and $dfTCI_t$ represent the discounting factors for cash flows and capital costs, respectively. It is worth mentioning that the biomass procurement costs, as part of the CF_t definition have been modified compared to the original model since the biomass acquisition relies on sale price level of the farmers. Accordingly,

$$BPC_t = \sum_{i} \sum_{g} \sum_{s} Pbl_{(i,g,s,t)} \cdot Lvs_{(i,g,s)} \tag{6.21}$$

where the biomass procurement cost (BPC_t) is evaluated by multiplying the linearized quantity, $Pbl_{(i,g,s,t)}$, of biomass i from the farmer in g at time t of the s available levels by the parameter containing the price levels, $Lvs_{(i,g,s)}$, for the farmer in region g.

6.4 Results and Discussion

The optimization problem for a fair profit allocation in a 2-enterprise corn-based ethanol SC was solved by means of the CPLEX solver in the GAMS® modelling tool.

In order to apply the linearization procedure, minimum profit requirements at different transfer prices (reported in Table 6.2) were determined solving the optimization problem which has been previously described in Chapter 2 for a single enterprise at a time (i.e. farmers and biorefinery). Table 6.2 reports the minimum profit values for the two enterprises at the chosen.

Once the minimum profit requirements were established we proceeded with the maximization of the enterprise profits ($Max\hat{\Phi}$). The outcome of the optimization procedure for each enterprise implementing the linearized Nash objective function, were 2.971 €$/GJ_{EtOH}$ for the biomass growers ($\Pi_{farmers}$) and 1.034 €$/GJ_{EtOH}$ for the biorefinery consortium. The λ multipliers used for the linear approximation took values for $\lambda_{f(1)}, \lambda_{f(2)} = 0.982$, and $\lambda_{b(2)} = 1$.

The results obtained for a two enterprise SC with and without the inclusion of a Nash GT approach are compared in Figure 6.3. The first stacked bars were obtained when the optimized problem aimed at the maximization of an overall profit ($\Pi_G = \Pi_{biorefinery} + \Pi_{farmers}$). The second ones were obtained after the Nash optimization. As is clear in Figure 6.3 the proposed approach ensures a more equal profit-split between the two enterprises involved in the SC.

It is interesting to note that the introduction of a Nash-type approach allows the farmers to choose different price levels along the time horizon. The overall system profit embedding a Nash approach matches very close the value obtained from a pure optimization of the enterprise profit summation, which results in a better economic performance of the supply chain as a whole. Table 6.3 shows the dynamic of participation of the farmers over the entire time horizon as the ethanol demand is increased, thus emphasizing that each farmer can move freely through the diverse levels of price along the time horizon.

Table 6.2: *Corn price levels and corresponding minimum profit for farmers and biorefinery.*

Level (S)	Price (€/tonne)	$\Pi_{farmers}$ (€)	$\Pi_{biorefinery}$ (€)
1	100	2.20E+08	1.00E+06
2	145	6.90E+08	3.19E+08
3	175	1.16E+09	6.37E+08

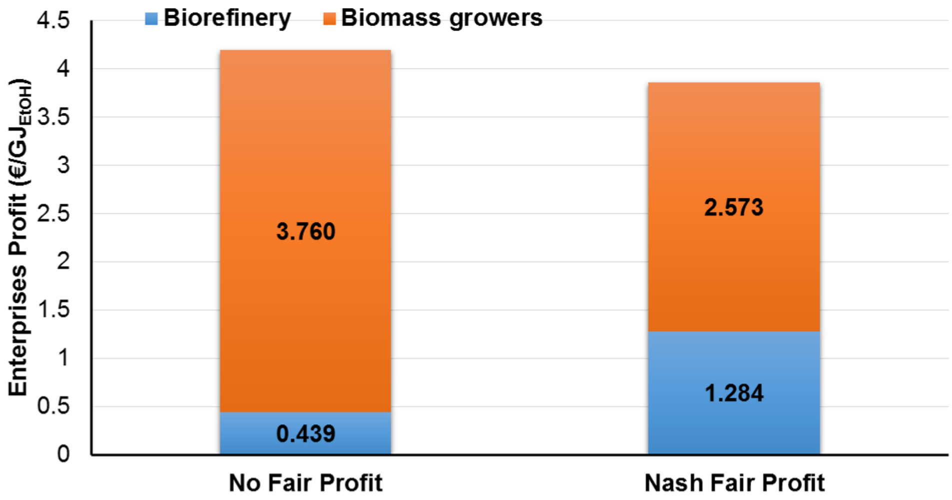


Figure 6.3: *Profit share before and after Nash supply chain optimization and the overall improvement after fair split.*

Table 6.3: *Evolution of farmer participation over time horizon.*

Farmers in (g)	Price (€/tonne)	Time Periods				
		1	2	3	4	5
17	100	X				
	175		X	X	X	X
24	145	X				
	175		X	X	X	X
28	100	X				
	175		X	X	X	X
29	175	X	X	X	X	X
39	100			X	X	
	145					X
60	110	X	X	X	X	X

