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—

CICLO XXII

**SUPPLY CHAIN MODELLING FOR THE ECONOMIC AND LIFE
CYCLE ANALYSIS AND OPTIMISATION OF BIOETHANOL
FIRST-GENERATION PRODUCTION PROCESSES**

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“It is no good crying over spilt milk, because all the forces of the universe were bent on spilling it”

W. Somerset Maugham

“Invincibili sono quelli che non si lasciano abbattere, scoraggiare, ricacciare indietro da nessuna sconfitta, e dopo ogni batosta sono pronti a risorgere e a battersi di nuovo”

Erri De Luca

Foreword

The fulfilment of the research project addressed in this Thesis has involved the financial and intellectual support of many people and institutions, which the author sincerely acknowledges.

Most of the research activity that led to the achievements outlined in this Thesis has been developed at the Department of Chemical Engineering Principles and Practice of the University of Padova (DIPIC), under the supervision of Dr. 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.

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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

Zamboni, A.; F. Bezzo; N. Shah (2009). Spatially explicit static model for the strategic design of future bioethanol production systems. 2. Multiobjective environmental optimization. *Energy & Fuels*, **23**, 5134–5143.

Zamboni, A.; N. Shah; F. Bezzo (2009). Spatially explicit static model for the strategic design of future bioethanol production systems. 1. Cost minimization. *Energy & Fuels*, **23**, 5121–5133.

Franceschin, G.; A. Zamboni; F. Bezzo; A. Bertucco (2008). Ethanol from corn: a technical and economic assessment based on different scenarios. *Chemical Engineering Research & Design*, **86**, 488–498.

Papers Submitted for Publication in International Journals

Dal Mas, M.; S. Giarola; A. Zamboni, F. Bezzo (2009). Strategic design and investment capacity planning of the bioethanol supply chain under price uncertainty. *Biomass & Bioenergy*.

Publications/Abstracts in Conference Proceedings

Zamboni, A.; F. Bezzo; N. Shah (2009). Supply chain optimization for bioethanol production system in Northern Italy: Environmentally conscious strategic design. In: *Computer-Aided*

Chemical Engineering 27, 10th International Symposium on Process Systems Engineering, Elsevier, Amsterdam, Paesi Bassi, 2037–2042.

Dal Mas, M.; A. Zamboni, F. Bezzo (2009). Bioethanol production in Northern Italy: supply chain design and capacity planning under uncertainty. *17th European Biomass Conference & Exhibition – From Research to Industry and Markets, 29 June – 3 July*, Hamburg, Germany.

Zamboni, A.; N. Shah; F. Bezzo (2009). Analisi e ottimizzazione della filiera di produzione di etanolo da mais. In: *Atti Convegno GRICU 2008 – 14-17 Settembre 2008*, Le Castella (KR), Italia, 1389–1394.

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Franceschin, G.; M. Sudiro; A. Zamboni; F. Bezzo; A. Bertucco (2007). Energy and economic assessment of bioethanol production by a dry milling process. In: *AIDIC Conference Series Vol.8*, 141–150.

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Abstract

In the last decade, we have been assisting to a global redefinition of the world energy system. Firstly motivated by severe concerns about environmental health and global warming, it found its real impetus in a more complex question. Although commonly considered as tightly related to oil depletion, it is rather a multifaceted interconnection of different issues, which could be generally labelled as the supply security question, and of which the oil shortage represents a contributing part. Thus, asking when oil runs out is not the only question and definitely not the main concern related to energy supply. As wisely stated by the Sheikh Ahmad Zaki Yamani about thirty years ago, “the Stone Age did not end for lack of stone, and the Oil Age will end long before the world runs out of oil”. In our opinion, this intriguing prediction represents the hot-spot of the question: how vital is it for policy makers to accelerate the end of the oil age and how that might be achieved?

After a fierce debate centred on the most viable way to manage the transition, renewable energy sources were eventually indicated as a realistic alternative to the conventional fossil sources. In particular, biomass conversion into biofuels was promoted as the best suitable option within the transport sector. At the governmental level, ambitious policies were conceived to drive the transition toward the new frontier. For example, the EU commission was determinant in pushing its Members through the imposition of minimum blending quotas of biomass-based fuels within the conventional fossil-derived ones. The latest EU guidelines also fixed new environmental standards setting at 35% the minimum *Greenhouse Gas* (GHG) emissions savings to be performed by biofuels with respect to the fossil-based ones they are meant to substitute.

Among the possible choices to reach the targets, bioethanol is currently acknowledged as the most appropriate solution for a short-term gasoline substitution, although during its history has known some discredits and oppositions by both the public opinion and part of the academic community. The core of the question stands in whether the ethanol production is actually capable to give the right answer in terms of energy supply security (as global warming mitigation and market penetration).

Therefore, decision makers should be driven by specific tools capable of steering the design of the novel biofuels systems considering production costs and environmental impact minimisation (or profits and financial sustainability maximisation) as undisputed paradigms. They should also adopt wider approaches which go beyond the limited company-centric view of the business and extends the scope of the analysis at the entire *Supply Chain* (SC).

Very limited work was found in literature addressing the use of quantitative methodologies for the strategic design of biofuels infrastructures. Therefore, the research project was thought to cover this lack of knowledge through the development an original methodology to embody the *Supply Chain Management* (SCM) tools application and mathematical programming within a biofuels SCs optimisation framework.

Accordingly, the aim of this Dissertation was to contribute in providing for modelling tools capable of steering the design of first generation bioethanol SCs through a full set of optimisation features. The work focused on the development of *Mixed-Integer Linear Programming* (MILP) models to assist the policy-making on biofuels industry at strategic and tactical level. The final objective was to deliver a suitable design and planning tool based on the approaches commonly applied to SC strategic design and planning under economic, financial and environmental criteria. Agricultural practice, biomass supplier allocation (domestic or foreign), production site location and capacity assignment, logistic distribution and transport characterisation were simultaneously taken into account within the same modelling framework. This also included different features for spatially explicit siting of supply networks nodes, capacity planning and a stochastic formulation was implemented to handle the effect of market uncertainty. Finally, with concerns to the environmental impact of cultivation practice a further aspect was deepened by assessing and minimising the global warming effect of fertiliser application in cropping biomass. The economics of the entire network was assessed by means of *Supply Chain Analysis* (SCA) techniques, whereas the environmental performance of the system was evaluated in terms of GHG emissions, by adopting a *Well-to-Tank* (WTT).

The emerging Italian corn-based ethanol was chosen as a demonstrative real world case study so as to assess the actual model capabilities in steering strategic policies on different interest level.

Riassunto

Gli ultimi due decenni sono stati caratterizzati da profondi cambiamenti negli equilibri economici e geopolitici mondiali. Uno dei motori di questa trasformazione è stata sicuramente la crisi del sistema di approvvigionamento energetico globale, di cui riscaldamento globale e carenza di petrolio sono solo due delle molteplici sfaccettature. Il cuore della questione può essere riassunto da una dichiarazione dello Sceicco Ahmad Zaki Yamani (all'epoca presidente dell'OPEC), il quale, circa trent'anni fa, asserì che "l'Era della pietra non finì per la mancanza di pietra, così come l'Era del petrolio finirà molto prima che il mondo esaurisca il petrolio". La vera domanda, quindi, non è tanto quando il petrolio terminerà, ma in che termini agire nell'interpretare e guidare il profondo cambiamento in atto. Tutto ciò ha generato in tutto il mondo un acceso dibattito per stabilire quale fosse la via migliore per gestire la rivoluzione del settore energetico mondiale e individuare quelle risorse di energia rinnovabile in grado di rappresentare l'alternativa più plausibile al sistema di approvvigionamento tradizionale. Tra queste, l'utilizzo della biomassa per la produzione di combustibili liquidi è stata universalmente indicata come la miglior alternativa ai vettori fossili comunemente utilizzati nel settore dei trasporti.

Recentemente, la Commissione Europea ha assunto un ruolo determinante nell'incoraggiare gli Stati Membri all'adozione di programmi ambiziosi volti alla promozione dell'utilizzo di combustibili alternativi: questo si è tradotto in politiche di vario tipo, caratterizzate da un'immissione obbligatoria sul mercato di quote sempre maggiori di combustibili prodotti da biomassa. Standard europei ne regolano la qualità in modo da garantire il perseguimento degli obiettivi energetici e ambientali comunitari. In particolare, un requisito fondamentale è la capacità di riduzione delle emissioni del 35% rispetto alla produzione dello stesso quantitativo energetico di combustibile fossile che andranno a sostituire.

Tra le alternative possibili, il bioetanolo è generalmente considerato la soluzione più pratica e perseguibile (almeno in un'ottica di breve-medio periodo) per sostituire la benzina convenzionale. Nonostante alcuni evidenti vantaggi, vi sono, tuttavia, una serie di questioni di tipo economico, ambientale e di accettazione sociale che ne hanno sinora rallentato l'effettiva penetrazione nel mercato dei carburanti per autotrazione. Il nocciolo della questione è il dubbio se effettivamente il bioetanolo sia in grado di fornire la giusta risposta alle esigenze di sicurezza di approvvigionamento imposte dalla questione energetica. La risposta a questa questione impone l'adozione di strumenti quantitativi in grado di valutare le reali prestazioni del sistema di produzione. In particolare, questi strumenti dovrebbero essere pensati per fornire supporto tecnico a livello politico e manageriale per gestire e progettare i nuovi

sistemi di produzione di biocombustibili. Tali strumenti richiedono l'adozione di un approccio più esteso al problema che sia quindi in grado di estendere l'analisi all'intera filiera produttiva (*Supply Chain*, SC). La ricerca bibliografica ha evidenziato evidenti lacune in materia di progettazione strategica di infrastrutture produttive per biocombustibili e, in particolare, in termini di metodologie quantitative per affrontare il problema.

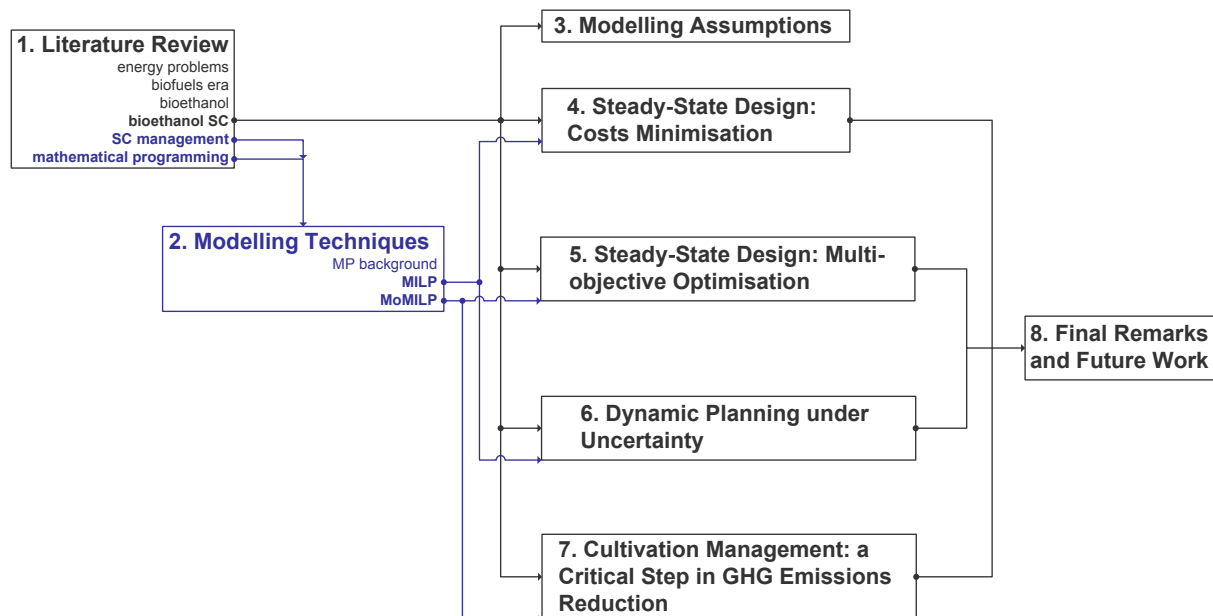
Il progetto di ricerca discusso in questa Dissertazione ha avuto come obiettivo quello di coprire questa lacuna e sviluppare una metodologia originale per l'accoppiamento di gestione delle SC (*Supply Chain Management*, SCM) e programmazione matematica. Il lavoro si è focalizzato sulla definizione di modelli a variabili miste lineari e intere (*Mixed-Integer Linear Programming*, MILP) per l'analisi di sistemi produttivi per il bioetanolo di prima generazione, in grado di essere utilizzati come efficaci strumenti di supporto alle politiche decisionali in materia di biocombustibili. L'obiettivo finale è quello di realizzare uno strumento di progettazione e pianificazione industriale basato sui comuni approcci alla progettazione strategica di filiere produttive, secondo criteri di tipo economico, finanziario e ambientale. I modelli MILP sono stati sviluppati e utilizzati per descrivere e ottimizzare la gestione delle fasi di lavorazione agricola per la produzione di biomassa, la strategia di approvvigionamento della stessa (produzione autarchica o importazione), la locazione e le dimensioni dei siti di produzione (di biomassa e biocombustibile), la distribuzione logistica e la tipologia del sistema di trasporti. Inoltre, la costruzione dei modelli è stata basata su una georeferenziazione delle variabili di progetto. Una formulazione di tipo stocastico è stata incorporata per gestire l'effetto dell'incertezza delle condizioni di mercato sulle prestazioni finanziarie. Infine, è stato approfondito un aspetto relativo all'impatto ambientale delle fasi agricole della catena produttiva così da minimizzare le emissioni di gas serra derivanti dall'impiego di fertilizzanti azotati.

Gli aspetti economici dell'infrastruttura produttiva sono stati valutati mediante approcci di analisi della filiera di produzione (*Supply Chain Analysis*, SCA), mentre le prestazioni ambientali del ciclo produttivo sono state stimate attraverso un approccio di analisi del ciclo di vita (*Life Cycle Analysis*, LCA) di tipo *Well-to-Tank* (WTT). I modelli sviluppati sono stati applicati per studiare la possibile organizzazione della produzione di bioetanolo da mais in Nord Italia.

La struttura della Tesi esposta segue lo schema logico riportato nella Figura seguente.

Nel primo Capitolo sono presentate le basi bibliografiche del progetto di ricerca. Partendo dall'analisi delle problematiche principali che riguardano le recenti crisi del sistema di approvvigionamento energetico globale, il lettore è accompagnato attraverso un percorso che porta alla descrizione delle principali soluzioni prospettate per risolvere il problema in un contesto più specifico, che è quello del settore dei trasporti. In particolare, la produzione di biocombustibili viene analizzata ponendo particolare attenzione al bilancio tra pro e contro emersi nel valutare le sue effettive potenzialità nel sostituire la produzione di combustibili

tradizionali. Si passa poi ad un'analisi bibliografica focalizzata sulla produzione di bioetanolo mediante tecnologie di prima generazione, volta a porre in luce i principali problemi da affrontare al fine di realizzare gli obiettivi europei in materia di biocombustibili.



Il Capitolo 2 è dedicato alla descrizione dello stato dell'arte della programmazione matematica e a fornire una base teorica per la formulazione di modelli di ottimizzazione di SC. Sono qui presentati gli approcci algoritmici al SCM, dando un rilievo particolare alla formulazione matematica di modelli di tipo MILP e alla costruzione logica degli algoritmi di soluzione. Infine, sono approfondite alcune tecniche specifiche come la programmazione matematica multi-obiettivo (*Multi-objective Mathematical Programming, MoMP*) e l'ottimizzazione di tipo stocastico.

Il Capitolo 3 conclude la parte introduttiva della Dissertazione. In questo Capitolo, infatti, sono dichiarate le principali ipotesi relative al modo di affrontare sia la progettazione dei sistemi di biocombustibili, sia la costruzione dei modelli matematici per l'ottimizzazione degli stessi. Viene presentata una descrizione generale delle principali componenti della catena produttiva di bioetanolo e sono discussi i criteri di valutazione economica e ambientale dei nodi della filiera. Il riferimento è il caso reale considerato in questo studio, ovvero la produzione di bioetanolo da mais in Nord Italia.

Nel Capitolo 4 si affronta il primo problema di progettazione. Questo prevede lo sviluppo di un modello MILP stazionario e georeferenziato per la progettazione strategica di SC di bioetanolo secondo un criterio di minimizzazione dei costi operativi. Vengono descritti i principali problemi legati alla progettazione del sistema e la formulazione matematica proposta per il modello di ottimizzazione. Il modello costruito viene poi applicato all'analisi del caso studio reale descritto al Capitolo 3.

Il Capitolo 5 tratta lo sviluppo di modelli di ottimizzazione ambientale. Il modello MILP descritto nel Capitolo 4 è preso come base per l'implementazione di criteri di ottimizzazione ambientale considerati contemporaneamente a quelli di tipo economico attraverso tecniche MoMP. Sono prese in considerazione differenti soluzioni per lo sfruttamento dei sottoprodotti del processo di produzione di bioetanolo come possibili alternative tecnologiche per l'abbattimento di costi ed emissioni.

Nel Capitolo 6 viene presentato un ulteriore sviluppo del modello al fine di renderlo adatto alla pianificazione degli investimenti a lungo termine e a gestire il rischio d'investimento dovuto all'incertezza delle condizioni di mercato. Si descrive, pertanto, lo sviluppo di un modello MILP di tipo dinamico e stocastico per l'analisi finanziaria e la riduzione del rischio d'investimento nella pianificazione della produzione di bioetanolo. L'implementazione al caso studio si focalizza sull'analisi delle dinamiche di mercato con riferimento ai costi d'acquisto della biomassa e ai prezzi di vendita di etanolo e sottoprodotti.

Il Capitolo 7 descrive lo sviluppo di un ulteriore modello matematico per il miglioramento delle prestazioni ambientali del sistema produttivo in esame, al fine di allinearne le performance agli standard europei in materia di emissioni di gas serra. Un modello di tipo MILP è concepito per l'ottimizzazione delle pratiche agricole (in particolare dell'utilizzo di fertilizzanti azotati) e delle tecnologie di sfruttamento dei sottoprodotti secondo criteri di tipo ambientale e finanziario. Il modello sviluppato è applicato per la massimizzazione del profitto e la minimizzazione delle emissioni di gas serra della produzione di etanolo da mais.

Il Capitolo 8 conclude la discussione della ricerca sviluppata con la presentazione dei principali risultati conseguiti e l'analisi di alcuni dei potenziali sviluppi futuri per proseguire la ricerca sull'argomento.