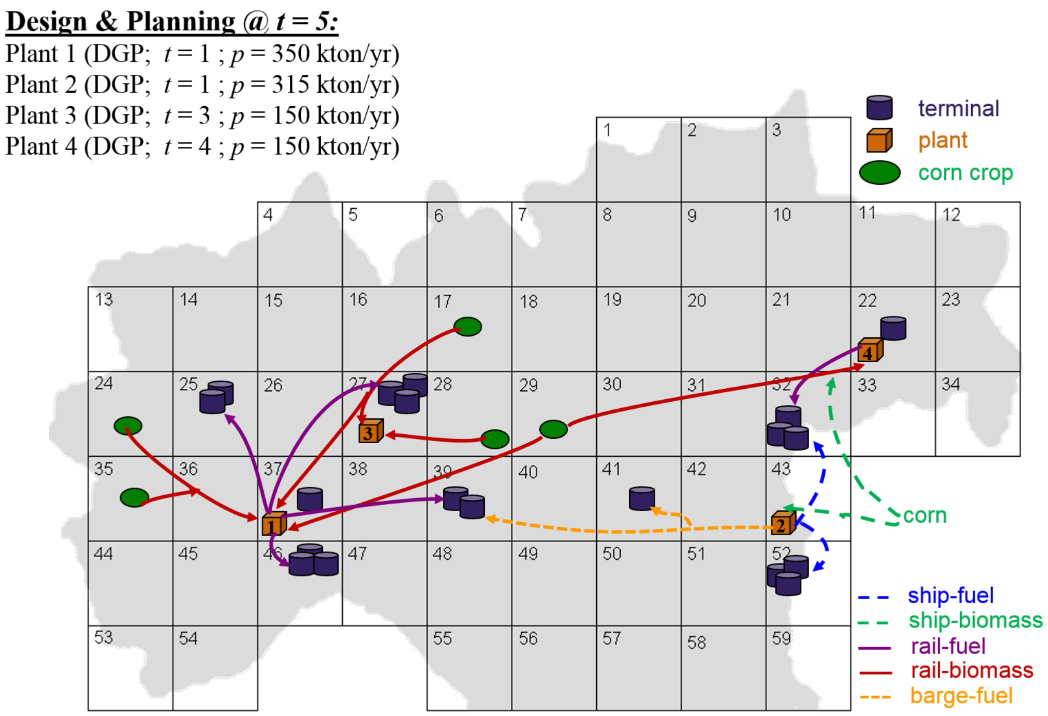


Figure 6.4: *Design and planning strategy at time period $t = 5$ under Nash optimization supply chain.*

In terms of design and planning, the SC configuration at the final period is represented in Figure 6.4. The optimal solution involves the establishment of four DGP bioethanol production plants operating at full capacity (over 250 kton/year). One facility is located on the coastline, although the system also relies on biomass importation. At the end of time period 5, the observed amount of imported biomass was about 42%, which reduced significantly the biomass supply costs, due to the lower price of the imported corn.

Furthermore, an analysis within the Nash modelling framework was performed by fixing the price levels over the time horizon (Table 6.4). It has been necessary to increase the original first corn price level (which was set to 100 €/ton) to 130 €/ton, since prices below 130 €/ton do not allow the system to reach the minimum profits established according to the Nash optimization.

From the results, it emerges that the fairest split of the profit is obtained at the lowest corn price, where the biorefinery consortium receives about 40% of the total and the farmers' enterprise holds the 60%.

However into the modelling framework exists a constraint where the total production of biofuel ($TP_{(t)}$) must be equal to the total demand of biofuel ($TD_{(t)}$) that is increased

Table 6.4: *Enterprise profit under fixed price.*

Fixed Price	$\Pi_{farmers}(€/GJ_{EtOH})$	$\Pi_{biorefinery}(€/GJ_{EtOH})$
Low (130 €/tonne)	2.319	1.442
Average (145 €/tonne)	2.799	1.130
High (175 €/tonne)	2.904	1.034

over the time horizon ($TP_{(t)} = TD_{(t)}$), thus in certain manner this equation restricts the economic performance of the biorefinery enterprise. Therefore, implementing the constraint as $TP_{(t)} \geq TD_{(t)}$, allows the production of biofuel could be greater than the biofuel demand over time horizon. The outcome of the analysis previous described is shown in Figure 6.5. As can be observed in a clear way in this instance for the lowest price there is a small

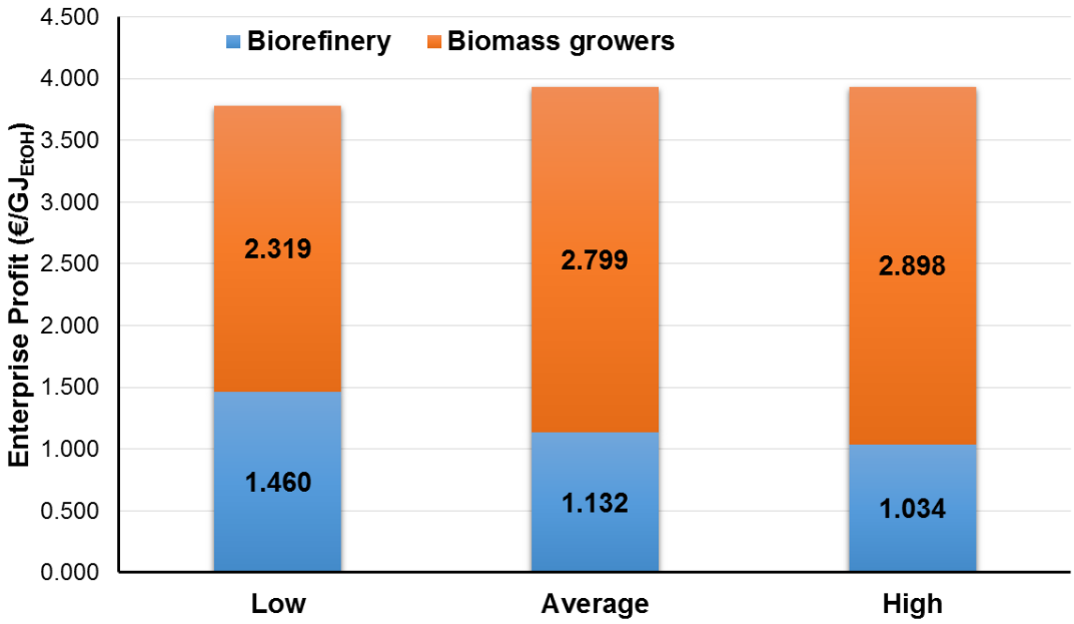


Figure 6.5: *Profit share at different fixed price levels (production constraint).*