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List of Symbols

Acronyms

<i>CHP</i>	Combined Heat and Power
<i>CVaR</i>	Conditional Value-at-Risk
<i>CY</i>	Corn Yield
<i>DDGS</i>	Distiller's Dried Grains with Solubles
<i>DDGSY</i>	Distiller's Dried Grains with Solubles Yield
<i>DGP</i>	Dry-Grind Process
<i>EC</i>	European Commission
<i>eNPV</i>	expected Net Present Value
<i>ETBE</i>	Ethyl Ter-Butyl Ether
<i>EU</i>	European Union
<i>EWO</i>	Enterprise-wide Optimisation
<i>EY</i>	Ethanol Yield
<i>FCF</i>	Free Cash Flow
<i>GDP</i>	Gross Domestic Product
<i>GMO</i>	Genetically Modified Organism
<i>GHG</i>	Greenhouse Gas
<i>GIS</i>	Geographic Information System
<i>GrSCM</i>	Green Supply Chain Management
<i>GWP</i>	Global Warming Potential
<i>LCA</i>	Life Cycle Analysis
<i>LP</i>	Linear Programs

<i>LPG</i>	Liquid Propane Gas
<i>MARR</i>	Minimum Accepted Rate of Return
<i>MIP</i>	Mixed Integer Programming
<i>MILP</i>	Mixed Integer Linear Programming
<i>MINLP</i>	Mixed-Integer Non-Linear Programming
<i>MoMP</i>	Multi-objective Mathematical Programming
<i>MoMILP</i>	Multi-objective Mixed Integer Linear Programming
<i>MP</i>	Mathematical Programming
<i>MTBE</i>	Methyl Ter-Butyl Ether
<i>ND</i>	Nitrogen Dosage
<i>NLP</i>	Non-Linear Programs
<i>NPV</i>	Net Present Value
<i>TI</i>	Total Impact
<i>OECD</i>	Organisation for Economic Cooperation and Development
<i>PSE</i>	Process Systems Engineering
<i>PY</i>	Protein Yield
<i>ROI</i>	Return On Investment
<i>SC</i>	Supply Chain
<i>SCA</i>	Supply Chain Analysis
<i>SCM</i>	Supply Chain Management
<i>SMrepl</i>	Soy-Meal replacement factor
<i>SSF</i>	Simultaneous Saccharification and Fermentation
<i>SY</i>	Starch Yield
<i>TTW</i>	Tank-To-Wheel
<i>VOC</i>	Volatile Organic Compounds

WTT Well-To-Tank

Sets

$b \in B$	set of burdens (CO ₂ , CH ₄ , N ₂ O)
$d \in D$	internal depots (distribution centres)
$g \in G$	set of square regions
$g' \in G$	set of square regions different than g
$i \in I$	set of products (biomass, biofuel)
$k \in K$	set of DDGS end-use options (soy-meal substitute, CHP fuel)
$l \in L$	set of transport modes (truck, rail, barge, ship or trans-ship)
$n \in N$	set of nitrogen dosages
$p \in P$	set of plant size intervals
$q \in Q$	set of corn purchase cost scenarios
$r \in R$	set of bioethanol market price scenarios
$s \in S$	set of life cycle stages
$t \in T$	set of time periods
$FTL_{i,g,l,g'} \subseteq L, \quad \forall i, g \text{ and } g'$	subset of feasible transport links for each product i via mode l between g and g'
	$FRL_{i,g,l,g'} = (i,g,rail,g') \Leftrightarrow g$ can be connected with g' by rail
	$FBL_{i,g,l,g'} = (i,g,barge,g') \Leftrightarrow g$ can be connected with g' by barge
	$FSL_{i,g,l,g'} = (i,g,ship,g') \Leftrightarrow g$ can be connected with g' by ship
	$FTSL_{i,g,l,g'} = (i,g,t-ship,g') \Leftrightarrow g$ can be connected with g' by t-ship

$Local_{i,g,l,g'} \subseteq L, \forall i, g$ and g' feasibility limitation of local transport links for each product i via mode l between g and g'

$$Local_{i,g,l,g'} = (i,g,l,g') \Leftrightarrow LD_{gg'} < 72 \text{ km}$$

$Total_{i,g,l,g'} \subseteq L, \forall i, g$ and g' total transport links allowed for each product i via mode l between g and g'

$$Total_{i,g,l,g'} = (i,g,l,g') = Local_{i,g,l,g'} + FTL_{i,g,l,g'}$$

$worst_{q,r} \subseteq q \cup R, \forall q$ and r combination representing the most unprofitable market scenarios that occur with a 10% confidence level.

$$worst_{q,r} = (q,r) = \{(2,1),(3,2),(4,3),(3,1),(4,1),(4,2)\}$$

Scalars

α	network operating period [d/y]
CCF	capital charge factor [y^{-1}]
DW	driver wage for tankers [€/h]
FD	fuel demand of tankers [km/L]
FP	fuel price [€/L]
γ	biomass conversion factor [$t_{\text{biofuel}}/t_{\text{biomass}}$]
GE	general expenses of tankers [€/d]
LA	land availability [ha]
LUT	load/unload time of tankers [h/trip]
M	maximum profit value, s.t. $M \gg PBT$
ME	maintenance of tankers [€/km]
MPd	DDGS market price [€/t]
MPe	market price of ethanol [€/t]
σ	DDGS production factor [$t_{\text{DDGS}}/t_{\text{biofuel}}$]

SP	average speed of tankers [km/h]
$SusP$	maximum percentage of domestic biomass suitable for fuel production
$TCap$	capacity of tankers [t/trip]
$TCap^*$	capacity of transport mode for local biomass transfer [t/trip]
TMA	availability of tankers [h/d]
$Trate$	tax rate
UTC^*	unit transport cost for local biomass transfer [€/tkm]
$UTCb$	unit transport cost for biomass supply [€/t]
$UTCe$	unit transport cost for ethanol distribution [€/t]
ζ	interest rate [%]

Parameters

AD_g	arable land density within region g [$\text{km}^2_{\text{arable land}}/\text{km}^2_{\text{region surface}}$]
BCD_g^{\max}	maximum cultivation density in region g [$\text{km}^2_{\text{cultivation}}/\text{km}^2_{\text{arable land}}$]
BCD_g^{\min}	minimum cultivation density in region g [$\text{km}^2_{\text{cultivation}}/\text{km}^2_{\text{arable land}}$]
c_{bs}	emission coefficient of burden b at stage s [unit of b /unit of reference flow]
CF_g	domestic biomass cultivation sites (binary parameter)
CI_k	capital investment for establishing production plants with DDGS end-use solution k [€]
CY_g	cultivation yield within square region g [$\text{t}_{\text{biomass}}/\text{d}\cdot\text{km}^2$]
d_b	damage factor for each burden b [$\text{kg CO}_2\text{-eq}/\text{unit of } b$]
δ_n	DDGS yield when a nitrogen dosage n is applied [$\text{t}_{10\%m}/\text{t}_{DM}$]
$DD_{d,g}$	delivery distance between terminals and drop zones [km]
DEM_g	fuel demand for each region g [t/d]

ε_t	discount factor at time t
$etperc_t$	ethanol market penetration value in mass percentages at the time t
εCap_t	discount factor for couples of equal cash flow at the time t
εFCC_t	discount factor for capital costs at the time t
$f_{ec,n,k}$	emissions credits coming from soy-meal replacement when a nitrogen dosage n is applied and DDGS is used as valuable alternative k
f_s	global emission factor for stage s [kg CO ₂ -eq/unit of reference flow]
γ_n	alcohol yield when a nitrogen dosage n is applied [t _{EiOH} /t _{DM}]
GS_g	square region g surface [km ²]
GY_n	grain yield per hectare when a nitrogen dosage n is applied [t _{DM} /ha]
inY_t	initialisation array for cost allocation of the starting SC at the time $t = 1$
$LD_{g,g'}$	local delivery distance between grids g and g' [km]
μ_n	soy-meal replacement factor when a nitrogen dosage n is applied [t _{sm} /t _{10%<i>m</i>}]
$MPd_{n,k}$	DDGS market price [€/t] when a nitrogen dosage n is applied and DDGS is used as valuable alternative k
MPe_r	ethanol market price in the scenario r [€/t]
ND_n	nitrogen dosage value related to the interval n .
$Q_{i,l}^{max}$	maximum flow rate of product i by transport mode l [t/d]
$Q_{i,l}^{min}$	minimum flow rate of product i by transport mode l [t/d]
$\pi_{q,r}$	probabilities of 16 (q,r) scenarios [%]
$PCap_p^{max}$	maximum biofuel production capacity of plant size p [t/d]
$PCap_p^{min}$	minimum biofuel production capacity of plant size p [t/d]
PCC_p	capital cost of establishing conversion plants of size p [€]

$\tau_{l,g,g'}$	tortuosity factor of transport mode l between g and g'
$TCap_{i,l}$	capacity of transport mode l for product i [t/trip]
$TCap^*$	capacity of transport mode for local biomass transfer [t/trip]
THR_d^{\max}	max terminal throughput allowed [t/d]
$UCRd_{n,k}$	costs reduction per unit of DDGS when used as valuable alternative k and related to a nitrogen dosage n [€/t _{10%m}]
$UPCb_g$	unit production costs for biomass in region g [€/t]
$UPCb_n$	unit production costs for biomass when a nitrogen dosage n is applied [€/t _{BM}]
$UPCc_q$	unit purchase costs for biomass in the scenario q [€/t]
$UPCe_n$	unit production costs for ethanol when a nitrogen dosage n is applied [€/t _{EtOH}]
$UPCe_p$	unit production costs for biofuel through plants of size p [€/t]
$UPCf_p$	unit production costs for biofuel through plants of size p [€/t]
$UTC_{l,i}$	unit transport cost for product i via mode l [€/tkm]
$\omega_{n,k}$	exceeding electric power per unit of DDGS produced [kW/t _{10%m}] when a nitrogen dosage n is applied and DDGS is used as alternative k

Continuous variables

$ADD_{t,g,g'}$	actual delivery distance between grids g and g' via mode t [km]
BC	annual by-products allocation credits [€]
BPC	corn production annual costs [€]
D	depreciation charge [€]
$D^I_{i,g}$	imported demand for product i in region g [t/d]
$D^L_{i,g}$	demand for product i in region g satisfied by local production [t/d]

$D_{i,g}^T$	total demand for product i in region g [t/d]
$D_{i,g,t,q,r}^{imp}$	demand for product i in region g at time t for scenario (q,r) satisfied by importations [€/month]
$D_{i,g,t,q,r}^{loc}$	demand for product i in region g at time t for scenario (q,r) satisfied by local production [€/month]
$D_{i,g,t,q,r}^{tot}$	total demand for product i in region g at time t for scenario (q,r) [€/month]
$DEM_{fuel,g,t,q,r}$	actual market demand for ethanol in region g at period t and scenario (q,r) [€/month]
$DEMT_d$	actual fuel demand at terminal d [t/d]
DNI	discounted net incomes [€]
EPC	ethanol production annual costs [€]
F_s	reference flow for stage s [units/d]
FC	fuel costs for blended fuel delivery [€/d]
FCC	facilities capital costs [€]
FCC_t	facilities capital costs at time t [€/y]
$FOC_{t,q,r}$	facilities operating costs at time t for scenario (q,r) [€/month]
GC	general costs for blended fuel delivery [€/d]
I_s	daily impact for stage s [kg CO ₂ -eq/d]
LC	labour costs for blended fuel delivery [€/d]
MC	maintenance costs for blended fuel delivery [€/d]
NPV	net present value [€]
$NPV_{q,r}$	net present value of the scenario (q,r) [€]
Obj_{NPV}	expected net present value [-€]

Obj_{CVar}	conditional value-at-risk [-€]
Obj_{NPV}	net present value [-€]
Obj_{TDI}	total daily impact [kg CO ₂ -eq/d]
$P_{i,g}^T$	production rate of product i in region g [t/d]
$P_{i,g,t,q,r}^{tot}$	production rate of product i in region g at time t for scenario (q,r) [€/month]
$Pb_{n,k}$	total production of biomass [t/y] when a nitrogen dosage n is applied and DDGS is used as valuable alternative k
PBT	profit before taxes [€]
$PBT_{t,q,r}$	profit before taxes at time t for scenario (q,r) [€/y]
PC	production operating costs [€/d]
$Pd_{n,k}$	total production of DDGS [t/y] when a nitrogen dosage n is applied and DDGS is used as valuable alternative k
$Pe_{n,k}$	total production of ethanol [t/y] when a nitrogen dosage n is applied and DDGS is used as valuable alternative k
$Pf_{p,g}$	biofuel production rate through plants of size p in region g [t/d]
$Pf_{p,g,t,s,r}$	biofuel production rate through plants of size p in region g at time t for scenario (s,r) [€/month]
$PPot_g$	potential domestic biomass production for each region [t/d]
$Q_{d,g}$	fuel flow rate from terminal d to drop zone g [t/d]
$Q_{i,g,l,g'}$	flow rate of product i via mode l between g and g' [t/d]
$Q_{i,g,l,g',t,q,r}$	flow rate of product i via mode l between g and g' at time t for scenario (q,r) [€/month]
TAR	total annual revenues [€]
$TAR_{t,q,r}$	total annual revenues at time t for scenario (q,r) [€/y]

TAX_t	production operating costs [€]
TC	transport costs [€/d]
$TC_{t,q,r}$	transport costs at time t for scenario (q,r) [€/month]
TCI	total capital investment [€]
TD_i	total demand of product i [t/d]
$TD_{i,t,q,r}$	total demand of product i at time t for scenario (q,r) [€/month]
TDC	total daily operating and capital costs [€/d]
TDI	total daily impact [kg CO ₂ -eq/d]
TI	total impact [kg CO ₂ -eq]
TOC	transportation operating costs for blended fuel delivery [€/d]
$TOC_{t,q,r}$	total operating costs at time t for scenario (q,r) [€/y]
TP_i	total production of product i [t/d]
$TP_{i,t,q,r}$	total production of product i at time t for scenario (q,r) [€/month]
$TPot$	total potential domestic biomass production [t/d]

Integer variables

$NTU_{i,l,g,g'}$	number of transport units of mode l for product i between g and g'
$NTU_{i,g,l,g',t,q,r}$	number of transport units of mode l for product i between g and g' at time t for scenario (q,r)
NTU_l	number of local transport units for biomass within region g
$NTU_{l,g,t,q,r}$	number of local transport units for biomass within region g at time t for scenario (q,r)

Binary variables

V_t	1 if taxation has to be applied at time t , 0 otherwise
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$W_{n,k}$	1 if a nitrogen dosage n is applied and a DDGS end-use k is adopted, 0 otherwise
$X_{i,g,l,g',t,q,r}$	1 if product i is to be shipped from region g to g' by means of mode l at time t for scenario (q,r) , 0 otherwise
$X_{i,g,l,g'}$	1 if product i is to be shipped from region g to g' by means of mode l , 0 otherwise
$Y_{p,g}$	1 if a conversion facilities of size p is to be established in region g , 0 otherwise
$Y_{p,g,t}$	1 if a conversion facilities of size p is to be established in region g at the time t , 0 otherwise
$Y_{p,g,t}^{plan}$	1 if the establishment of a new conversion facilities of size p is to be planned in region g during time period t , 0 otherwise
$Y_{p,g}^{start}$	1 if a conversion facility of size p is established in region g in the starting SC configuration, 0 otherwise
$Z_{d,g}$	1 if drop zone g is to be served by terminal d , 0 otherwise

Chapter 1

Literature Review

The objective of the discussion presented in this Chapter is to provide a motivational and literature background to the research project. Core drivers, limitations and key challenges of the European energy system are presented to the readers, with a particular view on fuel supply in the transport sector. The current status of biofuels production as conventional fuels substitutes and the main shadows on the future development are debated here, together with the most promising solutions over the short and medium-long term. Next, a review of the main literature on matter of bioethanol is reported, focusing the attention on the main drawbacks affecting the first generation production as well as the best technological pathway to achieve the European goals on biofuels. Successively, an overview of the engineering approach developed to overcome the question raised in the discussion is presented. Particular focus is dedicated to the mathematical programming tools devised by the *Process Systems Engineering* community. Finally, motivation and aim of the project are declared in relation to the background issues emerged from the previous discussion.

1.1 Energy outlook

Without any doubt, energy is the driving force in all natural phenomena. Every human being and actor of our ecosystem exists and evolves by unconsciously feeding on several energy sources at different levels so as to pursue its personal growth. As a consequence, energy provision is, as it has always been, the core business for each society as it evolved through the history.

Since the human civilization took shape, man has been able to improve and expand his energy consumption: wood combustion provided heat and fossil fuels in form of oil were used for lightning, while wind, water and draught animals provided mechanical energy (Sørensen, 1991). This energy system mainly based on renewable sources was progressively displaced as the industrial revolution broke through in the 19th century. The following advent of the steam engine and the steady boom of coal consumption soon took over the conventional way to produce energy with the renewable sources losing out under the fierce competition of cheaper and higher-quality new forms of energy. Not only costs and a higher energy density had been

determining this transition toward solid fossil fuels. Also the intermittence of energy supply through sun and wind led to the end of the game now asking for a more stable degree of provision. Another radical change of course occurred with the discovery of oil: its higher energy density, a lower carbon-to-hydrogen ratio as well as its very adaptability to cheaper and easier way of transport (e.g. pipelines and tanks) determined a progressive shift away from coal to more suitable fluid fuels. Thus, oil became the world's dominant energy source by the middle 20th century (Ausubel, 2000). All the mentioned issues together with the great versatility of oil as raw material for chemicals production did let suppose the beginning of a new golden era with oil playing the undisputed leading part on the world energy stage.

However, pretty soon it came to light the first sign of a deep lack of stability in the energy system as conceived: the oil shocks of the 1970s revealed the heavy dependence of energy supply on unreliable producers and determined a substantial weakening of the tight link between energy consumption and economic growth that generated a global debate on energy security (Goldemberg *et al.*, 2001). Hence, the inherent structure of an energy system mainly relying on importations was brought into question. As a consequence, the ensuing challenge of trying to change the current paradigm brought out a wide range of alternative solution to provide energy in all its forms, also reformulating the interests on renewable conversion techniques. However, as the crisis phased out and the fear faded all these viable solutions were set aside and the world economy shifted back to the former energy supply system. There had been several reasons behind this step back: the major are the cost of any of the new alternative not even getting close to compete with fossil fuels; besides, the transient nature of the crisis posed certain limitations on the way to think about the future perspective of energy question.

However, recent implications regarding the energy question have been calling back upon a permanent shift of paradigm ruling a global redefinition of the energy system. Renewed issues about security on oil supply and the ever greater demand of fossil source of energy from developing countries along with more recent concerns on global warming (and environmental pollution in general) have been pushing the world community to put into focus alternative energy systems: economical, environmental and social criteria have been, hence, put together to formulate a new way to conceive the global energy system not only as a paradigm of today but also as a must-do for the future.

1.1.1 *The energy supply question*

The current status of the energy supply is quite problematic as the global revolution evolves. The energy supply question is on the top of the world policy agenda and a thorny debate is still open on the most viable way to manage the transition. In order to better understand the question, it is worth looking back to the roots of the problem so as to throw light on the present situation and onto the range of solutions proposed for the near future.

Possibly, the core of the problem brings back to the age-old question of the market imbalance between energy demand and supply capabilities. In particular, in dealing with energy demand there are several factors that affect its trends in a single country as well as across the world. Population and *Gross Domestic Product* (GDP) are probably the two major drivers of demand growth. Concerning with global population, it has known a global increase of 66% since the early 1970s so as to reach over 6.6 billion people. Over the same time period, global GDP grew by 167%, twice as much as the increase in population (IEA, 2009). According to the existing link between energy and GDP (Reister, 1987), the abovementioned trend reveals an unrelenting ascent of energy consumption over the last years that is doomed to continue in the future. As a consequence, although the world economy has become less energy intensive (an average increase of 1.5% per year in the global GDP per capita has been followed by a 0.5% per year increase in energy supply per capita), the world energy consumption is expected to grow by 44% over the 2006 to 2030 period (EIA, 2009), as illustrated in Figure 1.1.

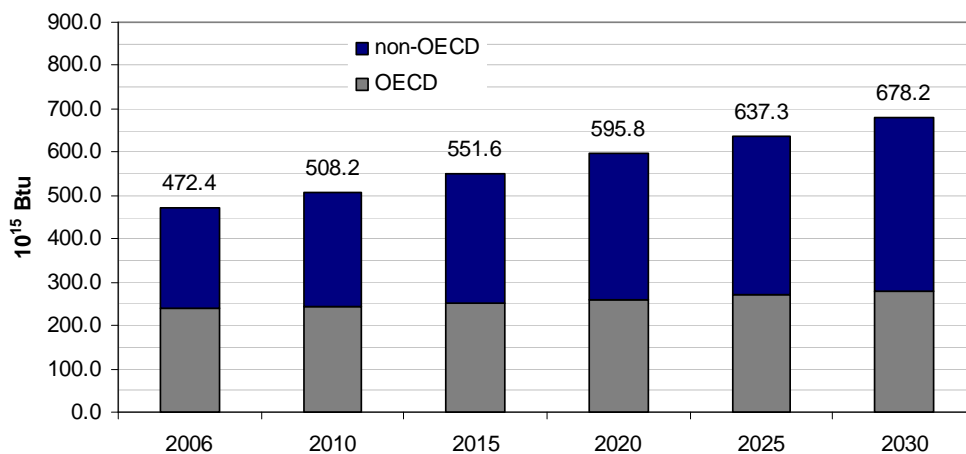


Figure 1.1 World total energy consumption, 2006-2030 (EIA, 2009).

Energy consumption will slowly grow (2.2%) in the nations belonging to the Organisation for Economic Cooperation and Development-OECD (including among the others North America, Mexico, Europe and Asia) but it will soar (4.9% per year) in the non-OECD countries (China and India) in order to feed the growing trend. Even considering the effect of the current world-wide economic downturn still dampening the demand for energy, the upcoming return to the normal standard, as anticipated after 2010, will spark again the usual growth trend in income and in energy demand.

So far, global energy needs have been mainly supplied by harnessing fossil fuels (liquid fuels and other petroleum, natural gas and coal) as primary energy source. As Figure 1.2 reports, among the suitable alternatives, liquids (mainly oil derived gasoline and diesel but also a quite small part of biofuels) are expected to provide the largest share of world energy consumption over the projection period, although the slight decrease of their share quota from 40% in 1990

to 32% in 2030 (EIA, 2009). In particular, this quota is almost totally meant to supply the needs of transport sector, which is also accounting for the largest increment (about 80% of the total) in total liquid demand as projected by 2030: indeed, about the 70% (EIA, 2009) of the world oil flow is used up to fuel automotive vehicles. In light of this, it is easy to understand how oil consumption is estimated to grow from 85 million to about 107 million of barrels per day over the 2006-2030 time period.

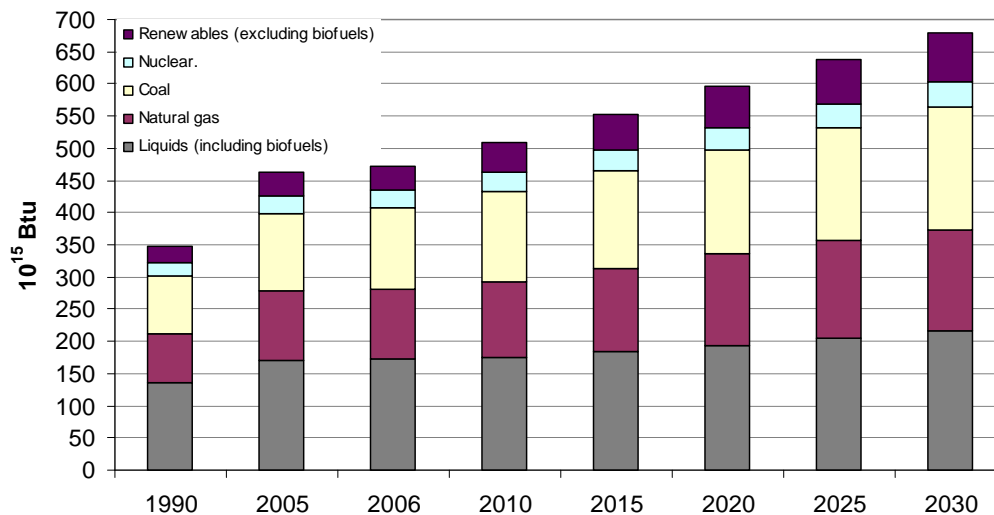


Figure 1.2 World total energy consumption by fuel source, 1990-2030 (EIA, 2009).

Unfortunately, oil is not an endless good and recent concerns about its actual availability have been alerting the world community. For over 50 years a lot of studies have been focusing on the longevity of petroleum reserves although none of them can be deemed as the “definitive” prediction on the peak of oil production (as evident from the diagram depicted in Figure 1.3) (ASPO International: www.peakoil.net).

As a consequence, this great uncertainty on future oil reserves as well as the geopolitical unreliability of many producers region have been contributing to characterise an uncertain global scenario that has thereby progressively affected the oil price, which has skyrocketed in the last few years only partially dampened by the recent economic crisis (Figure 1.4 (Data 360: www.data360.org)).

In addition to this, severe concerns about environmental health and global warming have recently come into play: in particular, GHG emissions resulting from the continuous use of fossil energy sources are projected to increase the carbon dioxide concentration in the atmosphere by 50% by 2020 (Service, 2004). This would worsen an already concerning situation in which the carbon dioxide level of 370 ppm has been deemed to be responsible for the 0.6°C rise in the average global surface temperature since the 19th century (where the CO₂ level was about 280 ppm) (Service, 2004).

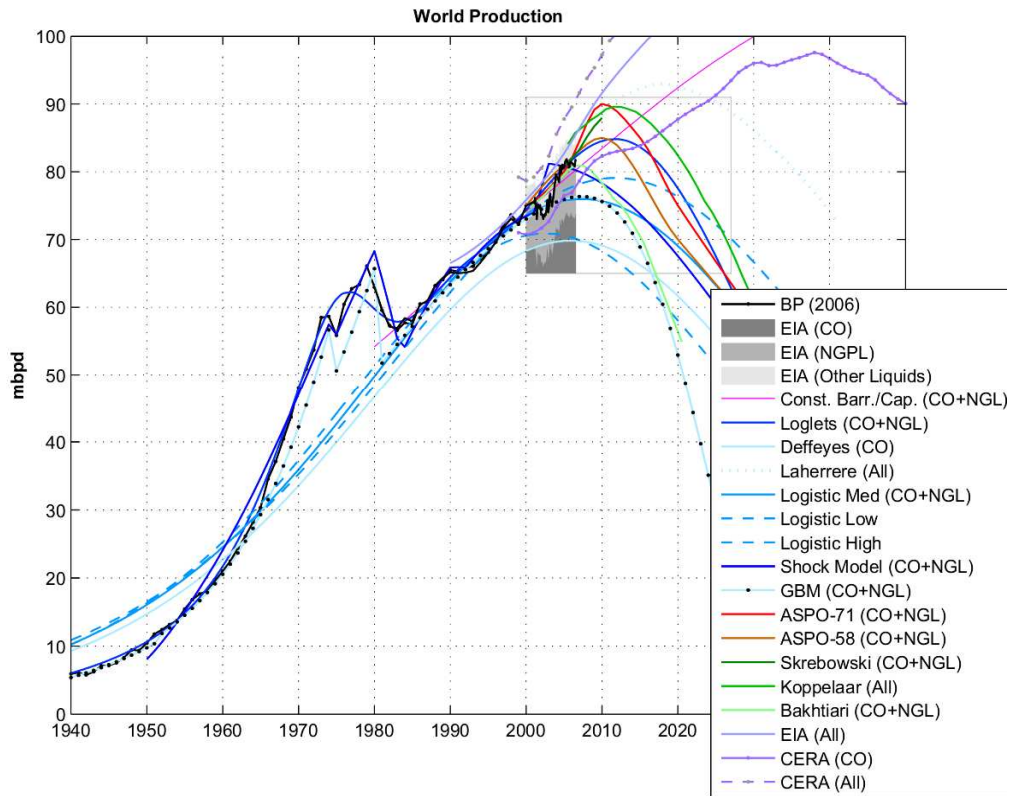


Figure 1.3 Predictions on the peak of oil production according to different studies (ASPO International: www.peakoil.net).

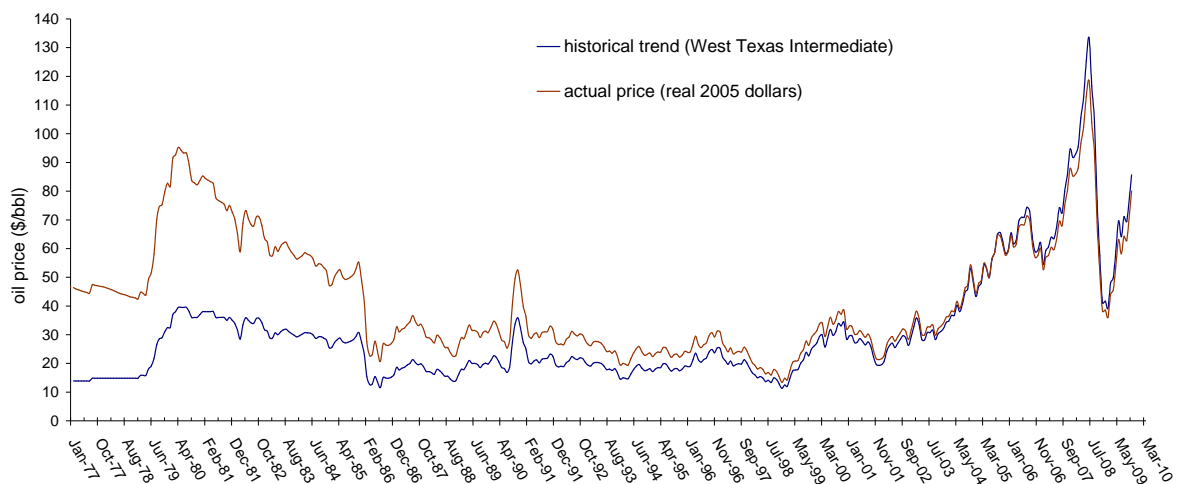


Figure 1.4 Spot oil price: historical trend vs. actual price (Data 360: www.data360.org).

All these issues meet together within the label of the energy supply security question. Accordingly, a viable solution cannot overcome the problem by only relying on the future possibility to find out new undiscovered oilfields and neither can it be extemporaneous and fragmented. Thus, it poses the necessary challenge to drive society toward a gradual release from the conventional reliance on fossil fuels, oil *in primis*, by adding new sources to the existing energy supply options. This target would allow achieving for both supply security and global warming mitigation if met through a well-thought traded-off set of different solutions aiming at renewability as well as certain reduction of carbon dioxide emissions. It is essential, then, for the world community to address this major energy challenge, incorporating different issues such as climate change, increasing dependence on oil imports as well as the access for all users to affordable and secure energy.

Renewable energy sources (i.e. hydropower, solar, wind, geothermal, and biomass) have been acknowledged as the most realistic alternative in a bid to spark a new industrial revolution that will deliver a low-energy economy, whilst making the energy we do consume more secure, competitive and sustainable. Their use would help reducing GHG emissions, diversifying energy supply and reducing our dependence on unreliable and volatile fossil fuel markets (in particular oil and gas). The growth of renewable energy sources might also stimulate employment in the industrial sector, the creation of new technologies so as improving our trade balance.

Among the other renewables, biomass has been encountering particular interest due to its versatility: energy plants (oilseeds, plants containing sugars) and forestry, agricultural or urban waste including wood and household waste can be used as suitable option not only in providing electric, mechanical and thermal energy, but also as a primary source to produce liquid biofuels for automotive purposes. The use of biomass can significantly contribute to reduce GHG emissions: in fact, the carbon dioxide it gives off when it is burned is traded-off by the amount absorbed when the plant was grown. However, generating net GHG savings tightly depends on the cultivation practice as well as on the fuel production processes in use.

1.1.2 *Energy policies*

In this still vague energy scenario, governments, private firms and research centres have been called to translate the new shift of paradigm into a well-advised policy steering the pathway from the conventional system towards a sustainable one. The EU Commission (EC, 2003), for instance, has been determinant in driving its Members to a general effort to comply with the commitments on climate change firstly pointed out by the Kyoto protocol. The new Directive (EC, 2009) on renewable energy set ambitious targets for all the EU Members aiming at reaching a 20% share of energy from renewable sources by 2020 and a 10% share of renewable energy in the transport sector.

The transport sector, indeed, has been addressed as one of the key issues within the energy agenda, accounting for the 67% of the overall oil consumption (EC, 2002) and being responsible for 21% of all GHG emitted in the European Union (EC, 2004). The so called Biofuels Directive (EC, 2003) and the following EU guidelines (EC, 2007) firstly set a compulsory minimum blending quota of biomass-based fuels at 2% by energetic content of the total conventional fossil-derived ones. That minimum level has been then required to increase to 5.75% in 2010 and up to the aforementioned 10% level by 2020. According to the latest EU standards laid out during the European Council held in Brussels in December 2008, biomass-based fuels are also required to cause a minimum of 35% (Londo *et al.*, 2009) (percentage that should increase up to 50% in 2017) GHG emissions savings. Following the Commission's Biomass Action Plan (EC, 2005), several Member States have also produced their own national action plans. Italy, for example, has complied with EU guidelines by setting the minimum blending fraction at 3% by energetic content for 2009 and 5.75% for 2010 (Italian Government, 2007).

1.2 The biofuels era

In view of the above, it appears that the global energy system will be shifting away from a fossil-based provision toward a more composite system where renewables and, in particular, biomass will play a crucial role. Within the transport sector (in particular road transport), notoriously exhibiting several limitations due to its intrinsic need for liquid energy carriers, biofuels have been indicated as one of the most promptly available options answering to the global energy supply question (Solomon and Johnson, 2009). Converting biomass crops into liquid fuels allows for air quality improvements (i.e., reduction of CO and VOCs emissions) as well as global warming mitigation by capturing into biomass a carbon-free and unlimited energy source such as solar energy. Furthermore, biomass may ensure a gradual release from oil dependence and a fair degree of supply security through a certain reduction of the import bill as well as through supplier and technology diversification. Eventually, the establishment of a biomass based fuel system can lead to a positive effect for the local economy by stabilizing the agricultural sector as well as by offering new development opportunities (Dunnett *et al.*, 2008).

Biofuels properly refer to liquid or gaseous fuels for the transport sector that are predominantly produced from biomass (Demirbas, 2008). A wide range of fuels can be produced from biomass resources including liquid vectors, such as ethanol, methanol, biodiesel, Fischer-Tropsch diesel, and gases, such as hydrogen and methane. In these years, a lot of interest has been directed toward the development of feasible solutions to convert biomass into suitable energy carriers, also drawing on the precious know-how dating back to past history. Therefore, already existing technologies have been adopted and brand new ones

devised and then deeply assessed as suitable alternative to oil-based fuels. This did result in a large number of feasible options each one harnessing different biomass as well as suitable in different forms and mixtures within the conventional fuels. Liquid biofuels that have been developed and then broadly used so far, may be classified according to the following product categories: (i) alcohols; (ii) vegetable oils, Fischer–Tropsch diesels and biodiesels; and (iii) biogasoline, bio-oils and bio-synthetic oils. Another useful classification is based on the technology applied to produce biofuels. The feedstock typology is also an important way to classify biofuels (Table 1.1 (Demirbas, 2009a)).

Table 1.1 *Classification of biofuels based on their production technology (Demirbas, 2009a).*

Generation	Feedstock	Example
First generation	Sugar, starch, vegetable oils, or animal fats	alcohols, vegetable oil, biodiesel
Second generation	Non-food crops, cereals straw, wood, solid waste, energy crops	alcohols, bio-oil, Fischer–Tropsch diesel
Third generation	Algae	Vegetable oil, biodiesel
Fourth generation	Vegetable oil	Biogasoline

First generation options include biofuels made from sugar, starch (i.e. bioethanol), vegetable oils, or animal fats (i.e. biodiesel) using conventional technology. They are usually limited in their ability to achieve targets for oil-product substitution, climate change mitigation, and economic growth (except for bioethanol from sugar cane), because their performance strictly depends on the technological and geographical context they refer to. Second generation biofuels harness a wider range of suitable feedstocks such as lignocellulosic materials including cereal straw, forest residues, bagasse, and purpose-grown energy crops (i.e. vegetative grasses and short rotation forests). They exhibit several advantages and avoid many of the concerns facing first generation options offering greater cost reduction potentials in the longer term. Algae fuel, also called third generation biofuel, is a possible solution which envisages the use of algae-extracted oils as a prompt fuel itself or in form of biodiesel when processed via transesterification. Finally, an appealing fourth generation option is based on the conversion of vegetable oil and bio-diesel into bio-gasoline using most advanced technology (Demirbas, 2009b).

1.2.1 *The dark side of biofuels*

Despite the broad range of suitable alternatives and their potential benefits, any biomass-based pathway toward fossil fuels substitution exhibits several constraints on its effective penetration within the conventional routes of the global energy supply system and has already

known oppositions. As depicted in Figure 1.5 (USDA, 2008), data regarding the European global use of biofuels clearly reveal that the EU goals on market penetration are still quite far away.

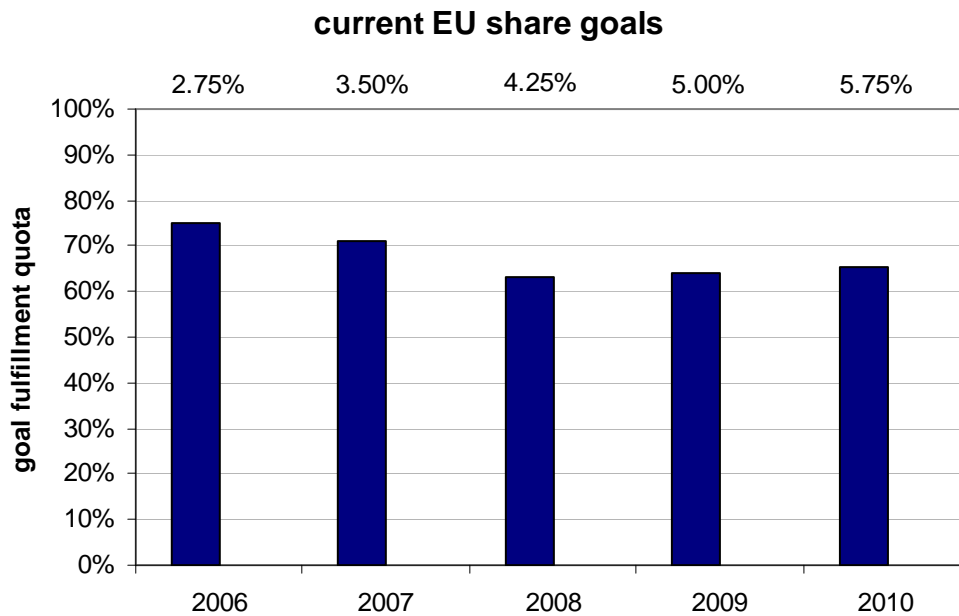


Figure 1.5 *Estimated fulfilment of current share goals for EU-27 Biofuels (USDA, 2008).*

The reasons behind this trend are manifold. As a start, first generation technologies still generate several doubts on whether they are sustainable from an economic and environmental point of view (Granda, 2007). On the other hand, second generation technologies are still economically immature to be competitive within the market. Even worse, algae and fourth generation options, although indicated by many as the future leading technologies, still suffer of serious technological limitations. However, the most critical issue relates to the fierce competition for land resources with other biomass based energy sectors (i.e. biomass for heat and power supply) as well as within the sector itself (i.e. bioethanol vs. biodiesel) and even more with the food industry. Land competition is deemed to be contributing to the recent rise in food prices (EEA, 2009) (the OECD estimates that current and proposed biofuel support measures in the EU and US might increase average wheat, corn and vegetable oil prices by about 8%, 10% and 33%, respectively, in the medium term). A similar rise is also observed in the prices of non-food biomass used in other industrial application. Although equally or even more important factors affect this trend (i.e. droughts in key producer countries, increasing meat consumption and rising oil price), it did generate a worldwide criticism against first generation technologies and biofuels in general. Finally, it is also worth mentioning that the lay-down of radical new infrastructures usually require both great capital expenditures and

potentially long time to be established as well as likely difficulties arising from the new system integration within the conventional one.