profit increment of the biorefinery reaching an economic performance of 1.460 $€/GJ_{EtOH}$, representing an profit increase for the biorefinery while still achieving a better fair profit share for both parties since the constraint on biofuel production was amended.

6.5 Final Remarks

A modelling framework which utilizes a separable programming approach to implement the game theoretical concepts developed by Nash was proposed. The purpose was to guarantee fair profit allocation in the design and planning of a two-enterprise biofuel supply chain. The proposed method guarantees fair profit levels of the separate enterprises while an optimum total profit of the entire supply chain is achieved. The transfer prices for biomass selling-acquirement which allow a fair split of the profits between the two enterprises are mostly located in the higher price level (i.e. 175 €/ton). However, the proposed method guarantees that even at a low corn price over the time horizon (130 €/tonne) better economic performance is achieved.

The integration of GT aspects in SC optimization tools could support the decision making among the stakeholders involved in the planning of bioenergy systems. As a matter of fact, these tools could enable the definition of planning strategies from which every single enterprise could benefit. This would facilitate the bargaining among the stakeholders as well as help the planning of bioenergy system capable achieve a better overall performance when a fair profit split is guaranteed.

CHAPTER 7

Conclusions and Future Research Directions

The advantages and contribution of the solution approaches proposed to the Thesis objectives have been opportunely highlighted along this document. This chapter aims at highlighting the most promising achievements on this project. Trends and challenges for possible future research lines are outlined.

7.1 Major Contributions

It is paramount and with some urgency of humankind to make use of renewable resources to cover the growing demand for energy in a sustainable fashion and thereby alleviate the environmental/socio/political issues driven by the use of fossil fuels. Particularly, the shift towards more sustainable and competitive fuels in the transportation sector represents a demanding task for both practitioners as for researchers within a more conscious society in the near future. However, not only the establishment of a new system of energy supply is imperative, but also new political actions are advocated in order to be integrated into a global structure to address the issues associated with the production of biofuels.

As has been presented and discussed in the preceding chapters, the design of systems for biofuel production has confronted and tackled several and multifaceted problems, such as economic profitability and environmental sustainability. Such scope must be dealt through a comprehensive methodology by incorporating the general stages of the production chain (supply chain), from the cultivation of biomass up to fuel distribution, all of this in accordance with the principles of supply chain management (SCM). The new capital spending in biofuel production systems should be driven by purposefully designed decision-making tools with foundation on multi-criteria analysis, by means of mathematical programming (MP) and, particularly, mixed integer linear programming (MILP) modelling frameworks.

Thus, this Thesis represents a further step in an attempt to tackle these challenges and devise holistic support models for integrated SCM. Major contributions are outlined in the following.

⇨ ***Enlargement of the technological space and its assessment.***

The integration of anaerobic digestion of solid residues after biomass conversion has been considered and included in the SC model through a spatially explicit and multi-period MoMILP modelling framework. Moreover, the improvement of dry-grind process in terms of environmental and economic performances through alternative usages of first generation by-products has been assessed. According to the optimization results (Chapter 2), this technology option could conveniently contribute to the overall energy balance and ensure a viable trade-off between the interests in conflict to help the design and planning of feasible and sustainable multi-echelon biofuels SCs.

At the same time, carbon trading scheme was introduced as a potential means to promote biofuels production technologies where emissions allowances are traded at an uncertain price/cost depending on the technology potential on emission savings. From the results it emerges that at the current CO_2 price the economic acknowledgement of the emissions would hardly promote environmental performance improvement. Therefore, for a improved carbon trading mechanism it is necessary to have better economic benefits for improving the emission trading market.

⇨ ***Quantification of uncertainty through the implementation of novel price forecasting methods.***

Four models to predict the prices of the commodities involved in bioethanol production were implemented. These models were applied directly to forecast corn and ethanol prices along the supply chain lifetime, while other corelations were defined to predict the prices of second-generation-technology raw materials, such as corn stover and miscanthus, and of by-products of ethanol production processes, such as distiller's dried grains with solubles (DDGS) and electricity (Chapter 3). Six different technologies involving corn as raw materials were included in the simulation model, four of them recurring to a stillage fermentation module to produce electricity (Chapter 2). The optimal bioethanol supply chain layout was calculated under the four prediction models in order to assess the supply chain robustness to changes in price evolution dynamics. The results of the simulations proved that minimal differences in the optimal supply chain design occur if prices follow different evolution paths and therefore part of the investment risk is mitigated: in fact, investors can be confident on the fact that the chosen supply chain is optimal also if commodity prices behave differently.