Notwithstanding this, the biofuels unquestioned potential to perform a unique range of services within any future energy-system portfolio (Farrell *et al.*, 2006), ranging from energy carriers for automotive purposes to heat and power supply, as well as their undeniable capabilities to offer real economic and environmental benefits call for a new effort aiming at the whole fulfilment of the EU share targets. This goal might be matched by using a wide range of suitable alternatives, being them biodiesel, biomethanol, bioethanol, pure vegetable oil, ETBE or any other energy vector that can be labelled as biofuel. At the moment, only sustainable biomass fuels however, such as ethanol and bio-diesel, can directly contribute in decreasing oil reliance in the short term (Solomon *et al.*, 2007).

1.3 Bioethanol

Among the suitable alternatives, bioethanol is currently acknowledged as the most appropriate solution for a short-term gasoline substitution and accordingly it has assumed a leader position within the biofuels market: in 2007, roughly 45 Mt of bioethanol have been produced for automotive purposes in the world, three quarters of which was generated in the United States and Brazil by means of first generation technologies (Cardona and Sánchez, 2007), and customers' demand is expected to more than double in the next 10 years (Demirbas, 2009c). On the other side, the European contribution still hesitate to take off accounting for 1.4 Mt with a further production capacity of 2.4 Mt under construction (European Bioethanol Fuel Association. <http://www.ebio.org/statistics.php>). Different ethanol-gasoline blends are suitable within the fuel market, ranging from E10 (a mixture of 10% ethanol and 90% gasoline by volume) to E85 (a mixture of 85% ethanol and 15% gasoline by volume). In the US approximately 99% of ethanol is used in E10 fuel (EIA, 2003). Still, in Brazil all of the gasoline put in the market must have at least a 25% anhydrous alcohol blend (E20) and about 40% of the total vehicle fleet run on pure ethanol (Knight, 2006).

Ethanol and ethanol-gasoline blends (gasohol) have a long history: it was in the late 1800s that Henry Ford built the first engine and cars that could be fuelled by ethanol. In 1908 the Ford Model T was first equipped with a flexible fuel engine capable of alternatively run on alcohol, gasoline or gasohol blends (Kovarik *et al.*, 1998). However, the actual expansion of ethanol market dates back to the first boom occurred in the late 1970s when an embryonic ethanol industry was started-up in US as the renewable answer to the momentary shortage of oil supply. However, this emergency solution to the global oil crisis was building up on frail basis: modelled after the beverage industry and thus characterised by small plant size and poor design features, as the oil market scenario was re-established by the mid-1980s the corn-based bioethanol production system begun to run into economic sustainability problems

which determined a global failure notwithstanding the great governmental support (Jacques *et al.*, 2003). Meanwhile in Brazil a similar revolution was occurring with the so-called 'Proalcohol' program (launched in 1975): initially promoting the use of a fuel blend (a mixture named gasohol) of anhydrous ethanol (produced from sugar cane) within gasoline, it quickly changed its targets switching to hydrous ethanol used in its pure form as a fuel gasoline substitute. The system, however, was very stiff and when the market got into spots in the late 1980s, consumers began to switch back to conventional cars in which gasoline (still blended with a minimum level of ethanol) could be used. To most, it looked like the gasohol boom was over (Jacques *et al.*, 2003).

However, in the 1990s some domestic as well as international events combined together to bring about the steady re-launch of the business. The main driver was beyond doubt the Kyoto Protocol in which most industrial nations agreed to face the first signs of global warming by targeting a global GHG emissions reduction through a substantial cut down of the fossil fuels consumption. Other national specific events, though, also gave a big push: in the United States, for instance, MTBE (methyl ter-butyl ether, an oxygenated additive necessary to substitute carcinogenic substances previously used to increase the octane content) was banned due to some concerns on its possible carcinogenic nature as well as to its detection in groundwater. The new laws provided for the substitution of this substance with more environmental-friendly oxygen boosters, such as bioethanol or bio-ETBE (Jacques *et al.*, 2003). All the rest is recent history: new concerns about oil depletion and security on energy supply brought to the actual status in which bioethanol industry is a well-established reality within the liquid fuel sector.

1.3.1 Production technologies

Biomass-derived carbohydrates (hemicellulose and cellulose) can be converted into sugars by hydrolysis and then fermented into alcohol by the action of microorganisms, usually yeast (Demirbas, 2008). First generation technologies, in wide use today, involves the direct fermentation of sugars from sugar cane to ethanol as well as the saccharification and subsequent fermentation of cereals starch. The fermentation is then followed by distillation and separation stages. The basic chemical reactions during biomass fermentation are the followings:



They occur in presence of catalysts of various nature, although the most common is *Saccharomices Cerevisiae*. This is the more mature and the only industrial technology and

represents the easiest way to obtain bioethanol. However, the less abundant biomass availability and more expensive feedstocks together with other issues related to the harsh conflict with food industry did contribute to spark the development of alternative production technologies looking at more abundant and non-food raw materials such as agricultural and forestry residues, woody biomass, energy crops and organic industrial waste, the so called second generation technologies.

A wide variety of processes for the production of ethanol from cellulosic materials have been studied so far and are currently under development (Piccolo and Bezzo, 2009), and great innovation have been made on the paradigm of converting lignocellulosic biomass into hydrocarbon fuels in general (Regalbuto, 2009). Most of the recent research efforts aim toward the concrete endeavour to ensure a sustainable and viable transition from the first generation bioethanol system toward a second generation one.

1.3.2 *Bioethanol: open issues*

At the moment, bioethanol production through first generation technologies is at the highest ever production levels, although during its history has known many valleys and peaks as well as some discredits and oppositions by both the public opinion and part of the academic community. In particular, bioethanol production from starchy materials, i.e. corn and wheat, was believed (Chambers *et al.*, 1979), and still is (Patzek, 2006; Campbell *et al.*, 2009), not to perform efficiently from an energetic standpoint and to use more energy than it actually provided as fuel. Many studies have been addressing these issues (Marland and Turhollow, 1995; Lorenz and Morris, 1995; Graboski, 2002; Shapouri *et al.*, 2002; Pimentel and Patzek, 2005; Kim and Dale, 2005a), all of them estimating over the entire life cycle (from the biomass growth to the fuel distribution) the net energy required to produce ethanol. This resulted in a conflicting range of different conclusion probably more suitable to tighten the debate up than to clarify the question. In a focussing review of these works, Hammerschlag (2006) tried to look at the problem by a more objective point of view through the formulation of a normalized performance indicator. In a quite similar way, Eaves and Eaves (2007) also took up the analysis by extending the review to a wider range of works. This way to assess the problem allowed highlighting the reasons behind the wide variance of the studies outcomes: first of all a great difference in the underlying assumptions (in some cases even based on old and biased data) was pointed out; on the other hand, some studies did not take into account the energy credits allocation to side-productions (i.e. the distiller dried grains with solubles, DDGS). Notwithstanding this, even using more focused indicators, the simple assessment of the energy value of the production process may lead to lose the point out of the question: the actual value of the service provided by bioethanol as liquid fuel within the more general context of energy supply security goes beyond its mere evaluation as a simple industrial product. As asserted by Dale (2008), net energy as it has been used in the media and as is

generally understood by the public is both irrelevant and misleading. Net energy is irrelevant because it falsely assumes that all energy carriers are equally valuable. The core of the question stands in whether the biomass conversion into a liquid fuel for automotive purposes (i.e. ethanol) is actually capable to give the right answer to the energy supply question, involving more complex issues like global warming mitigation and oil substitution within the market.

In light of this, more insight on the real nature of the problem should be attributed to those studies addressing the environmental as well as the economic performance of bioethanol production in relation to its capabilities to penetrate the fuel market in terms of both economic sustainability and competitiveness.

In dealing with the environmental question, many researchers agree on ascribing to bioethanol production certain positive impacts, the most common of which being the reduction of GHG emissions. However, the actual carbon footprints of such a system is still debated and the capabilities of first generation bioethanol productions to global warming mitigation have been long scrutinised (Farrell *et al.*, 2006; Kim and Dale, 2005b; Delucchi, 2006; Malça and Freire, 2006; Reijnders and Huijbregts, 2007; Kim and Dale, 2008; Romero Hernández *et al.*, 2008; Davis *et al.*, 2009; Gnansounou *et al.*, 2009; Petrou and Pappis, 2009). Most studies concluded that ethanol derived from starchy biomass, such as corn and wheat, can sustainably contribute to oil displacement (Farrell *et al.*, 2006), although the effective environmental impact tightly relates to the technological and geographical context which the system perform in. For example, GHG emissions from corn-based ethanol production can be estimated between 3% and 86% (Davis *et al.*, 2009) lower than the emissions from gasoline production, depending on how the ethanol is produced. In particular, it is broadly remarked how this wide range of uncertainty is determined by the difference in options used to provide the energy needs of the process (Granda *et al.*, 2007) as well as by the great variability in agricultural production conditions, in terms of climate, properties of soil, cropping management and cultivation practice in general (Kim and Dale, 2008). Again, an important role on the impact of bioethanol production on global warming is also played by the end-use of valuable sub-products and thereby by their emission credits allocation as their market penetration may avoid the production, and hence the related emissions, of the goods they are going to replace. However, the utilization of biomass for biofuels also counts for other negative impacts on environment: for instance, it would increase acidification and eutrophication particularly because of nitrogen (and phosphorus) related burdens from the soil during cultivation (Kim and Dale, 2005b). Thus, particular importance has been given to fertiliser application having brought into question the sustainability of corn-based ethanol production (Robertson *et al.*, 2008): it is also one of the primary sources for nitrogen losses from soil (i.e. N_2O , NO_x and NO_3^{-1}) which can contribute to GHG emissions. For example, the largest source of N_2O in the United States is the agricultural soil management activity (e.g., fertilizer application and other

cropping practices) (Kim and Dale, 2008). Besides, the abundant use of chemical fertiliser often relates to intensive biomass production practices: this issue always entwines with the ethical questions of biodiversity preservation and with the prevention of using GMO to boost land yield.

To complicate even more this already knotty situation it also contributes the question related to land use change. Delucchi (2006) in a very focused well-to-wheel analysis of biofuels production systems argued that the assignment of ever more cultivated lands to intensive energy crops would increase the overall GHG emission with respect to the previous production practice: this is due to indirect land use change effects of the conversion of undisturbed land elsewhere in the world and the resulting GHG emissions. However, although it is acceptable to account for the direct effect of land use change and on the consequent emissions, on the other hand the indirect effect is highly controversial for many reasons. For example, according to Searchinger *et al.* (2008), indirect land use change essentially would make biofuel industries responsible for the environmental consequences of decisions over which they have no control.

The issue of economic feasibility of ethanol as a fuel has been under considerable debate, too (Karuppiah *et al.*, 2008; Hettinga *et al.*, 2009). The economics of bioethanol production by first generation technology strongly depends on the feedstocks supply costs (ranging approximately between 50 and 80% of the total production cost according to the specific biomass (Petrou and Pappis, 2009)) and thus suffers from the strong market price variability of raw materials. Although corn-based production is broadly considered a mature industry, fluctuating oil market prices calls for a strong governmental action through national subsidies as well as through mandatory blending quota so as to fill the competitiveness gap with gasoline. Besides, the business profitability deeply relies on the side incomes coming from DDGS production as animal feed substitute (or alternatively from electricity produced using DDGS to fuel a power station). As a consequence, the expansion of bioethanol industry has been tempered by changing market conditions (Schmit *et al.*, 2009) and, in particular, the high variability of both DDGS and corn prices have been pushing companies through a disinvestment decision trend.

Moreover, even though ethanol can be blended with gasoline without significant difficulties in using the existing distributing infrastructure (Bernard and Prieur, 2007), the transition from an oil-based fuel system to a biomass-based one represents a complex strategic design problem.

Despite all of these controversial issues, bioethanol from starchy biomass represents a well-balanced trade-off among very few alternatives that can provide a certain degree of security in energy supply. Hence, it likely represents the most advised option to achieve over a short-term horizon the aforementioned European goals in matter of oil displacement. This is even

clearer if first generation ethanol is viewed as a preliminary step towards better performing second generation biofuels.

As recently observed (Petrou and Pappis, 2009), there is a need for an integrated analysis based on several issues that may help defining a more comprehensive view of biofuels production systems. Therefore, especially in those countries where first generation production is not yet established, a preliminary assessment of such systems is of the utmost importance in order to overcome the abovementioned drawbacks affecting the bioethanol production practice. Hence, decision makers and major stakeholders involved in biofuels policies development should be driven by preliminary analysis and evaluations of the interactions within the system under assessment. The minimisation of production costs and environmental impact or the maximisation of profits and financial sustainability ought to be taken as undisputed paradigms in pursuing a well-advised strategy through a wider approach which goes beyond the limited company-centric view of the business and extends the scope of the analysis at the entire supply chain.

1.4 Supply Chain Management

The term SC may be used to identify the integrated process wherein a number of various business actors (i.e., suppliers, manufacturers, distributors, and retailers) works together in an effort to: (i) acquire raw materials, (ii) convert these raw materials into specified final products, and (iii) deliver these final products to retailers (Beamon, 1998). As depicted in Figure 1.6, the actors are connected through the flow of products and information. In order to provide end products to the customers, a network of actors is involved in activities (as purchasing, transforming and distributing) to produce goods and/or services (Stevens, 1989; Swaminathan *et al.*, 1996; Cooper *et al.*, 1997). All of these actors add value to the end product (Lummus, 1999).

The management of these flows across the entire SC, from suppliers to manufacturers, from final assemblers to distribution (warehouses and retailers), and ultimately to consumers, is what is commonly called SCM (Silver *et al.*, 1998). The term SCM is relatively new in the literature, appearing first in 1982 (Oliver and Webber, 1982). SCM is viewed by many as a highly novel management concept, but comparison with earlier work reveals similarities. Thus, the fundamental assumptions, on which SCM rests, are significantly older (Cooper *et al.*, 1997). Modern views of SCM can be classified on different levels, according to the following categories (Papageorgiou, 2009):

- i. strategic and tactical level: SC design (infrastructure)
- ii. tactical and operational level: SC planning and scheduling

iii. operational level: SC control (real-time management)

each one of the above characterised by a well determined time horizon as well as a precise detail level. In a review focused on the advances and challenges facing the process industry in the future, Shah (2005) pointed out the vital importance to apply SC design to the “supply chains of the future”, among which the biofuels infrastructures are included, so as to provide useful support to national and international policy as well as to strategic decisions in industry.

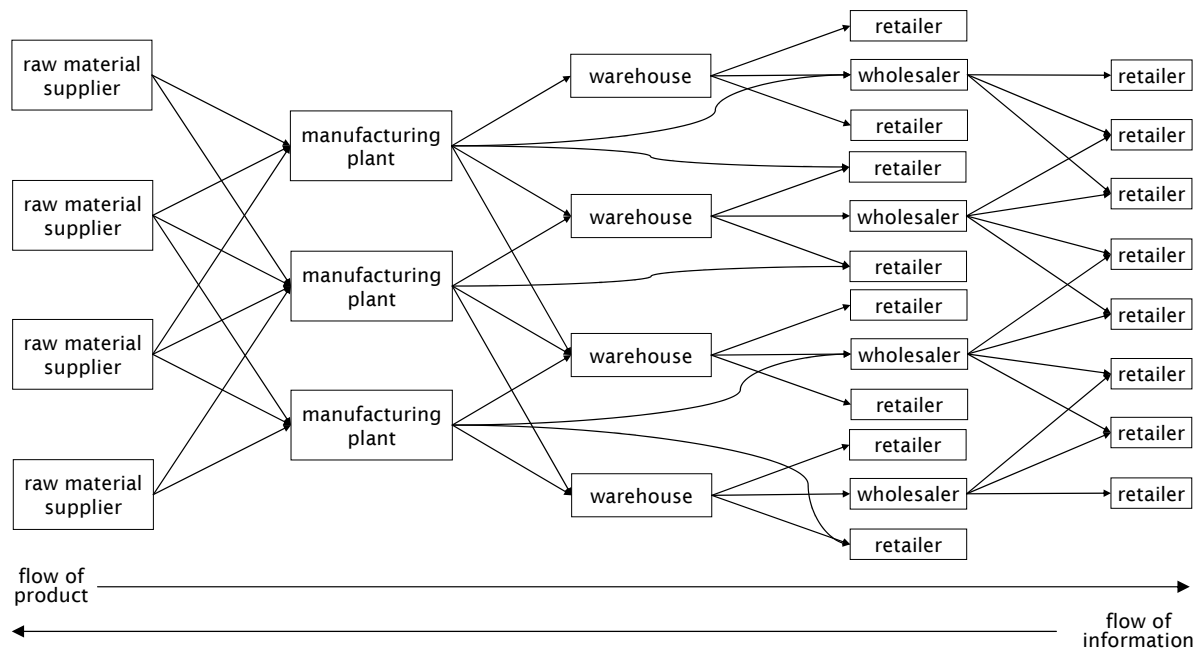


Figure 1.6 General SC outline.

The author also defines SC networks design as a strategic decision process about where to locate new facilities (production, storage and logistics), what supplier to use for each facility (sourcing decision). Accordingly, one or more of the following decisions need taking:

- i. number, size and location of manufacturing sites, warehouses and distribution centres
- ii. production decisions related to plant production planning and scheduling
- iii. network connectivity (e.g. allocation of suppliers to plants, warehouses to markets etc.).
- iv. management of inventory levels and replenishment policies
- v. transportation decisions concerning mode of transportation (e.g. road, rail etc.) and also size of material shipments.

Since the beginning of SCM history, a wide range of tools have been developed so as to ease the decision-making process involved in the strategic design of industrial SCs, in particular

oriented toward a modelling approach to the problem. SC models can be classified according to two main categories, (i) simulation-based and (ii) mathematical programming. Both of them represent a very useful approach to address high level problems such as the whole design of industrial infrastructures, and the choice of the best pathway depends on the task in hand. For example, simulation-based models are characterised by higher precision and thereby they are more time consuming. Hence, they might be particularly indicated in facing small-size problems concerning with a fixed set of few possible network configurations requiring a high level of detail in evaluating the dynamic operation of the system. On the other hand, mathematical programming models are less precise, but they are best suited when unknown configuration are involved in the study and are broadly advised, especially in the early stage of strategic design (Beamon, 1998). In particular, as stated by Kallrath (2000), *Mixed-Integer Programming* (MIP) represents one of the most suitable tools in determining the optimal solutions of complex SC design problems.