⇨ ***Policy assessment through supply chain management models.***

A whole chapter was dedicated to the analysis of the impacts on the optimal bioethanol supply chain design of the recent European Commission (EC) proposal to amend part of the existing directive that regulates the biofuel blending requirements (Chapter 4). First, the proposal was presented and discussed, then the original MILP model was modified to include the new accountability technique and two second-generation technologies, one based on an energy crop, the other on agricultural residues. This proposal gives more room to second generation technologies in the supply chain design, but the profitability was proved to be still far from being achieved. Cost reductions for second generation technologies were discussed in order to reach an economic breakeven for both types of technologies under the proposed demand scenario. Furthermore, the impact of this proposal on taxpayers and on fuel consumers was compared with the current directive scenario, in order to evaluate the positive aspects and the drawbacks of the proposed modifications to the existing directive.

⇨ ***Assessment of cooperation and competitiveness of different players through a Game Theory approach.***

In the age of globalization, the economic and industrial landscape has seen many radical changes. In such context, supply chains are becoming complex networks of a large number of entities that sometimes compete and sometimes cooperate to fulfill customer needs and to satisfy market requirements. Standalone supply chains, where each entity makes its decisions so as to maximize its own profits according to its own objectives, often lead to a loss of efficiency and fail to face the complexity of the economic environment they are facing with. Such scenarios, cooperative and non-cooperative, have been covered in the Chapter 5. The problems have been assessed through a game theory (GT) approach within the optimization based decision support system. The emerging results from the optimization demonstrate that game theory could conveniently help the decision-makers using more realistic pathways to the biofuel supply chain planning problems. Among the scenarios considered, the cooperative structures, where resources/service facilities are shared and decisions are made to maximize the global profit, suggests that, under certain conditions, to be more beneficial and efficient. Furthermore, from the competitive analysis could be used as a bargaining tool among the stakeholders in order to improve the decision making across different business scenarios. In this context, effective design tools could provide some assessment criteria for many companies to change their way of doing business by exceeding the border of standalone and individual actions toward collective actions and cooperative strategies. Therefore, building alliances appears as a successful strategy in modern supply chain networks, allowing the system to achieve a higher global performance.

However, this cooperative behaviour has raised a new research direction, since it is not clear how the profits should be distributed among the participating parties. In Chapter 6 this difficulty has been addressed through a modelling framework which utilizes Nash game-theoretic concepts. The purpose of the methodology has been to achieve solutions that fairly distribute profit between the enterprises at the same time as optimizing the supply chain objective variables and fulfilling the biofuel demand. The transfer prices for biomass selling-acquirement were used in order to distribute profits into the model with the interest agents in the supply chain. Without doubts, the fusion of game theory frameworks with supply chain management tools could support decision making among stakeholders involved in planning of new bioenergy systems.

7.2 Future Research Opportunities

Increasingly, the World liquid fuels supply is expected to rely on biofuels. In fact, over the next decade, it is expected that the biofuels will become an important part of the fuel mix for road transportation. In this meaning, many governments, corporations, and researchers see biofuels as a solution for tackling energy security, environmental and economic challenges associated with petroleum dependency. This is how large oil-consuming nations concerned about energy security, climate change and economic stagnation are driving global biofuels markets through a number of policy platforms, principally biofuels mandates.

Within this holistic picture, a number of possible suggestions for future work that relate to the work presented in this thesis are presented. The aim is to provide the reader with ideas about how a framework for future supply chain modelling and analysis could be accomplished based on the understanding gathered through the work to date. In order to build an integrated supply chain model for a real-life supply chain, several extensions are needed:

① One good opportunity is to expand the modelling capabilities (especially with concern to the description of the environmental impact) to provide some general tools to assess the effect of European Union (EU) or national policies.

② The research area dedicated to game theory is a rather new stream of research in supply chain management, and several future developments can be done. It could be interesting, introduce interactions among the supply chain participants through a leader-follower Stackelberg game under Nash equilibrium concepts.

③ Another crucial point of research would be to pursue a study of how the inherent power relations between supply chain partners could be incorporated so as to capture the actual negotiation principles involved and find a pragmatic approach to agreement in pricing policies that could be useful for any type of power relations.

④ An important development of the project might be directed towards strategic decisions related to power generation infraestructures establishment and technology selection which might be properly driven through adopting a comprehensive approach embedding all the SC phases according to SCM techniques.

It is expected that the future recommendations will enhance the usefulness of this research project and will result in the development of a fully integrated and comprehensive supply chain optimization model.

"*Interesting research raises more questions than it answers. It is controversial. It invokes responses like "that can't be true" or "this is obviously incomplete." Interesting research should initially leave the reader a little discontent, unnerved, or motivated to prove it wrong or at least incomplete*".

(Cachon (2012))

Appendices

APPENDIX A

Interaction between Indirect Land Use Change and Biofuel production

KEY feature introduced in this chapter contemplates the incorporation of the new approach proposed by the EC for the inclusion of emissions caused by iLUC. The general behaviour of the bioethanol SC is as the already proposed framework in the previous chapter, thus dealing with multiechelon, multiperiod, and spatially explicit features are intrinsic part of the formulation to steer decisions and investments through a global approach of a bioethanol SC. A demostrative case study is presented referring to the emerging Italian ethanol production. Results show the effectiveness of mathematical programming-based tools to provide decision makers with a quantitative analysis assessing the economic and environmental performances of different design configurations facing the new amendments proposed by EC.