1.4.1 *Mathematical Programming*

Mathematical Programming (MP) approaches to design problems traditionally belong to the history of the *Process Systems Engineering* (PSE) community. Firstly developed to assist in the operation and design of chemical processes, they were strictly focused on the company-centric view of the production stage level. However, the increasing awareness of the real opportunity of achieving efficiency improvements as well as higher economic benefits that may be obtained by adopting an integrated management of the interaction among the actors of the entire production system, have been motivating a global trend driving toward the extension of the paradigm boundaries in the PSE approach to optimisation. As a result, supply chain management has suddenly become a key issue in the PSE community. This has led to the development of new generation tools specifically devised to provide decision-making support within the scope of SCM (Guillén-Gosálbez and Grossmann, 2009). The fundamental concept behind these tools is the caption of the system behaviour (in terms of manufacturing sites, raw materials supply, logistics and distribution tasks) within the whole SC environment, with the final aim being the optimisation of the network topology according to some predefined criteria. Thus, the core of the methodology lays on the definition of appropriate performance measures so as to formulate consistent optimisation criteria to configure the system on. Profits and economics in general, have been traditionally pursued as optimisation criteria, and then production costs and/or business incomes have become the most widely used performance indicators (Beamon, 1998). However, very soon it showed up the need for other optimisation drivers so as to account for the multiple issues relating to the multifaceted problem of SCM where conflicting aspects may concur in determining the optimal configuration of the network. As a consequence, other goals have been added in the list of performance indicators. Customer responsiveness (Lee and Billington, 1993), flexibility

(Voudouris, 1996; Georgiadis and Pistikopoulos, 1999) and risk management (Aseeri and Bagajewicz, 2004; Guillén *et al.*, 2005) have been included as suitable criteria defined according to the different stakeholders needs within the business.

In the past decade, restricting environmental regulation imposed by governments has determined a global redefinition of industrial policies so as to comply with the new mandates. As a direct consequence, increasing attention has been directed towards the inclusion of pollution mitigation as part of the optimisation criteria driving the design of process systems. In addition, this trend has been recently accelerated by the growing awareness that improving the environmental sustainability of a production process may also improve its economic performance (e.g., sales may be positively affected by a better public perception of the product or operating cost reduction may be achieved by improving the process efficiency) (Azapagic and Perdan, 2000).

In view of above, there has been a paradigm shift to understand the design approach as well as the scope of the analysis of process systems. In fact, as pointed out by Cano-Ruiz and McRae (1998) in reviewing the state of the art of environmentally conscious design of chemical plants, a new approach that considers the environmental performance as a design objective rather than a design constraint may lead to the discovery of unexplored solutions that not only minimise ecological damage but also lead to overall economic profits. Yet, limiting the scope of the analysis to a company-centric view of the production system may result in misleading solutions, as may occur when a decrease of the local impact determines an increase in the overall ecological damage. These drawbacks have been overcome by including environmental responsibility principles within a more comprehensive approach analyzing the performance of a production system across the entire SC so as to generate a new branch of SCM, namely, the *Green Supply Chain Management (GrSCM)*. In an extensive review of over 200 scientific contributions encompassing various research areas, Srivastava (2007) remarks the importance of a more extensive use of mathematical programming to contribute to major advance in an environmentally conscious SCM.

One of the main driver in using MP lies also in the possibility of performing a simultaneous optimisation of different issues (Guillén-Gosálbez and Grossmann, 2009), thus enabling the exploration of a balanced trade-off between conflicting objectives. This requires the incorporation of multiple criteria decision-making techniques within the modelling framework, namely, *Multi-objective Mathematical Programming (MoMP)*. According to Mavrotas and co-workers (Mavrotas *et al.*, 2008), the methods for solving MoMP problems can be classified into three categories according to the phase in which the decision maker is involved in the decision process: the *a priori*, the *interactive* and the *a posteriori* methods. In both the *a priori* and the *interactive* method the objectives are weighted and grouped together in a single optimisation criterion, thus imposing to decision makers to express their preference before the solution procedure. This represents a limitation in the MoMP capabilities as the

whole set of different solutions may not be analyzed and assessed. This drawback is overcome adopting the *a posteriori* method, which provides a full set of feasible (non-inferior or Pareto optimal) solutions so that the decision makers can evaluate and decide the most viable alternative according to their needs.

The application of MoMP within the specific field of GrSCM is further motivated by the approach that it adopts: the evaluation of the SC performance in terms of ecological damage covers all the stage of the life cycle of the product, thus fitting with the needs of *Life Cycle Assessment* (LCA) techniques, broadly acknowledged as the best methodology to rigorously quantify the environmental burdens and their potential impact of a process, product or activity (Azapagic, 1999). However, including LCA techniques within a MoMP framework poses the problem to find the most appropriate approach to evaluate the ecological damage of the system. This issue asks for the adoption of appropriate indicators capable of measuring the environmental performance. To date much effort has been directed toward the analysis of the problem (Azapagic, 1999; Azapagic and Perdan, 2000; Pre´ Consultants, 2000) in order to define a broadly accepted standard. However, especially in applying the LCA theory to the SC optimisation, the best viable option is determined by analyzing the scope of the problem of interest as well as by a trade-off between a detailed and thorough comparison among alternative products (as required by LCA) and the minimisation of the calculation effort (needed to carry out the SC optimisation).

The same problems come up in assessing the risk on investment as well as the financial performance of a supply system. Moreover, this issue is further complicated by the uncertainty affecting economic issues, i.e. feedstocks purchase cost and products market price. The strong variability of such parameters might actually invalidate the modelling outcomes and lead to erroneous results in the post-processing stage when strategic policies should be formulated on those basis. Therefore, the previously mentioned deterministic modelling frameworks have been enforced by adding probabilistic features in a specific effort to handle the uncertainty. Comprehensive reviews on optimisation under uncertainty for process systems engineering applications can be found in the works by Sahinidis (2004), Cheng *et al.* (2005) and Li and Ierapetritou (2008). Most recent applications to process SCs are based on stochastic programming formulations (Liu and Sahinidis, 1996; Iyer and Grossmann, 1998; Tsiakis *et al.*, 2001; Guillén *et al.*, 2005). This approach, albeit exhibiting more thorough capabilities in addressing the uncertainty on modelling parameters, usually results in problem of considerable size and hence difficult to solve. As a consequence, the most recent academic efforts have been directed toward the development of alternative algorithms devised for the conceptual simplification of the solution procedure so as to make these optimisation problems easier to solve and then more appealing to a broader diffusion within an industrial environment.

1.5 Motivation and aim of the project

SCM tools have also been applied to the assessment of bioenergy systems with a broad success. Both simulation-based (e.g., Nguyen and Prince, 1996; De Mol *et al.*, 1997; Allen *et al.*, 1998; Caputo *et al.*, 2005; Hamelinck *et al.*, 2005) and MP (e.g., Dunnett *et al.*, 2007; Bruglieri and Liberti, 2008; Yu *et al.*, 2009) models have been exploited and tailored to optimise the design of novel biomass-to-energy supply networks under both economic and environmental criteria.

To the best of our knowledge, very limited work (Morrow *et al.*, 2006; Dunnett *et al.*, 2008) has been directed so far towards using MP optimisation models to design a bioethanol supply system. In fact, there are a lot of studies on the economic and environmental performance of bioethanol production from agricultural sources (Kim and Dale, 2005a; Morrow *et al.*, 2006; Kwiatkowski *et al.*, 2006; Kim and Dale, 2008; Dunnett *et al.*, 2008; Karuppiah *et al.*, 2008; Yu *et al.*, 2009). Some works (Kwiatkowski *et al.*, 2006; Karuppiah *et al.*, 2008) have been addressing the design of corn-based ethanol production, but limiting the analysis to the company level: the plant topology optimisation carried out in terms of unit connections and flows in each network stream aimed at minimising the energy requirement of the overall plant. Other works (Kim and Dale, 2005a; Kim and Dale, 2008) have adopted LCA approaches to evaluate both the economic and the environmental performance of the ethanol production from corn: however, notwithstanding the broader boundaries of the analysis embracing the entire life cycle of the production chain, the assessment was limited to a performance evaluation without tackling the design task. More comprehensive studies can be found within the area of second generation bioethanol production (Morrow *et al.*, 2006; Dunnett *et al.*, 2008; Yu *et al.*, 2009) aiming at the optimisation of whole infrastructure design. However, they seem to focus on the logistic optimisation in terms of biomass supply and product distribution rather than on the strategic design of the entire infrastructure.

It is therefore evident that all the research efforts devoted so far to the assessment of bioethanol production, have never had as a primary objective the optimisation of the entire supply chain in order to support the economic and environmentally conscious strategic design of corn-based systems. Besides, the use of MP optimisation have been only recently applied to the bioethanol SCs design, even though this has been limited to the production from woody biomass. This may be related to the opinion that first generation technologies, and corn-based production in particular, should be seen as a preliminary step toward the most promising second generation ones, by which they will be supposedly phased out. However, as recently observed (Hettinga *et al.*, 2009), corn-based ethanol production might incur in significant efficiency improvements due to the technological learning in the coming years, so as to make it competitive also against second generation technologies. In any case, as grain-based ethanol will remain in many nations' energy portfolio for quite a long time (Robertson *et al.*, 2008), it

is essential to propose a strategic approach aiming at boosting the overall economics and softening its environmental impact.

The aim of the project is hence to contribute in providing for decision-making tools capable of steering the strategic design of first generation bioethanol production systems through a full set of optimisation features. The work focuses on the development of MP models for SC optimisation problems to assist the policy-making on biofuels industry at strategic and tactical level. The final objective is to deliver a suitable design and planning framework based on the approaches commonly applied to the multi-echelon SC strategic design and planning under economic, financial and environmental criteria (Sahinidis *et al.* 1989; Tsiakis *et al.*, 2001; Hugo and Pistikopoulos, 2005; Almansoori and Shah, 2006). Agricultural practice, biomass supplier allocation (domestic or foreign), production site location and capacity assignment, logistic distribution and transport characterisation will be simultaneously taken into account within the modelling framework to design the optimal network configuration under different optimisation criteria ranging from environmental to financial and economics ones. The framework will embody different features for spatially explicit siting of supply networks nodes (Almansoori and Shah, 2006) and capacity planning of strategic fuel systems (Hugo and Pistikopoulos, 2005). A stochastic formulation will also be implemented to handle the effect of uncertainty (Tsang *et al.*, 2007a). Finally, with concerns to the environmental impact of cultivation practice a further aspect will be deepened by assessing and minimising the global warming effect of fertiliser application in cropping biomass.

The economics of the entire network will be assessed by means of SCA techniques, focusing on biomass cultivation site locations, ethanol production capacity assignment and facilities location as well as transport system optimisation. The environmental performance of the system will be evaluated in terms of GHG emissions, by adopting a WTT (CONCAWE, 2007) approach in order to consider the operating impact over the entire life cycle.

The emerging Italian corn-based ethanol will be assessed as a demonstrative real world case study so as to assess the actual model capabilities in steering strategic policies on different interest level according to the stakeholders focus. In particular, Northern Italy will be considered as the geographical benchmark and the dry grind process will be assumed as the standard technology for ethanol production.

Chapter 2

Modelling Techniques

This Chapter aims at providing theoretical background on the main modelling techniques this research project have been dealing with. SC optimisation and related issues such as SC design and synthesis are firstly introduced. Successively, mathematical programming tools are briefly outlined as algorithmic approaches to SCM, by putting particular focus on MILP. Next, a review of the main algorithms devised for MP problems solution is presented, with a particular reference to MILP problems and to the branch and bound solution algorithm. Finally, more specific modelling features are addressed through a brief overview on MoMP and on stochastic optimisation.

2.1 Supply Chain Optimisation

Strategic design and network planning of biofuels systems fall within the broader category referred to as SCM. Within the various disciplines that constitute SCM, optimisation based methodologies have been recently attracting a great deal of attention from industry and academia (Grossmann, 2004). In particular, their high versatility to address a wide range of problems, from strategic (i.e. logistics network design) to tactical ones (i.e. inventory and transportation decisions), all the way through operational problems (i.e. production scheduling and vehicle routing), have made them widely used in decision-making support. SC optimisation methodologies can, indeed, radically enhance logistics and supply chain performance through the effective coordination of various decisions concerning the planning and the design procedure.

The design and planning of a supply network is defined by the set of activities springing from the conceptual decision to establish a production system until its actual development by selecting the proper sequence of activities and the corresponding network topology. The topology comprises the selected activity nodes and the connections between them. Network configuration synthesis is a fundamental task of the design and planning process: it represents the conversion of the conceptual idea into a more concrete flowsheet through the evaluation of alternatives. In order to gain insight into the concept, two definition of synthesis are here proposed:

- a. Biegler *et al.* (1997) in addressing process design describe synthesis as an iterative process with several steps: (i) concept generation; (ii) alternatives generation; (iii) analysis of alternatives; (iv) evaluation of alternatives; and (v) optimisation of design.
- b. Tveit (2006) states that the synthesis of (energy) systems can be defined as the process of generating many alternative conceptual flowsheets, often in the form of a superstructure, and selecting the topology and system parameters that give rise to the flowsheet that is optimal for a given objective or objectives.

Although referring to different system boundaries (the former is limited to process design whereas the latter embraces the entire supply system), both definitions evidence a common way to formulate the synthesis task within a general design process. In particular, the suggested procedure revolves around two main concepts, namely the formulation of network alternatives and the following selection according to a predefined optimisation criterion. Framing the problem through optimisation techniques entails the representation of the system alternatives by sets of equations which are functions of the design variables. Thus, the goal of optimisation is to solve the equations and to find the set of variables values that best satisfy the performance criterion.

As observed by Shapiro (2004) in addressing the questions facing supply chain planning, a major challenge in this area includes the development of specific modelling tools. This task often lead to the generation of large-scale problems, whose actual complexity strongly depends upon which methodology is chosen to formulate the problem. Several methodologies embracing hierarchical, simulation and hybrid (involving the simultaneous use of simulators and heuristic rules) approaches as well as mathematical programming (i.e. algorithmic approaches) have been devised within the scope of SC optimisation. As already mentioned in the previous Chapter, simulation and algorithmic approaches (Beamon, 1998) are the most extensively used in PSE.

Probably, the right answer to SC synthesis questions cannot be found in any single ‘silver-bullet’ modelling approach, but rather in an optimal combination of the different options. In this work, however, the attention will be focused on the algorithmic approaches as they represent the most suitable option in the early stage of systems design when the superstructure of the network is completely undetermined, as often happens when dealing with biofuels SCs.

2.2 Algorithmic approaches

When an optimisation problem is framed within the SCM scope, algorithmic approaches are among the most widely used modelling techniques. The implementation of an algorithmic methodology can be taken through the following consecutive three steps:

- i. postulation of a superstructure of alternatives simultaneously embedding all possible topologies
- ii. formulation of an optimisation model for the superstructure
- iii. solution of the optimisation problem to define the optimum configuration

The postulation of the general SC superstructure goes through the mathematical representation of the systems behaviour by means of a model which combines the physics of the network with logical relations, all expressed as algebraic equations. To determine the optimal configuration of the system the optimisation problem must be solved so as to minimise a predefined objective function (optimisation criterion) still holding the physical constraints (material or energy balances) and logical relations previously outlined. In other words, the superstructure representation generates a MP problem that must be solved with an ad-hoc solution algorithm.

As already mentioned MP problems deal with the optimisation of an objective function representing the performance criterion (i.e. costs, environmental impact, financial risk, etc) according to which the system should be configured. The algebraic formulation of a MP problem has the following general form:

$$\begin{aligned}
 \min \quad & f(\bar{x}) \\
 \text{s.t.} \quad & h(\bar{x}) = 0 \\
 & g(\bar{x}) \leq 0 \\
 & \bar{x} \in \mathfrak{R}^n
 \end{aligned} \tag{2.1}$$

where $f(\bar{x})$ is the objective function, $h(\bar{x})$ is the set of equations that describe the system behaviour (material or energy balances and logical constraints) and $g(\bar{x})$ is the set of inequalities that defines the logical constraints the specific network is subjected to. The variables array \bar{x} represents the set of design decision that will be defined by the problem solution (Grossmann, 2005a).

MP problems are usually divided into different classes depending on their characteristics and inherent structure. For example, they may be referred to as (i) *deterministic* when all the modelling parameters are known and specified, or as (ii) *stochastic* when at least one of them is uncertain and is assumed to follow a particular probability distribution (Beamon, 1998). MP problems may also be regarded as *Linear Programs* (LP) or *Non-Linear Programs* (NLP) depending on whether the functions are linear or not.

2.2.1 Mixed-Integer Programming

In dealing with SC networks design and planning, many of the decision that must be taken are discrete in nature (i.e. whether an activity exists within a 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. Hence, a combination of discrete and continuous variables must be embodied within the general mathematical formulation. As a consequence, Equation (2.1) now takes the *Mixed-Integer Programming* (MIP) form:

$$\begin{aligned}
 & \min f(\bar{x}, \bar{y}) \\
 & \text{s.t. } h(\bar{x}, \bar{y}) = 0 \\
 & \quad g(\bar{x}, \bar{y}) \leq 0 \\
 & \quad \bar{x} \in \mathfrak{R}^n, \bar{y} \in \{0,1\}^m
 \end{aligned} \tag{2.2}$$

where \bar{x} still represents the n -set of continuous variables, whilst \bar{y} is the m -set of discrete variables (which generally are binary variables) that take 0-1 values to define the design decisions. MIP models refer to as MILP models when all of the algebraic equations and inequalities are linear.

Finally, it is also worth mentioning that MILP problems, and their sub-sets, are usually regarded as steady-state models operating within a fixed time horizon. However, if a dynamic modelling is needed the model can be built as a steady-state multi-period problem through a linear formulation referring to a discretised time horizon (Kouvelis and Rosenblatt, 2000).

2.3 Solution algorithms

Once the mathematical postulation of the network superstructure as well as the optimisation model is built, the MP problem must be solved by means of a dedicated solution algorithm. To date there is no efficient method for solving problems of all classes, but many specialised algorithms have been devised in relation to the main categories which MP problems are divided into, namely LP, NLP, MILP and MINLP. Accordingly, the choice of algorithm is tightly dependent on the problem formulation and characteristics.

SCM problems solution, especially with concerns to bioenergy systems (Hugo and Pistikopoulos, 2005; Morrow *et al.*, 2006; Dunnett *et al.*, 2008; Bruglieri and Liberti, 2008; Yu *et al.*, 2009; Almansoori and Shah, 2009), has been recently dominated by linear modelling approaches (both LP and MILP). This has also been promoted by the availability of reliable commercial software such as GAMS (Brooke *et al.*, 1998), AMPL (Fourer *et al.*, 1992) and AIMMS (Bisschop and Entriken, 1993) for the solution of optimisation problems.

This section is in no way meant to cover the full area of MIPs algorithms. A fuller description can be found in many textbooks (i.e. Williams, 1993). The further discussion will focus on MILP-dedicated solution algorithms, which will be implemented in this Thesis.

Unlike LPs with the simplex algorithm (and its revised versions (Beale, 1968)), none universal algorithm has emerged for the efficient solution of all the MILP modelling range. Different algorithms measure better against different types of problems due to the computational complexities of the existing classes. Among the wide range of suitable options, most methods fall into one of the five categories reported below (Williams, 1985; Grossmann, 2005a):

- i. *Cutting planes* methods (Gomory, 1958; Crowder *et al.*, 1983; Van Roy and Wolsey, 1986)
- ii. *Enumerative* methods (Land and Doig, 1960; Balas, 1965; Dakin, 1965; Geoffrion, 1969)
- iii. *Pseudo-Boolean* methods (Hammer and Rudeanu, 1968; Granot and Hammer, 1972; Hammer and Peled, 1972)
- iv. *Branch and bound* methods (Williams, 1993)
- v. *Benders decomposition* methods (Benders, 1962).