A.1 Motivation

The bioenergy has been promoted over the past decades as an option to climate change mitigation through the replacement of fossil fuels and also as a source to reduce the world's dependence on the oil, and also as a source to reduce the dependence of the regarding oil, which is a natural source and consequently limited. Accordingly the biofuels have been identified as a feasible option in matter of sustainability and competitiveness in order to offer the right choice for global transport. With liquid fuels likely to remain the primary energy source for road transport for at least the next few decades, biofuels are widely recognised as an important means of lowering the greenhouse gas emissions of transport.

A.2 Problem definition and main assumptions

Controversy, meanwhile, emanates primarily from the fact that ILUC cannot be empirically observed, and must therefore be rendered "visible" through modelling. In spite of this complexity and controversy, modelling work has shown iLUC to be capable in *theory* of generating significant GHG emissions, which in some cases could be significant enough to render biofuels carbon footprint *double* that attributable to petrol or diesel (Searchinger et al., 2008). Up to this point, most studies attempting to quantify the magnitude of iLUC used an economic approach to address it (Searchinger et al., 2008; Edwards et al., 2010; Kløverpris et al., 2008; Tyner et al., 2010; Bergsma et al., 2006; Laborde, 2011) merging into the same modelling framework the economic and biophysical (agricultural) systems. Borne predominantly by the use of partial and general equilibrium models as shown in Witzke et al. (2008). However such models and therefore the estimations have resulted in widely differing predictions about the emissions caused by iLUC and where the land use changes will occur, partly because of differences in the treatment of the considerations as input data and the interaction among bilateral trade and behaviour of the supply. Having stated the above, no model has been implemented yet below a national level or for predicting the spatial relocation of displaced activities (Gnansounou and Panichelli, 2008; Fritsche and Wiegmann, 2011).

Recently, the European Commission has proposed for the first time that the estimated global land conversion impacts will be considered when assessing the greenhouse gas

Table A.1: *Estimated iLUC emissions from biofuel and bioliquid (Europarl, 2013).*

Feedstock group	Estimated iLUC emissions (Kg CO2-eq/GJ)
Cereals and other starch rich crops	12
Sugars	13
Oil crops	55

performance of biofuels. The proposal sets out iLUC factors for different crop groups (Table A.1). These factors represent the estimated land use change emissions that are taking place globally as a result of the crops being used for biofuels in the EU, rather than for food and feed. Simply put, all biofuels that use land will get an iLUC factor. Feedstock that do not require agricultural land for their production (i.e. waste, residues, algae) and those that cause direct land use change (i.e. in which case operators need to calculate their actual emissions) are exempt from the factors. Under the new rules, the estimated emissions from iLUC factors, are to be included in Member States' and fuel suppliers' reporting of GHG savings under the EU Renewable Energy Directive (RED) and the Fuel Quality Directive (FQD) respectively (Europarl, 2013). The aim of the proposal is to start the transition to biofuels that deliver substantial GHG savings when also estimated iLUC emissions are reported. The aims of the proposal are to:

- limit the contribution that conventional biofuels (with a risk of iLUC emissions) to achieve the targets in the RED;
- improve the GHG performance of biofuel production processes (reducing associated emissions);
- encourage a greater market penetration of advanced biofuels (low-iLUC) and so contribute more to the targets in the RED than conventional biofuels;
- improve the reporting of GHG emissions by obliging Member States and fuel suppliers to report the estimated iLUC emissions of biofuels.

The Commission is of the view that in the period after 2020 biofuels which do not lead to substantial GHG savings (when emissions from iLUC are included) and are produced from crops used for food and feed should not be subsidised.

The GHG associated with changes in the carbon stock of land resulting from iLUC are not subject to reporting requirements under the current legislation. Both Directives (RED and FQD) invite the Commission to review the impact of indirect land-use change on GHG and, if appropriate, propose ways to minimise it whilst respecting existing investments made in biofuels production. Consequent to this invitation, the Commission identified a number of uncertainties and limitations associated with the available numerical models used to quantify iLUC, while recognizing that the iLUC may reduce the GHG emissions savings resulting from biofuels and bioliquids, and as such, recommended that this issue was to be addressed under a careful approach.

In light of the foregoing, the leading aim in this chapter is to introduce the iLUC factor proposed by the European Comission into the modelling framework already developed in Chapter 2. The design process is conceived as an optimization problem in which the whole production system is required to complying with the two objective functions: (*i*) the maximization of the financial performance of the business, expressed in terms of the NPV, and (*ii*) the minimization of the impact on global warming (in terms of overall GHG emissions) in operating the system. The biofuel supply chain in question is referred as in Chapter 2.

A.3 Mathematical Features

The framework of the model has been laid down following the previous formulation as a MoMILP problem under common criteria adopted in the design of bioethanol multiechelon, multiperiod SC strategy level. An important key feature is addressed in the present proposed approach involving the inclusion into the modelling structure of the factor representing emissions caused due the iLUC that has been proposed by the European Comission. The core mathematical modelling is set forth below, proposing both objective functions definition followed by special feature introducing the iLUC factor.

A.3.1 Economic and Environmental objective functions

The economic objective function (Obj_{Eco}, [€]), is estimated in terms of the NPV of the system and needs to be maximized in configuring the production network to optimize business profitability. It is calculated by summing the discounted annual cash flows (CFt, [€]) for each time period t minus the capital investment ($TCIt$, [€]) when a production facility is established. Accordingly:

$$Obj_{Eco} = -NPV \tag{A.1}$$

$$NPV = \sum_t (CFt \cdot dfCFt - TCIt \cdot dfTCIt) \tag{A.2}$$

where $dfCF_t$ and $dfTCI_t$ represent the discounting factors for cash flows and capital costs, respectively. On the other hand, the enviromental objective (Obj_{Env}) is expressed through the definition of the total impact (TIt, [kg of CO_2-eq/time period]) over time, which is estimated by summing up the GHG emission rate for each LCA stage s as well as the effect of emission credits coming from by-products end-use ($Imp_{(s,t)}$, [kg of CO_2-eq/time period]):

$$Obj_{Env} = TIt = \sum_s Imp_{(s,t)} \tag{A.3}$$

$$Imp_{(s,t)} = \sum_s f_{(s)} \cdot F_{(s,t)} \tag{A.4}$$

where the impact rate $Imp_{(s,t)}$ is determined by applying an impact factor, $f_{(s)}$ [kg CO_2-eq/unit], for stage s, to a reference flow, $F_{(s,t)}$ [units/time period], which is specific to LCA stage s at time t.

A.3.2 iLUC issues

Pursuant to by the EC recently (Europarl, 2013), this proposal forms part of the highly anticipated EU plans to tackle the impact of biofuels on iLUC. Therefore the estimated iLUC emissions should be included in the reporting of GHG emissions from biofuels under Directives 98/70/EC and 2009/28/EC, and is introduced as follows into the modelling framework:

$$iLUC_t = \sum_k \sum_g iF \cdot F_{(s,t)} \tag{A.5}$$

where the iLUC factor for the feedstock group (iF), in the case of this work the corn utilized as a biomass to produce ethanol corresponds to a value of 12 kg of CO_2 per GJ.

A.4 Case Study

The emerging bioethanol fuel SC in Northern Italy has been chosen as a case study to show the model capabilities in steering the strategic design of biofuels systems. According to this, the SC analysis and LCA approaches proposed in Chapter 2 have been taken in consideration to evaluate the specific modelling parameters and for representing actual economic and environmental data.

A.5 Results and discussion

The problem was solved by means of the CPLEX solver in the GAMS® modelling tool. In the following discussion, a preliminary part is devoted to presenting the strategic investment decisions according to the simultaneous optimization framework of GHG emissions savings including the iLUC effect and economic profitability. In the second part, a sensitivity analysis on the proposed factor is performed. Subsequently a comparison of several iLUC factors taken from literature on the SC configuration is presented and discussed.

A.5.1 Simultaneous environmental and economic optimization

It is interesting to observe the effect of the iLUC factor on the simultaneous environmental and economic performances through the MOO, due to this factor, emerges from the optimal configuration in terms of economic performance (point A in Figure A.1) entailing a marginal NPV of 1.19 €/GJ_{EtOH} against a global environmental impact of 103.6 kg CO_2 eq./GJ_{EtOH} which implies that this point A is completely out of any chance of meeting the environmental targets of the EU. The SC configuration would involve the establishment of ethanol plants either exploiting a standard DGP process ($k = 1$) or relying on an alternative thin stillage valorization route and on natural gas supplement for energy needs (DGP-TS_{NG}, k = 6).

On the other hand, the environmental solution represented by point D in Figure A.1 reduces the marginal impact to 40 kg CO_2 equiv./GJ_{EtOH} representing a 54% of GHG reduction, still maintaining a good economic performance which involves a marginal NPV of 0.79 €/GJ_{EtOH}. Therefore, this solution emerges as the best supply chain design in terms of the environmental performance, which would be sufficient to meet the 2017 target (set to 50%). Thus, the EU GHG emission reduction target would be achievable when all the DDGS is devoted to bioenergy production (as with the technology DGP-CHP, $k = 2$).

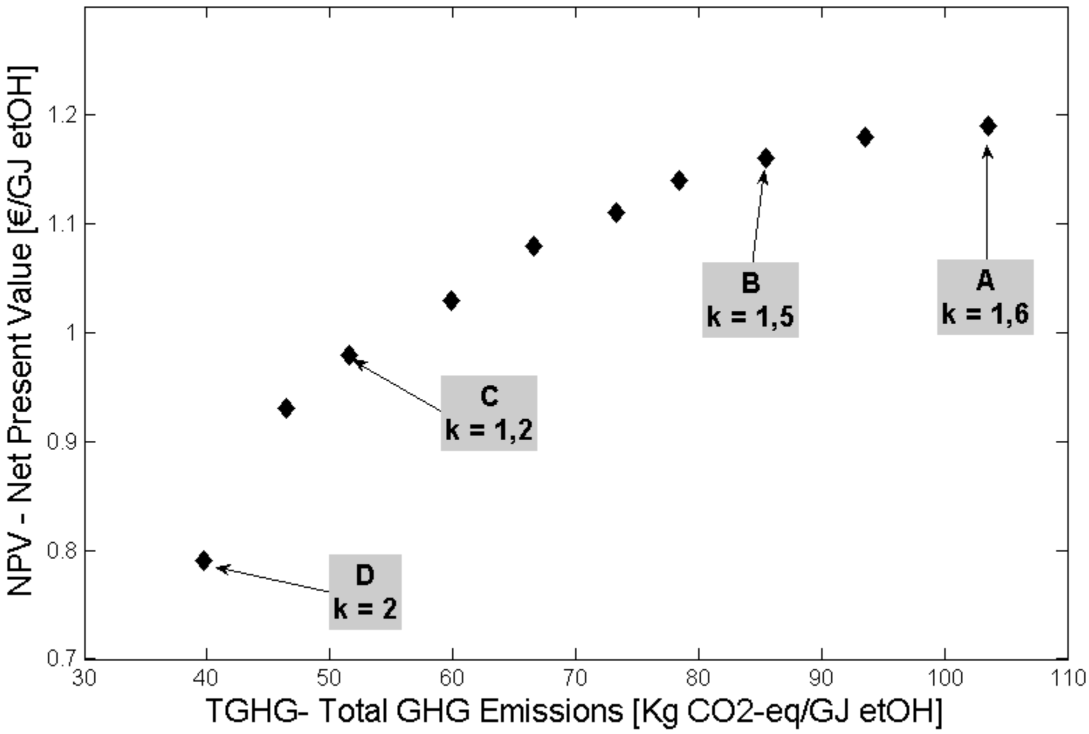


Figure A.1: *Pareto set of optimal solutions: simultaneous optimization under NPV maximization and GHG emissions minimisation criteria (k = production technology) considering the iLUC factor.*