All these methods, albeit with different features and various facets, are based on the common underlying idea to transform the MILP problem into a set of LP sub-problems which can be then solved through the simplex algorithm. This is achieved through the LP relaxation technique which allows transforming an integer problem into a linear one by simply turning the binary variables into continuous ones varying between 0 and 1 ($0 \leq y \leq 1$, referring to Equation (2.2)). All of the above methods present their own pros and cons, although the most common drawback relates to the prohibitive computational efforts when the methods are applied to large size problems. Consider, for example, an MILP problem counting only one continuous variable ($n = 1$, with reference to Equation (2.2)) and twenty binary variables ($m = 20$, referring to Equation (2.2)): the enumerative methods require the solution of more than one million LP sub-problems (2^m).

The branch and bound methods have proved the most successful in general on practical large scale MILP problems. They involve a well-thought combination of different features of the abovementioned options (in particular, enumerative and cutting planes features), which allows for the efficient solution of large size problems without exceeding in the computational effort. Commercial software for MILP solver (i.e. OSL, CPLEX and XPRESS) are also available and can be used to solve problems with million of binary variables (if enough time and CPU memory is provided).

2.3.1 Branch and bound algorithm

The main idea behind the branch and bound algorithmic procedure is to use a divide and conquer strategy to decision-making by generating partial solutions to the problem and eliminating unpromising regions of the solution space. The resulting algorithm would allow for a limited, although still exhaustive, enumeration of LP sub-problems within which is guaranteed to find the optimal solution.

The branch and bound algorithm consists of a procedure which rests on the LP relaxation theory and is developed through different iterative steps that will be described below (Pistikopoulos and Adjiman, 2001).

LP relaxation theory

Consider the general MILP problem described by Equation (2.2). The LP relaxation entails to change all the m binary variables into continuous ones ranging within the 0-1 interval. Accordingly, Equation (2.2) takes the form:

$$\begin{aligned}
 \min \quad & f(\bar{x}, \bar{y}) \\
 \text{s.t.} \quad & h(\bar{x}, \bar{y}) = 0 \\
 & g(\bar{x}, \bar{y}) \leq 0 \\
 & \bar{x} \in \mathfrak{R}^n, \bar{y} \in \mathfrak{R}^m \\
 & \bar{x} \geq \{0\}, \{0\} \leq \bar{y} \leq \{1\}
 \end{aligned} \tag{2.3}$$

Let us consider now two relaxed problems, P_i and P_j , in which a number k' and k'' (both lower than m) of binary variable \bar{y}' and \bar{y}'' are fixed before relaxing the problem. Accordingly, the two problems formulation can be expressed as:

$$\begin{aligned}
 \min \quad & f(\bar{x}, \bar{y}) \\
 \text{s.t.} \quad & h(\bar{x}, \bar{y}) = 0 \\
 & g(\bar{x}, \bar{y}) \leq 0 \\
 & \bar{x} \in \mathfrak{R}^n, \bar{y} \in \mathfrak{R}^m \\
 & \bar{x} \geq \{0\}, \{0\} \leq \bar{y} \leq \{1\} \\
 & \bar{y}' \in K_i, \text{ fixed}
 \end{aligned} \tag{2.4}$$

and:

$$\begin{aligned}
 & \min f(\bar{x}, \bar{y}) \\
 & \text{s.t. } h(\bar{x}, \bar{y}) = 0 \\
 & \quad g(\bar{x}, \bar{y}) \leq 0 \\
 & \quad \bar{x} \in \mathfrak{R}^n, \bar{y} \in \mathfrak{R}^m \quad (P_j) \\
 & \quad x \geq 0, 0 \leq y \leq 1 \\
 & \quad \bar{y}'' \in K_j, \text{ fixed}
 \end{aligned} \tag{2.5}$$

with the set of K_j fixed variables including the set K_i ($K_i \subset K_j$ and $\dim\{K_j\} \leq m$). Let us define f^* as the solution value of the objective function for the MILP problem (3.2), while f_i^* and f_j^* denote the solutions of problems (P_i) and (P_j) , respectively. Stated that the more a problem is constrained (or the larger the number of fixed variables), the higher the optimal value of the objective function to be minimised, then the following properties must hold:

- a. if P_i is infeasible, then P_j is infeasible
- b. if P_j is feasible, then P_i is feasible
- c. if P_j is feasible, then $f_j^* \geq f_i^*$
- d. if any y is integer in the solution of P_j , then $f_j^* \geq f^*$

The branch and bound algorithm takes advantage of these properties to explore and reduce the solution space into which to enumerate the LP sub-problems. The basic methodology behind the iterative procedure is described in the following (Figure 2.1 is taken as graphical reference).

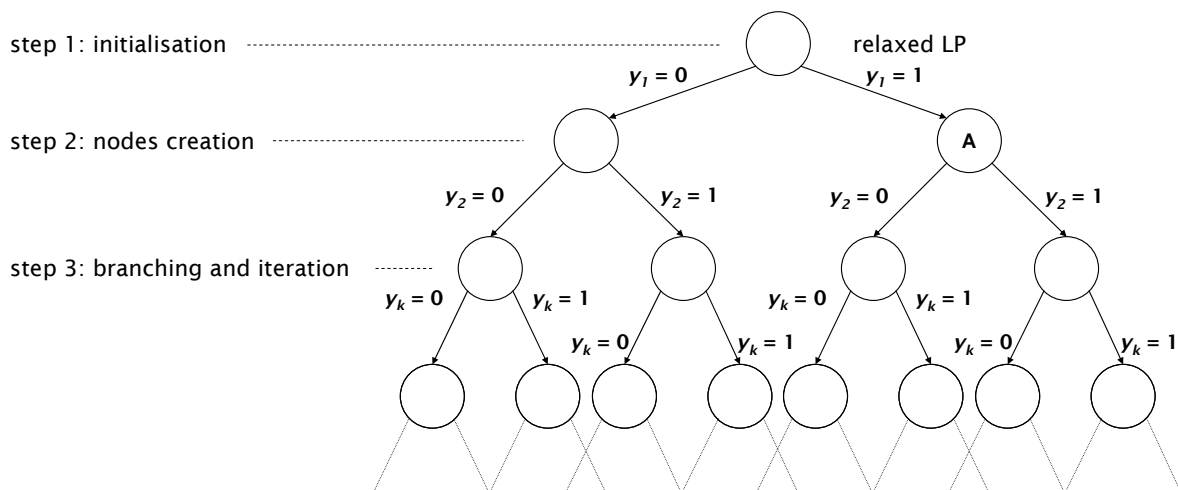


Figure 2.1 Branch and bound tree (Pistikopoulos and Adjiman, 2001).

The algorithm is initialised by solving the fully relaxed LP problem, P_0 , defined by Equation (2.3). Without fixing any y variable the solution might entail two situations: (i) f_0^* is the

solution of the MILP problem, if all the binary variables result to be integer; otherwise (ii) f_0^* represents the *lowest* of the *lower bound* of the solutions space (Property (d)).

The second step involves the creation of two sub-problems (or *nodes*) by fixing only one of the binary variables, y_l , still keeping the other variables relaxed. The solutions of the two sub-problems gives two tighter lower bounds ($f_l^*(y_l = 0)$ and $f_l^*(y_l = 1)$), the minimum of which constitutes the *new lower bound* of the problem (f_{min}) (Property (c)). If the solution of the relaxation is integer, it provides an *upper bound* of the problem (f_{max}) (Property (d)). If $f_{max} - f_{min} < \varepsilon$ (convergence test), the solution is found. Otherwise, if one of the $f_l^*(y_l)$ solutions is greater than f_{max} , the whole branch deriving from the corresponding node (i.e. node A, if $f_l^*(y_l = 1) > f_{max}$) cannot lead to the optimal solution anyway, and thus must be cut from the solutions tree. On the other hand, any node with a lower bound less than f_{max} is added to the lists of nodes that need to be further analysed. This involves the selection of a new node among the remaining to be used to create two new nodes by fixing another binary variable. The procedure is re-iterated and repeated until the convergence test is fulfilled.

It is worth mentioning that different performance in the algorithm can be achieved depending on the alternative criteria that may be used at each step to decide which node to be selected or how to branch the tree (which binary variable to fix). Thus, different approaches and methods combinations can be implemented to adapt the algorithm performance to the MILP problem which needs solving.

2.4 Multi-objective optimisation

As already mentioned, the solution procedure of SC optimisation problems is ruled by the minimisation of an objective function representing the single optimisation criterion previously chosen to configure the system. In dealing with the design of biofuels systems, decision makers can formulate a wide variety of design requirements and objectives according to the numerous stakeholders' needs that should be taken into account through the design pathway (i.e. network efficiency, environmental impact, economic performance in terms of cost minimisation or profitability maximisation, and so on). Usually SC designers have been adopting a modelling strategy envisaging the obtainment of a unique objective modelled after the algebraic form represented in Equation (2.2). However, it is also possible to include more than one objective in a more comprehensive and versatile design process by embodying multiple criteria embracing a wider set of design requirements. These problems are referred to as multi-objective optimisation problems and their main peculiarity is their inherent capability to model possible optimisation criteria, or rather, stakeholders' preferences. These new modelling features can be mathematically expressed through what is called MoMP formulation, according to which p optimisation functions are taken into account simultaneously:

$$\begin{aligned}
& \min f_j(\bar{x}, \bar{y}), \forall j \in \{1, 2, \dots, p\} \\
& \text{s.t. } h(\bar{x}, \bar{y}) = 0 \\
& \quad g(\bar{x}, \bar{y}) \leq 0 \\
& \quad \bar{x} \in \mathfrak{X}^n, \bar{y} \in \{0, 1\}^m
\end{aligned} \tag{2.6}$$

Unlike single-objective problems, which always result in a single solution $(\bar{x}, \bar{y})^*$ (when a solution exists), MoMPs produce a matrix of multiple solutions, all likewise optimal (or sub-optimal), due to conflicts between objectives. In other words, referring to the mathematical formulation of Equation (2.6), the solution of p objective functions $f_j(\bar{x}, \bar{y}) : \mathfrak{X}^{n \times m} \rightarrow \mathfrak{R}^l$ is a subset Z of space \mathfrak{R}^p called feasible objective region. The elements of Z are called objective vectors, $\bar{z} = [(\bar{x}, \bar{y})_1, (\bar{x}, \bar{y})_2, \dots, (\bar{x}, \bar{y})_p]^T$, which represent the whole set of sub-optimal solutions. This calls for the definition of a new optimality criterion. A common way of defining optimality is the Pareto optimality, which can be defined as follows (Miettinen, 1999):

Definition 2.1: A decision vector $(\bar{x}, \bar{y})^*$ is Pareto optimal if there does not exist another (\bar{x}, \bar{y}) such that $f_i(\bar{x}, \bar{y}) \leq f_i(\bar{x}, \bar{y})^*$ for all $i = 1, \dots, p$ and $f_j(\bar{x}, \bar{y}) < f_j(\bar{x}, \bar{y})^*$ for at least one objective j . Otherwise, $(\bar{x}, \bar{y})^*$ is non-optimal.

In other words, a solution is Pareto optimal if it is not possible to find another feasible solution so as to improve one objective without necessarily worsening at least one of the others.

There are usually many Pareto optimal (or non-inferior) solutions, and the whole set of them is referred to as Pareto surface. All the solutions laying onto the Pareto surface are mathematically equal and depend on the decision makers to select as the “right” solution. According to the design process stage in which decision makers express their preference, it is possible to distinguish three different families of methods (Collette and Siarry, 2003):

- i. *A priori* methods
- ii. *Progressive* (or interactive) methods
- iii. *A posteriori* methods.

In the a priori methods, the trade-off between objective functions is determined before the execution of the optimisation model. This is achieved by weighting the different objectives within a single objective function. Although their simplicity in terms of execution, these methods have known criticism concerning with the difficulties to be able to accurately quantify (either by means of goals or weights) preferences in advance. In the progressive

method, interactive phases of dialogue with the decision makers are interchanged with phases of calculation so as to head, after few iterations, toward the most preferred solution. These methods, although applying specific techniques to model the decision makers requirements, exhibit two main drawbacks: first of all, decision makers need to be involved in the optimisation process continuously in order to adjust the objective criteria as long as new results become available; secondly, because of this iterative process, decision makers never see the whole range of possibilities, but only the effect of their preferences at that stage of the optimisation. On the contrary, the a posteriori methods do generate the whole set of efficient solutions (all of them or a sufficiently broad representation) and then the decision makers select the preferred one. The only drawback that we must emphasize here is that the computational effort needed to generate a full representative set of Pareto optimal solutions might be prohibitive. However, with the recent availability of ever better performing computational facilities the a posteriori methods have been receiving more and more attention.

2.4.1 The ε -constraint method

Among the available a posteriori alternative options, the ε -constraint method (Steuer, 1986) resulted as the most widely applied in multi-objective optimisation problems due to its aptitude to be implemented into the MP modelling language and to fit with the available solution algorithms. The ε -constraint method has several advantages over the others (Mavrotas, 2009):

- i. it allows obtaining a more rich representation of the efficient set of solution
- ii. it allows producing unsupported efficient solutions in *Multi-objective MILP* (MoMILP) problems (Steuer, 1986; Miettinen, 1999)
- iii. it does not suffer of scaling problems for grouping together the objective functions
- iv. the number of the generated efficient solutions can be controlled by properly adjusting the number of grid points in each one of the objective function ranges

The mathematical formulation of this method builds on the main idea (Cohon, 1978; Chankong and Haimes, 1983) to optimise one of the objective functions using the others as constraints in the constraint part of the model. Accordingly, Equation (2.6) can be reformulated as:

$$\begin{aligned}
& \min f_1(\bar{x}, \bar{y}) \\
& \text{s.t. } f_j(\bar{x}, \bar{y}) \leq \varepsilon_j, \quad \forall j \neq 1 \\
& \quad h(\bar{x}, \bar{y}) = 0 \\
& \quad g(\bar{x}, \bar{y}) \leq 0 \\
& \quad \bar{x} \in \mathfrak{X}^n, \bar{y} \in \{0,1\}^m \\
& \quad \varepsilon_j \in \{\varepsilon_j^L, \varepsilon_j^U\}, \quad \forall j \neq 1 \\
& \quad j \in \{1, 2, \dots, p\}
\end{aligned} \tag{2.7}$$

where:

$$\begin{aligned}
& \varepsilon_j^L = \min f_j(\bar{x}, \bar{y}), \quad \forall j \in \{1, 2, \dots, p\} \\
& \text{s.t. } h(\bar{x}, \bar{y}) = 0 \\
& \quad g(\bar{x}, \bar{y}) \leq 0 \\
& \quad \bar{x} \in \mathfrak{X}^n, \bar{y} \in \{0,1\}^m
\end{aligned} \tag{2.8}$$

while ε_j^U is the maximum value among the $(p-1)$ values for $f_j(\bar{x}, \bar{y})$ when all $f_i(\bar{x}, \bar{y})$ ($\forall i \neq j, i \in \{1, 2, \dots, p\}$) are minimised without constraints.

In the literature, several versions of the ε -constraint method have been proposed to improve its performance or to adapt it to a specific type of problems (Ehrgott and Ryan, 2002; Laumanns *et al.*, 2006; Hamacher *et al.*, 2007). This work will refer to the MoMILP solution approach proposed by Hugo and Pistikopoulos (2005) following the works by Papalexandri and Dimkou (1998) and Dua and Pistikopoulos (2000). The proposed algorithm is illustrated in Figure 2.2. It involves three preliminary steps (1 to 3) in which the constraining parameters (ε_j) are evaluated, and the feasible range is set, by solving p single-objective problems. Next, step 4 involves the discretisation of the ε -parameter space into $NQ^{(p-1)}$ sufficiently small intervals and the further application of the ε -constraint method at each parameter interval realization. Accordingly:

$$\begin{aligned}
& \min f_1(\bar{x}, \bar{y}) \\
& \text{s.t. } f_j(\bar{x}, \bar{y}) \leq \varepsilon_j, \quad \forall j \neq 1 \\
& \quad h(\bar{x}, \bar{y}) = 0 \\
& \quad g(\bar{x}, \bar{y}) \leq 0 \\
& \quad \bar{x} \in \mathfrak{X}^n, \bar{y} \in \{0,1\}^m \\
& \quad \varepsilon_j \in \{\varepsilon_j^1, \dots, \varepsilon_j^q, \dots, \varepsilon_j^{NQ}\}, \quad \forall j \neq 1 \\
& \quad j \in \{1, 2, \dots, p\}
\end{aligned} \tag{2.9}$$

where:

$$\varepsilon_j^1 = \varepsilon_j^L, \quad \varepsilon_j^q = \varepsilon_j^L + q \cdot \frac{\varepsilon_j^U - \varepsilon_j^L}{NQ} \quad \text{and} \quad \varepsilon_j^{NQ} = \varepsilon_j^U \quad (2.10)$$

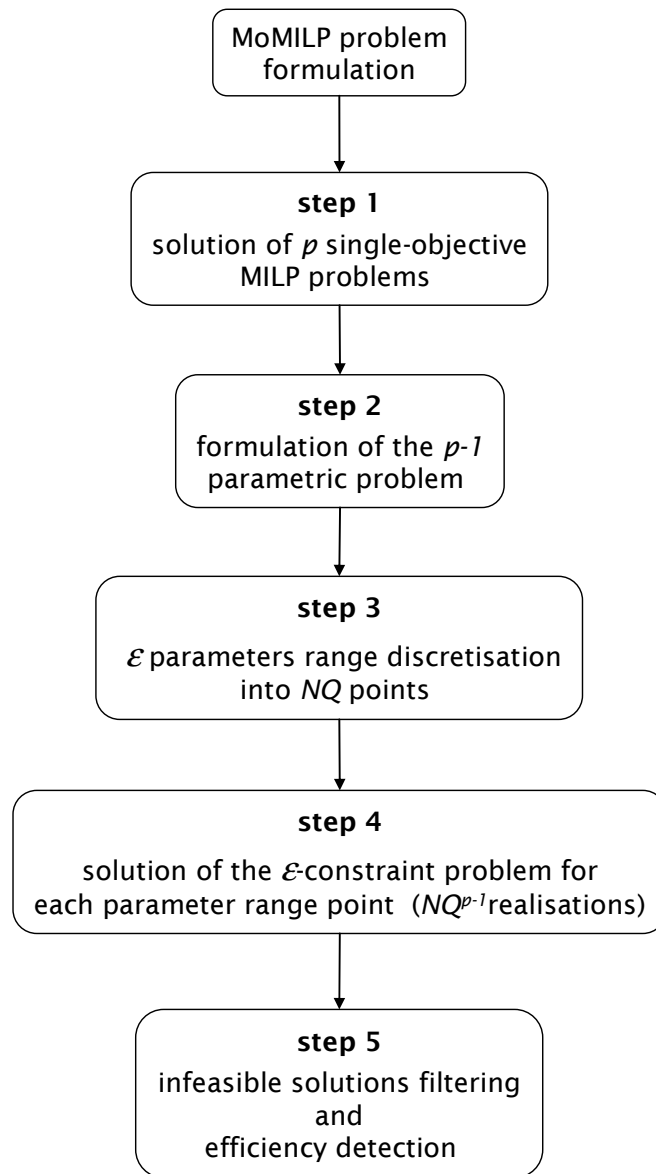


Figure 2.2 Information flux for the multi-objective optimisation algorithm.