It should be noted that the cases including the iLUC factor maintain their economic performance in both instances as in Section 2.6.1 presented before. However, this new inclusion of emissions produces a more significant effect on the environmental performance of the supply chain, since the target for the optimum setup would be only reachable the target of 50% for 2017. Nevertheless the selection of technologies in both instances are the same; for the economic performance the system design would involve the establishment of 6 production plants combining the standard DGP production plant ($k = 1$) and the technology involving the anaerobic digestion of the thin stillage ($k = 6$) on natural gas supplement for energy needs. The design of the system for the environmental solution proposes the installation of 6 production plants implicating only the technology based on DGP-CHP ($k = 2$) where the whole DDGS is devoted to power generation.

A.5.2 Sensitivity Analysis on iLUC

It is noteworthy that the implementation of the iLUC impact affects only the environmental issue of the SC as expected, therefore, sensitivity analysis on the value proposed by the EC has been conducted in order to determine the effect that the variation of this value could produce in the configuration of SC.

The outcomes in terms of total impact from this analysis for both economic and environmental solutions, TI_{Eco} (point A in Figure A.1) and TI_{Env} (point D in Figure A.1) respectively, are presented in Table A.2. It is possible to emphasize that even if the value of the factor proposed by EC is increased by 66%, the selection of the optimal technology for both solutions remains the same. On the other hand the best solution in terms of the environmental performance is based on the technology DGP-CHP ($k = 2$).

Table A.2: *Sensitivity analysis on the iLUC factor.*

iLUC (kg CO2/GJ)	TI_{Eco} (kg CO2/GJ)	Technology (k)	TI_{Env} (kg CO2/GJ)	Technology (k)
8	99.55	1,6	35.63	2
12	*103.6*	*1,6*	*39.7*	*2*
16	107.6	1,6	43.7	2
20	111.5	1,6	47.8	2

It is noteworthy the behaviour of optimal environmental solution (point D in Figure A.1) in terms of its environmental performance facing the ILUC factor sensitivity. This because even when is taken into consideration the highest value for the iLUC factor assumed as 20 kg CO_2/GJ, the supply chain configuration in terms of optimal technology selected (DGP-CHP, $k = 2$) remains the same (see Table A.2). Therefore, the whole system could withstand the environmental thresholds through the set up and establishment of this technology (Figure A.2).

Conversely, the environmental performance of the economic optimal solution (point A, TI_{Eco}) is more severely affected by the inclusion of the iLUC factor, as can be easily spotted in Figure A.1. From the analysis of the effect of varying the iLUC factor (see Table A.2)in the optimal economical solution shows that for all cases is jeopardized the acceptance by EU, since the optimal configuration of the supply chain falls short of meeting the thresholds

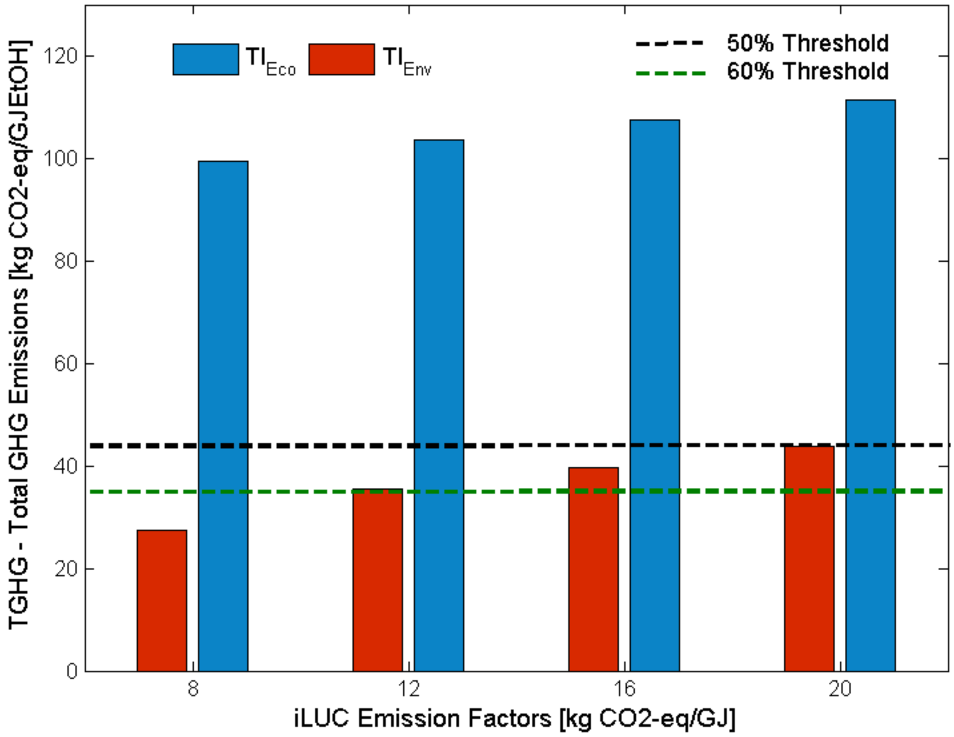


Figure A.2: *Total impact iLUC factor.*

imposed (Figure A.2).