It is important to note that the ε -constraint method can neither guarantee feasibility nor efficiency and both conditions need verifying once the complete set of solutions has been obtained. Therefore, an additional post-processing phase (step 5) for detecting efficiency (based on the concepts of Pareto optimality) has to be included as part of the overall multi-objective optimisation algorithm.

2.5 Stochastic optimisation

The discussion addressed so far has been dealing with modelling issues regarding deterministic optimisation techniques in which all the model parameters are known. However, it is quite common in designing biofuel systems (or, indeed, any other system) to make decisions in presence of uncertainty (i.e. on raw material costs, market price and activities burdens). Hence, decision makers have to measure against optimisation problems which depend on undetermined parameters sets. Within the scope of SC design and planning, the PSE community has long been involved in the development of dedicated tools and a variety of ways to formalize the uncertainty has been then devised, together with different approaches for solving optimisation problems under uncertainty. These include scenario-based multi-period formulations (Tsiakis *et al.*, 2001), stochastic programming (Dempster *et al.*, 2000; Gupta *et al.*, 2000; Gupta and Maranas, 2003; Lababidi *et al.*, 2004), supply chain dynamics and control formulations (Bose and Pekny, 2000; Perea-López *et al.*, 2001; Cheng and Duran, 2004), and fuzzy decision-making (Petrovic *et al.*, 1999; Chen and Lee, 2004). In a review of state-of-the-art and opportunities for optimisation under uncertainty, Sahinidis (2004) categorises all the existing modelling approaches into three main families:

- i. *Stochastic programming* (recourse models, robust stochastic programming and probabilistic models)
- ii. *Fuzzy programming* (flexible and possibilistic programming)
- iii. *Stochastic dynamic programming*

The main difference between these methods is the underlying philosophy which they adopt to handle the uncertainty. In the stochastic programming case, for example, uncertainty is modelled through discrete or continuous probability functions. On the other hand, fuzzy programming considers random parameters as fuzzy numbers and constraints are treated as fuzzy sets. Dynamic programming, instead, considers the uncertainty as an inherent part of the modelling environment: this involves the formulation of a discrete time system that evolves over a discrete time periods each one characterised by different scenarios with a defined probability.

Among the suitable alternatives, the use of stochastic programming for SC design and planning has been showing increasing interest (Sodhi and Tang, 2009). The stochastic programming approach adopted in this work is a MILP with fixed recourse, also known as scenario analysis technique (Birge and Louveaux, 1997). This approach is based on the main idea to consider simultaneously multiple scenarios of an uncertain future, each with an associated probability of occurrence. Under the assumption of discrete distributions of the uncertain parameters, this approach seeks network configurations that are good (nearly optimal) for a variety of scenarios of the design parameters at the expense of being sub-

optimal for any one scenario (Santoso *et al.*, 2005). Hence, optimisation entails maximisation or minimisation of expected objectives, where the term “expected” refers to multiplying performance measures associated with each scenario by its probability of occurrence. Accordingly, given a set s of possible scenarios for the design parameters, the stochastic modelling features can be mathematically expressed through the following MILP formulation:

$$\begin{aligned}
 \min \quad & \mathbb{E}(f(\bar{x}, \bar{y})) = \sum_s \omega_s \cdot f_s(\bar{x}, \bar{y}), \quad \forall s \in \{1, \dots, w\} \\
 \text{s.t.} \quad & h(\bar{x}, \bar{y}) = 0 \\
 & g(\bar{x}, \bar{y}) \leq 0 \\
 & \bar{x} \in \mathfrak{X}^n, \bar{y} \in \{0,1\}^m
 \end{aligned} \tag{2.11}$$

where $\mathbb{E}(f(\bar{x}, \bar{y}))$ is the expected objective, $f_s(\bar{x}, \bar{y})$ the single objective function related to scenario s and ω_s is the discrete probability value for the occurrence of scenario s parameters conditions.

Chapter 3

Modelling Assumptions

The objective of the discussion presented in this Chapter¹ is to provide a comprehensive description of the bioethanol SC in terms of economic and environmental issues. A general outline of the production network components is firstly drawn. The subsequent sections specifically address the economic and environmental evaluation of the network nodes of the bioethanol SC in relation to a real world case study, namely the emerging corn-based ethanol production in Northern Italy. The detailed characterisation of the related SC node categories in terms of modelling parameters through SCA and LCA techniques is finally reported.

3.1 The bioethanol SC

The objective of the work addressed in this Thesis is the development of a general modelling framework to design and plan strategic SCs such as biofuels production systems. Dealing with such an optimisation problem usually entails a wide range of decisions with concern to the best network configuration to be established in order to achieve the desired performance.

As already stated in Chapter 1, SCs can be generally viewed as production networks including a number of facilities, namely logistic nodes, such as suppliers, production sites and demand centres. In a similar context, a biofuel SC is defined as a network of integrated nodes that are mutually connected and work together in the endeavour to satisfy the customer demand of a specific fuel. As depicted in Figure 3.1, a general biofuel supply network can be divided into two main substructures: the first one concerns with the upstream fuel production and involves biomass cultivations, biomass delivery and fuel production sites; the latter is related to the downstream product distribution to the demand centres. Between the end-nodes there can be a broad variety of production technologies, transportation modes, and logistic choices. Therefore, the decision process toward the best SC design involves the optimal choice among the possible combinations of these network nodes. As already evidenced, the design outcomes

¹ The topic addressed in this section is part of publications Franceschin *et al.* (2007a), Franceschin *et al.* (2008), Zamboni *et al.* (2009a) and Zamboni *et al.* (2009b), Zamboni *et al.* (2009c) and Zamboni *et al.* (2009d).

are not unique as they strongly depend on the specific conversion technology and even more on the geographical context in which the system is going to be operating.

Accordingly, the modelling framework development cannot be exempted from a preliminary work oriented to a rigorous characterisation of the production system under assessment which reckons with specific geographical and technological issues. The methodology adopted in this work refers to the classical SCA (for economic evaluations) and LCA techniques (in relation to environmental analysis).

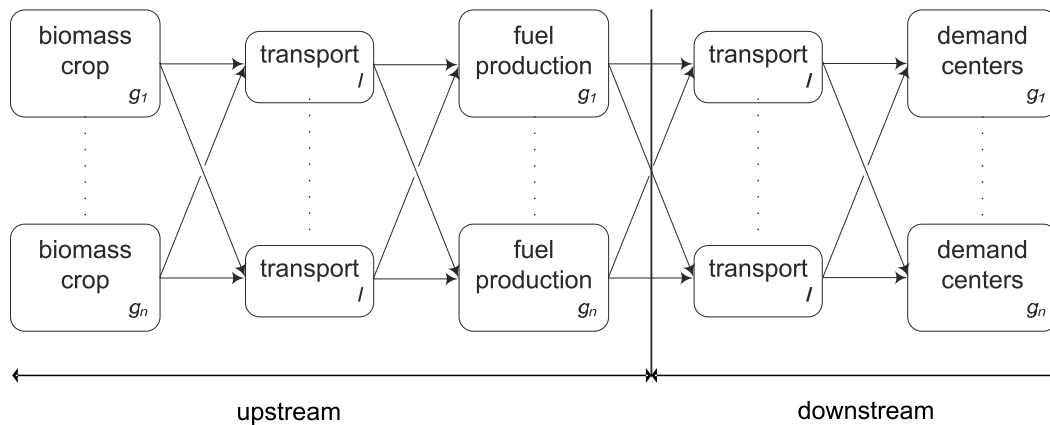


Figure 3.1. *Biofuels network superstructure.*

3.2 Case study

The specific features which the entire project is referred to reckon with the formulation of a representative case study embodying the geographical as well as the technological benchmarks which the modelling framework has been based on.

The emerging corn-based ethanol production system in Northern Italy was chosen to the scope. First of all, in complying with EU guidelines on biofuels, the current Italian energy policy sets the minimum blending fraction of bioethanol within gasoline at 3% by energetic content for 2009 and 5.75% for 2010 (Italian Government, 2007). Moreover, the region under investigation represents a self-sufficient area in terms of conventional fuel supply infrastructure as well as a promising biomass production belt with concern to soil conditions, corn yield and farming practices. Additionally, the existing distribution infrastructure includes a full-scale range of transport options available for industrial purposes. These are likely reasons why some Italian companies have been planning the establishment of first generation ethanol production facilities scheduling corn as suitable biomass. Presently, four ethanol plants are under planning and their probable location and size was considered in this work. In particular, a 110,000 t/y production plant is assumed to be built up in the industrial area close

to the Venice harbour (element $g = 32$ in the grid that will be later described), a second 160,000 t/y facility should be established in Porto Viro ($g = 43$), a 160 kt/y plant is proposed in Tortona ($g = 37$) and, finally, a 100,000 t/y plant should be constructed in Trieste ($g = 34$).

3.2.1 Spatially explicit features

An important step in implementing a spatially explicit modelling framework is the territorial characterisation required to map all the possible network configurations within the area of study as well as to set a geographical benchmark for the model parameters. Northern Italy was discretised into a grid of 59 homogeneous square regions of equal size (50 km of length); each one represents an element identified by g (the grid is illustrated in Figure 3.2). One additional cell ($g = 60$) was added as a pseudo-region to represent the option of importing biomass from foreign suppliers. The actual land surface of each squared region (GS_g) was measured by considering the specific geographical configuration of the area (the estimated values are reported in Table A.1). Element 60 was assigned a fictitious (very large) value so as to represent a pseudo-region capable of an “unlimited” biomass production that may satisfy the domestic demand.

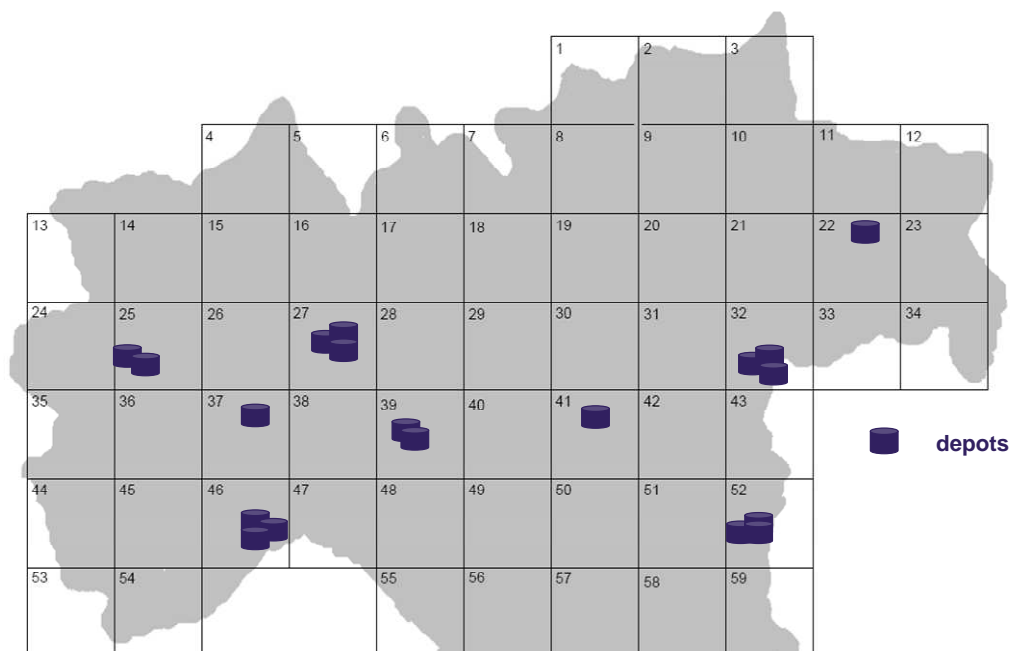


Figure 3.2 Grid discretisation and Northern Italy.

3.2.2 Demand centres

The characterisation of demand centres is another key issue in the preliminary assessment of SC systems as they are likely to represent the main driver of the optimisation process. When dealing with biofuels, it is very important to establish at which SC stage the conventional fuel is blended with a biomass-derived one. A recent Governmental report (INDIS, 2007) outlining the Italian fuel-for-transport infrastructure, highlights two important issues regarding gasoline distribution. First of all, the eight main companies operating in Italy (covering more than 95% of the whole market) exhibit a highly integrated SC; besides, present regulations make it very difficult to increase the storage facilities location and capacity. The Italian fuel SC is therefore a static network, within which the main bottleneck is represented by the storage structure. As a result, oil companies are forced to share terminals and to tightly schedule their product delivery to final customers. Secondly, downstream products (gasoline, diesel and LPG) are stored at *primary depots*, mainly located along seacoasts, and are then distributed to *internal depots*, located in the neighbourhoods of the main transport nodes (rail stations or highways), by means of pipelines. Finally, products are distributed from internal depots to filling stations mainly by road tankers. Furthermore, the hygroscopic nature of ethanol-gasoline mixtures suggests that ethanol should be added and blended with gasoline just before the final distribution stage.

Accordingly, the internal depots are assumed as the actual demand centres for bioethanol. Provided the usual demand driven nature of the problem of study, the demand assignment to blending centres must be solved before the SC optimisation as a typical secondary distribution problem carried out to define the ethanol demand at the blending nodes. The mathematical formulation, reported in details in Appendix B, has been based on the MILP modelling approach commonly applied in the optimisation of fuel distribution systems (Kong, 2002) and solved in GAMS (Rosenthal, 2006).

Northern Italy grids (regional elements g as defined above) have been hence characterised by a homogeneous blended fuel demand (DEM_g). Internal depots (d) are fuel suppliers that have to be assigned a certain number of drop zones to serve. DEM_g values have been extrapolated from provincial gasoline demand, and the maximum terminal throughput allowed (THR_d^{\max}) has been derived from internal depots throughput capacity. The actual throughput ($DEMT_d$) is assigned to each terminal by implementing the optimisation model. Once $DEMT_d$ is known, the ethanol demand (D_g^T) can be easily derived by fixing the blending percentage that characterise each demand scenario.

Data about provincial gasoline demand perspectives for 2009 and 2010 as well as internal depots location and maximum distribution capacity have been collected from Governmental web sites (Italian Government, 2008). It is important to discuss here a fundamental underlying assumption related to demand definition: the time-variant nature of ethanol demand is mainly determined by biofuels regulation rather than market. This justifies the approximation of

blended fuel demand to a mean constant value obtained as an average of the 2009 and 2010 demand perspective. Accordingly, Table A.2 resumes the input values of DEM_g used to implement the secondary distribution optimisation model. On the other hand, Table 3.1 reports the THR_d^{\max} values, while Figure 3.2 depicts the geographical location of the internal depots.

Table 3.1 Values for maximum depot throughput capacity (THR_g^{\max}).

depot d	region g	THR_g^{\max} (t/d)
a	22	1500
b	25	2000
c	27	4000
d	32	5300
e	37	2000
f	39	2000
g	41	1500
h	46	3000
i	52	4000

The optimal configuration of the logistic distribution from blending terminal down to demand centres (elements g), as resulting from the optimisation outcomes, is reported in Figure 3.3.



Figure 3.3 Blended fuel distribution system: optimal configuration for Northern Italy.

3.3 Supply Chain Analysis

Once the geographical location is characterised along with the market features in terms of gasoline and biofuel demand, a detailed SCA is needed. This allows tailoring the modelling framework to the specific case study under assessment, and involves the definition of the economics of the system in terms of modelling parameters related to the technological choices which the case study entails. Accordingly, the *goal and scope* of the system have to be defined with the necessary precision required by the representative value of the assessment that is going to be approached. Within the scope of mathematical programming this has to be carried out with a double purpose. The first one is to perform the economic, and successively environmental, optimisation: SCA (and LCA consequently) are needed as an endogenous tool to compare alternative topologies of the same production network. The second goal is to use the results obtained through optimisation to compare the performance of the obtained production system with that of an exogenous supply network (e.g., the conventional process that is aimed to replace). The unit for the performance measures, i.e. the *functional unit* of the system, needs to capture the nature of the service provided by products. Accordingly, when referring to alternative fuels, this should be defined as an absolute benchmark such as *km driven* or *GJ of energy* provided using those fuels in a combustion engine. On the other hand, to obtain a satisfactory estimation of the system performances, special attention has to be given to the choice of the SC stages to be included, i.e. the *system boundaries* definition. Hence, the set of SC stages s considered in the evaluation are given by biomass cultivation (bc), biomass transport (bt), fuel production (fp) and fuel distribution (ft), and expressed as:

$$s \in S \equiv \{bc, bt, fp, ft\}.$$

3.3.1 Biomass cultivation

As first generation production technology is assumed to represent the most convenient solution over a short-term horizon within the Italian industrial context, corn is recognised as the most suitable biomass for ethanol production. Spatially specific data regarding corn yields (CY_g) and corn crops fractions of the overall available land (BCD_g^{\max}) were retrieved from territorial data (ISTAT, 2007), whereas land availability (AD_g) were obtained through a GIS system (Corine Land Cover 2000[®]; APAT, 2006). Corn production costs ($UPCb_g$) were derived from actual data (CRPV, 2007): fixed costs were separated from yield dependent ones so as to create a grid-dependent set of parameters as illustrated in Figure 3.4, where every diamond represents the production cost as a function of the crop yield. The approach was also validated through actual data.

Table A.3 reports the whole set of input parameters assigned to describe biomass cultivation. To characterise imported corn, $UPCb_{60}$ was estimated from actual data representing the production costs of corn in Eastern European countries (deemed to be the most viable option for Italian ethanol producers).

The available corn cultivation data are not classified in terms of corn final utilization (either food or industrial purposes), and, therefore, a maximum biomass utilization quota was assumed: parameter $SusP$ was set equal to the estimation reported by the United States Department of Agriculture for corn production (USDA, 2005), in which the corn amount deployed for industrial purposes was projected to reach an asymptotic threshold of about 14% of the entire domestic production. The assumption seems quite reasonable considering that the region of study presents some similarities to the American corn belt with respect to soil conditions, corn yield and farming practices.

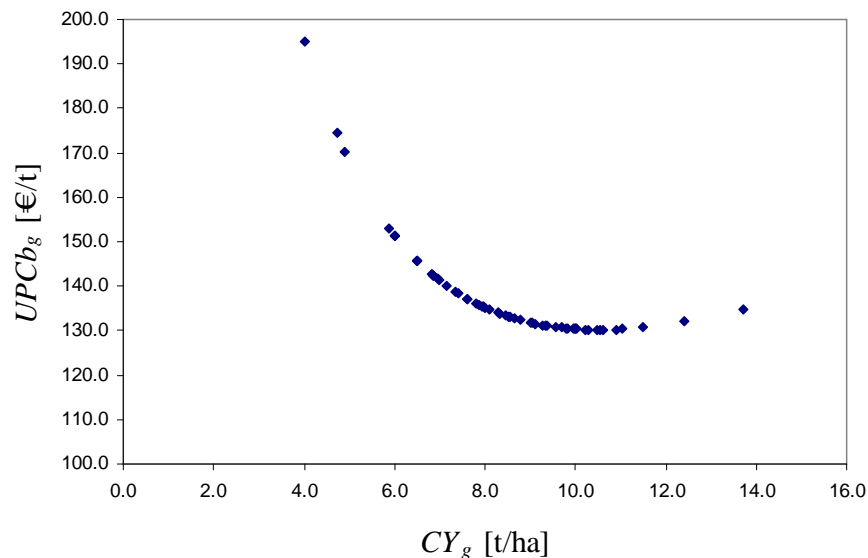


Figure 3.4 Unit production costs for corn cultivation ($UPCb_g$): parameters values are assigned by relating cost to the actual crop yield.