A.5.3 EC iLUC factor proposed *vs.* Literature factors

There is a growing recognition that the environmental impacts associated with iLUC could affect dramatically the performance of biofuel SC. Consequently, quantifying the emissions of GHG due to iLUC has been attempted and is currently hotly debated by many researchers. The debate centers on the ability of any model to accurately identify changes in land use that are directly attributable to biofuels initiatives.

In this instance other iLUC factors from literature (Audsley et al., 2010; Searchinger et al., 2008) have been introduced and have been compared with the one proposed by the EC. The table A.3 shows the iLUC factors taken into account.

As can be observed in the Figure A.3 showing the total emissions of the supply chain under iLUC issues for both extremes of the pareto curve representing the economic and environmental optimum solutions. Are noteworthy the quantitative outcomes emerging when applying the approach published by Searchinger et al. (2008) which is considered in

Table A.3: *Estimated iLUC emissions from different approaches.*

Approach	Estimated iLUC emissions (kg CO2-eq/GJ)
Audsley et al. (2010)	18
Searchinger et al. (2008)	106

the literature as unrealistically high value for the indirect issues. And indeed, the effect produced in the supply chain results in a total impact for economic optimum (TI_{Eco}) of almost the double, 197.5 kg CO_2 when is compared with that of the EC, and even more with respect to the environmental optimum (TI_{Env}) with 134.6 kg CO_2 against 40 kg CO_2 of the EC.

On the other hand, the results obtained by using the estimated factor by Audsley et al. (2010) are comparable or similar to the EC one, as can be observed from the Figure A.3, where the overall impact of the economic optimum configuration reaches 109.4 kg CO_2 while the environmental solution in its total impact presents 45.48 kg CO_2.

It should be noted that for the economic optimal solution (point A in Figure A.1 and identified as TI_{Eco} in Figure A.3) whatever the factor applied, the economic performance exceeds the threshold imposed of 60%. Conversely in two of the cases presented , i.e. for Audsley et al. (2010) and the EC proposal, the environmental performance reach the 47% and 54% respectively of GHG reduction of compared to gasoline.

A.6 Concluding Remarks

Achievement of the EU's goals for greenhouse gas reduction in transport fuels is dependent upon the use of biofuels. However, some stakeholders are concerned about the potential ILUC impacts of biofuels and are questioning the appropriateness of policies that encourage their use. From the results, it emerges that technology option which considered the DDGS fed to a CHP station stands as the optimal choice that could conveniently contribute to withstand the addition of a iLUC factor. Given the expressed concerns about the indirect exchange interaction between the land use change and bioethanol production, our study provides an analysis at "local level" along the northern territory of Italy generating a future

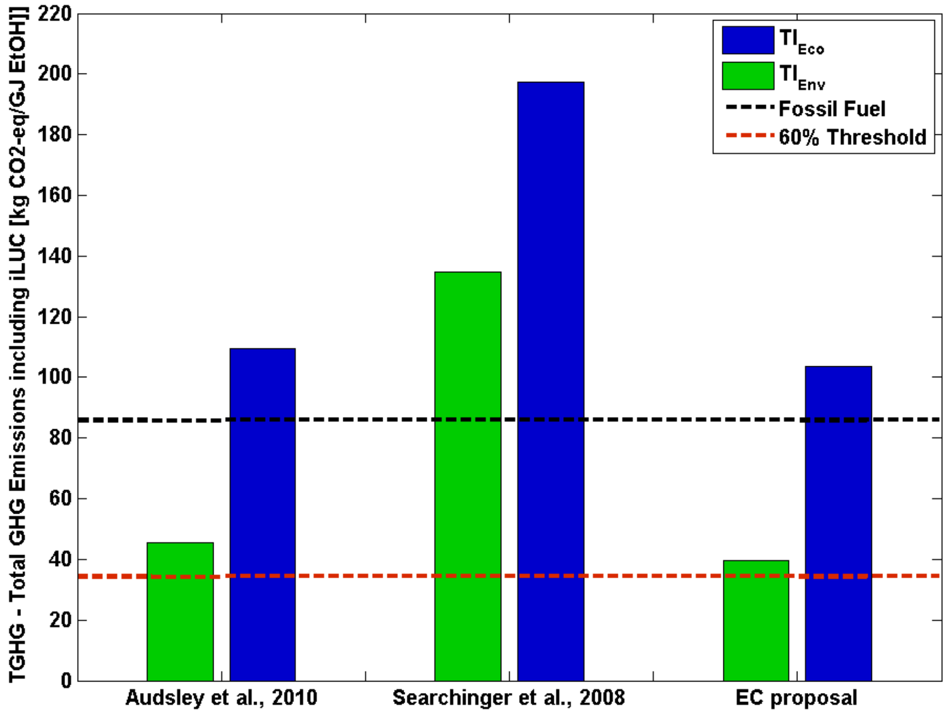


Figure A.3: *Total emissions for both economic and environmental optimal solutions considering iLUC.*

perspective of the response of the SC with respect to the iLUC factor projected by the EC.

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