3.3.2 Transport system

The Northern Italy industrial infrastructure includes a full-scale range of available alternatives such as trucks, rail, barges and ships, which have been defined as possible delivery means for both corn supply and bioethanol distribution. Trans-shipping was also included as a viable transport option for biomass importation. Finally, the internal transfer of biomass within each production element g was described assuming the employment of small road tankers. In this work, the transport system is assumed as an additional service provided by existing actors already operating within the industrial/transport infrastructure. As a consequence, transport costs only refer to the rental fees necessary to avail of the service. Transport related

parameters, such as unit transport costs ($UTC_{i,l}$) and transport means capacity ($TCap_{i,l}$) have been gathered from the literature (Buxton, 2008) and then validated with respect to available industrial data. Table 3.2 reports the transport related parameters as defined in the case study under assessment.

Table 3.2 Transport system input parameters.

mean l	$UTC_{i,l}$ (€/tkm)		$TCap_{i,l}$ (t)	
	ethanol	corn	ethanol	corn
small truck	-	0.270 [†]	-	5 [‡]
truck	0.500	0.540	23.3	21.5
rail	0.210	0.200	59.5	55
barge	0.090	0.120	3247	3000
ship	0.059	0.064	8658	8000
trans-ship	-	0.005	-	10000

[†] UTC^* referring to the notations adopted in the next Chapter

[‡] $TCap^*$ referring to the notations adopted in the next Chapter

Distances between elements g and g' ($LD_{g,g'}$) were evaluated by measuring the linear route linking the centres of each square cell (if allowed in the geographical context, otherwise the shortest viable route was considered). The average distance within a grid element was assumed proportional to the actual region surface. In order to better represent the actual delivery distance in relation to the transport mean, a tortuosity factor ($\tau_{g,l,g'}$) was also introduced to take account that the actual product transport route is not linear (but rather depend on the transport characteristics): $\tau_{g,l,g'}$, is a multiplication factor to be applied to the local linear distance ($LD_{g,g'}$) and depends on the transport mode l . As a matter of example, the delivery distance is generally different if covered by truck rather than by ship.

With reference to Figure 3.5, the definition of $\tau_{g,l,g'}$ for trucks is based on the assumption that the maximum distance between g and g' is the circle line b , whereas the shortest distance is the straight line a (i.e., $LD_{g,g'}$). Accordingly, $\tau_{g,l,g'}$ should range between 1 and 1.6. The value of the tortuosity factor was set equal to 1.2 when a highway linking g and g' is available (the same value was chosen for the tortuosity factor for railways), whereas its values was set equal to 1.4 if only local roads exist. In defining the barge and ship tortuosity factors, as the actual distance between harbours was known (and being a limited number of them), all $\tau_{g,l,g'}$ were specifically calculated (and are reported in Table 3.3).

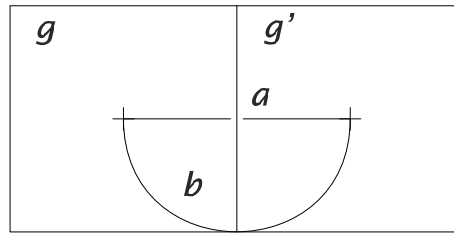


Figure 3.5 Tortuosity factor estimation.

Table 3.3 Tortuosity factor for barge and ship delivery routes.

elements linked	τ
<i>barge</i>	
38↔39	1.9
39↔40	1.0
40↔42	1.4
42↔43	1.8
<i>ship</i>	
32↔34	0.85
32↔43	1.18
32↔52	1.06
34↔43	0.66
34↔52	0.68
43↔52	1.54

3.3.3 Ethanol production

The most common processes in conventional corn-based ethanol production are known as Dry Grind Process (DGP) and Wet Mill. The DGP (Kwiatkowski et al., 2006) is usually the preferred choice and hence assumed in this work to characterise the production facilities. Ethanol production costs are sensitive to plant capacity due to the economy of scale effect on capital and operating costs. This important issue has been taken into account in estimating production and capital costs in devising a purpose-designed financial model.

This model avails of a process simulator (Aspen Plus™) to provide a sensible base case for the sensitivity and financial analyses. The base case refers to the standard fuel production capacity of 110,000 t/y which superstructure is represented in Figure 3.6. The raw material

(corn) is converted into the two products, ethanol and the DDGS, through five main process steps:

- i. Grinding, Cooking and Liquefaction
- ii. Saccharification and Fermentation
- iii. Distillation & Dehydration
- iv. Water evaporation and recycling
- v. Drying of the non-fermentable fraction

In the first plant section, the corn is milled down to the required particle size (< 2 mm) in order to facilitate the subsequent penetration of water and is sent to a slurry tank where it is also added with water. The slurry is “cooked” by using low-pressure steam: this allows for the simultaneous sterilisation of the slurry and the breakage of starch-hydrogen bonds so that water can be absorbed. The following liquefaction step is performed by the action of enzymes (α -amylase) on the exposed starch molecules. The effect is a random breakage of the carbohydrates linkages thus decreasing the viscosity. The mash from the liquefaction vessel is added to a backset stream and then cooled down, ready for the fermentation step.

In the fermentation reactor, a simultaneous saccharification and fermentation occurs (SSF): starch oligosaccharides are almost completely hydrolysed (99%) into glucose molecules by glucoamylase enzyme which action is catalysed by the yeasts (*Saccharomices Cerevisiae*).

The outlet stream from the fermenter (*beer*) contains also small quantities of sub-products such as acetaldehyde, methanol, butanol, acetic acid and glycerol.

Note that a large quantity of carbon dioxide is also produced: while most of it is immediately purged, the rest is supposed to be removed in a degasser drum prior to the distillation section. Since the gas purge stream is not free of ethanol, an absorption column is used to recover it and clean the gas before venting. The scrubbing water is recycled upstream to the slurry tank.

It is assumed that the distillation section involves three columns: the fermentation broth is split into two streams fed to two stripping columns at different pressure conditions (1.7 and 0.5 bar). The distillate products (with an ethanol content of about 50% by weight) are sent to the final rectifying column (5 bar). This last unit 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 required fuel grade (99.8%).

The condensing heat of the rectifier column supplies the reboiler energy demand at the 1.7 bar stripping column; in cascade, the heat of condensation of the distillate in this latter column is exploited to boil up the bottoms of the vacuum stripping column.

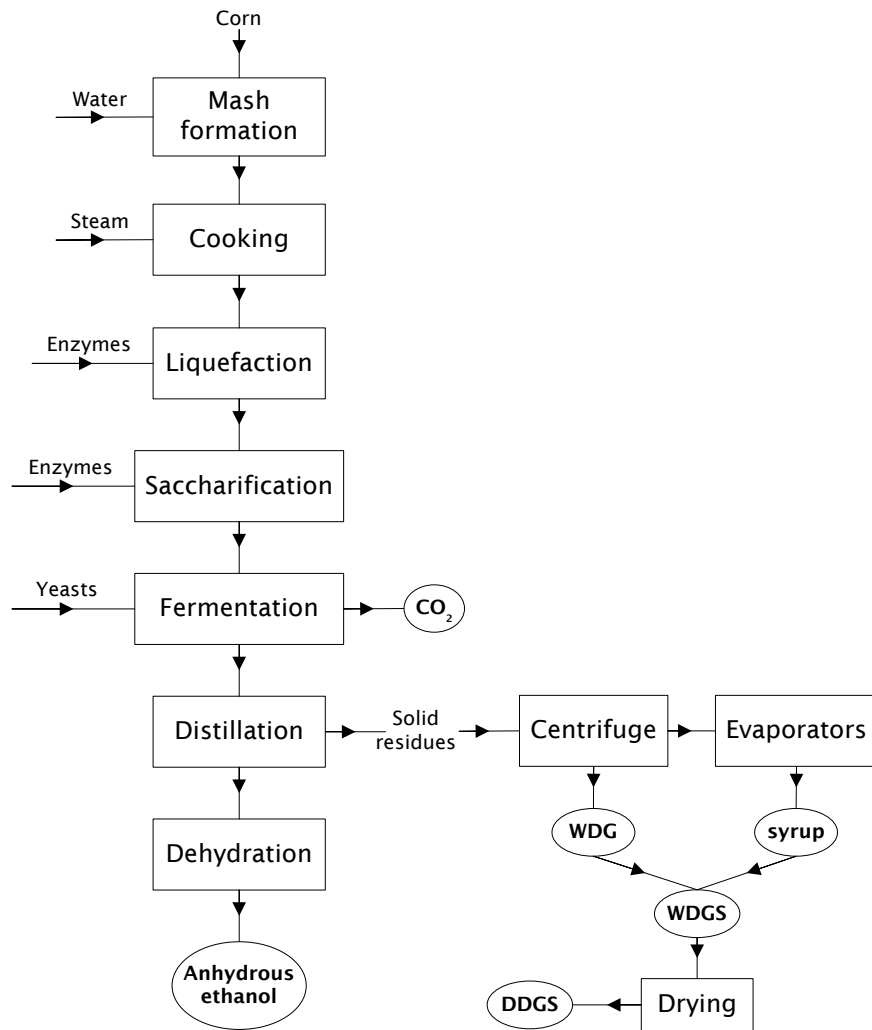


Figure 3.6 Block Flow Diagram of the Dry Grind process.

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 *backset*, while the rest is sent to a multiple-effect evaporator. Here it is concentrated 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 main by-product, namely DDGS, with a moisture content of about 10%, suitable as animal feed substitute or as a valuable fuel to produce heat and power. The process overall mass and energy balances are summarised in Table 3.4 and Table 3.5.

Since energy is the second largest terms among production costs, the process optimisation should first consider the possibility of meeting both electricity and steam demands by means of solutions able to increase the process energy efficiency. Combined Heat and Power generation (CHP) has been identified as a suitable alternative that could be applied to current technology in reaching solid cost savings and returns. Accordingly, we have been formulating

and evaluating three different options, which basically differ in the fuel choice: natural gas, vegetable oil and the DDGS itself. The main technical assumptions and fuels properties are summarised in Table 3.6.

Table 3.4 Overall mass balance.

	[kg/h]	[kg/kg _{EtOH}]
water	8,107	0.597
cooking steam	8,400	0.619
corn	41,875	3.085
enzymes (dry basis)	68.34	5.034 10 ⁻³

Table 3.5 Overall energy balance.

natural gas	1.15 [t/h]	0.085 [kg/kg _{EtOH}]
electric power	7 [MW]	515 [W/kg _{EtOH}]

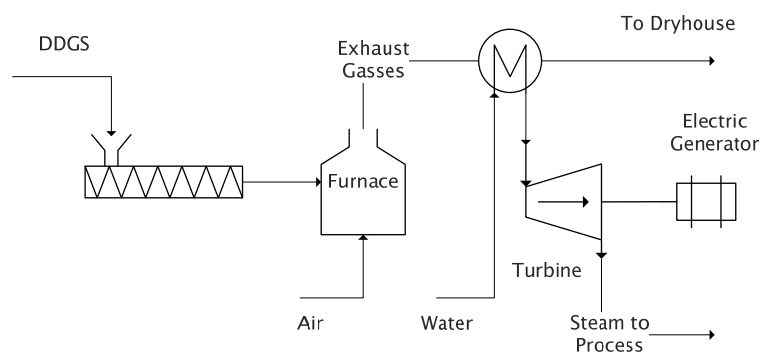
A different solution is represented by a vegetable oil power station, designed to meet electric power requirements and part of the heat power needs: in fact, such plants are not as efficient as gas CHP and it is not reasonable to get from them all the process steam, as a huge power station would be needed. Several commercial solutions are available, among which an engine capable of producing 8 MW of electric power and 4.1 t/h of steam has been chosen (Wartsila, 2006). The oil consumption is about 1,613 t/y. In this case, an additional gas-fed boiler for matching the steam demand is needed. Assuming its thermal efficiency equal to 80%, the natural gas consumption is equal to 3,565 t/y.

As a third choice the possibility of using the entire DDGS production (about 105,500 t/y) as fuel to provide both process heat and electricity has been taken into account. This solution allows producing 20 MW of electric power and all the heat power required by both the ethanol production and the DDGS drying section. It is important to highlight that, whereas the previous CHP solutions allowed the implementation of a rigorous computation thanks to the availability of technical data required, in the case of a DDGS burner the estimation of the biomass needs and energy outputs have been based on a set of efficiency parameters retrieved from the literature (Morey *et al.*, 2006). For instance, the electricity production was assessed by means of a *generation parameter* defined in terms of kWe per litre of ethanol produced. A schematic flowsheet of the DDGS heat and power plant are presented in Figure 3.7.

Table 3.6 Summary of the technical assumption and data for heat and power stations.

data	value
steam requirements	35.8 t/h 26.6 MW
electric power requirements	7 MW
DDGS drying power	11 MW
DDGS dryer efficiency	80 %
LHV _{GAS}	802 MJ/kmol
LHV _{OIL}	40.4 MJ/kmol
LHV _{DDGS} (dry basis)	20.9 MJ/kmol
exhausts Specific Heat	1.084 kJ/kg K
exhausts Temperature limit	< 100 °C
gas turbine	
electric power	25.2 MWe
thermal efficiency	34.6 %
exhausts mass flow	92.2 Kg/s
exhausts temperature (after turbine expansion)	488 °C
vegetable oil engine	
electric power	8 MWe
thermal efficiency	46 %
fuel flow	0.448 kg/s
exhausts mass flow	15.5 Kg/s
exhausts temperature (after engine)	347 °C
boiler efficiency	80 %
DDGS burner	
electric energy production	1.15 kWe/L _{EtOH}
heat energy production [§]	9.67 MJ/L _{EtOH}
DDGS required	0.31 kg/kg _{com}

[§] discharge temperature high enough to meet process needs

**Figure 3.7** CHP Station: DDGS burner.

The main goal of this part of the work was to assess the business scenario of a standard DGP so as to quantify the economics of the process. The quantification has been carried out by means of a financial analysis for both the base case and the alternative solutions proposed. A financial model (Douglas, 1988; Peters *et al.*, 2003) capable of both evaluating production costs (capital² and operational) and assessing the economic profitability has been developed.

Table 3.7 Summary of the parameters and data for financial modelling.

data	value
total capital investment (M€)	
standard process	70
gas turbine CHP plant	14.15
oil engine CHP plant	7.41
DDGS burner CHP plant	20.25
prices	
ethanol denaturated	0.58 €/L
DDGS	300 €/t
electric energy (sold to the grid)	25.9 €/MWh
corn	160 €/t
process water	0.041 €/t
denaturant	0.26 €/l
yeasts	0.516 €/kg
enzymes	5 €/kg (α -amylase) 3.5 €/kg (g-amylase)
urea	132.74 €/t
sulphuric acid	69.32 €/t
lime	51.62 €/t
utilities	
steam	14.31 €/t
natural gas	0.268 €/kg
electricity	0.103 €/kWh
vegetable oil	501 €/t
other costs	
labours	33,500 €/labour
maintenance	3 % TCI
administration	2 % Total Revenue
start up	10 % TCI

² The capital annualising has been done by means of a *straight line method* distributed in a 10 years plant life time.

Main parameters and data utilised in model formulation are reported in Table 3.7.

In the case of conventional corn-based ethanol production, incomes result from ethanol and DDGS sales (no electricity is sold to the grid), while production costs derive from the overall capital (annualized TCI) and operating costs (raw materials, chemicals, utilities, M&Os and general expenses). On the other hand, if a CHP plant is integrated to the process, electricity is potentially an additional product to be sold to the market. In the base case, it has been assumed that electricity and steam are acquired from an external supplier, so that the gas requirements are due exclusively to DDGS drying system.

If a renewable fuel is used then there is the possibility to obtain a financial support in terms of Green Credits. They represent the basic driver to adopt a CHP technology based on a renewable fuel. As a matter of example, let us consider the Italian situation (GSE, 2009): if a natural gas turbine is used, the selling price for the electricity is about 91.34 €/MWh (and it is permitted only for 15 hour a day, corresponding to 5,094 h/y); on the other hand, if a renewable fuel is chosen, a grant of 180 €/MWh for 24 hour a day (corresponding to 8,150 h/y) for at least 12 years is awarded.

In order to complete the economic analysis oriented to calculate the model parameters, a last analysis has been carried out by considering the effect of the plant capacity on the overall profitability. Previous data were based on an ethanol productivity of about 110,000 t/y (that is the production capacity of the first corn-based ethanol plant that is supposed to be operating in Italy). However, production costs are sensitive to plant capacity as there is an economy of scale effect on capital and operating costs. Economic theories (Douglas, 1988) agree about the fact that operating costs increase proportionately with the plant size, whereas this does not happen with capital cost that increases less rapidly. A commonly used relationship between capital cost (PCC) [€] and plant capacity ($PCap$, in this formula expressed as [kt/y]) is as follows:

$$PCC = a \cdot PCap^r \quad (3.1)$$

where a is a constant and r is the increasing factor, whose value ranges from 0.4 to 0.9 (Peters *et al.*, 2003). Recent works (Gallagher *et al.*, 2005) suggest a power factor of 0.836 for the ethanol industry, whereas a is (from industrial data) to be equal to 1.132.

To achieve a linear formulation (required by the mathematical modelling features as defined in the following Chapters), the plant capacity was discretised into four capacity intervals p . The operating limits ($PCap_p^{\max}$ and $PCap_p^{\min}$) were deducted from current industrial design (beyond those limits, operating a plant is either non-practicable or economically unsustainable). Once the discrete intervals were defined, the nominal sizes ($PCap_p$) were used to estimate PCC_p . The unit production costs (UPC_{fp}) for each different interval were estimated by using the economic model described above.

Biomass costs and capital investment depreciation charges were deducted from ethanol production costs as they will be comprised in the overall SC operating costs assessment. Table 3.8 summarises the model parameters related to each plant capacity size.

Table 3.8 Ethanol production stage parameters.

plant size p	$PCap_p$	$PCap_p^{max}$	$PCap_p^{min}$	PCC	$UPCf_p$
1	110	120	80	70	0.160
2	150	160	140	91	0.154
3	200	210	190	115	0.151
4	250	260	240	139	0.149

It is also noteworthy to assess the effects on the economics when either one of the two options for DDGS end-use (as animal feed substitute or alternatively as fuel for a CHP station) is adopted. Selling DDGS as an animal feed substitute, for instance, entails a cost allocation of 20% to discount from the entire SC overheads (Hammerschlag, 2006). The situation changes if it is used for CHP production as the cost allocation decreases to about 15% (according to the outcomes coming from the economic evaluation previously described); however, also the unit production costs $UPCf_p$ reduce substantially thanks to the energy savings. This required the redefinition of the $UPCf_p$ for each plant capacity range. Table 3.9 summarises the model parameters related to the biofuel production in the second instance.

Table 3.9 Ethanol production costs when DDGS is used to provide for the process energy needs.

plant size p	$UPCf_p$
1	0.060
2	0.049
3	0.041
4	0.029

3.4 Life Cycle Analysis

The environmental evaluation of the system performance requires an LCA assessment. This is carried out according to the principles and standards laid out by the International Standards Organization (ISO, 1997). The environmental performance measurement involves the GHG emissions bill, evaluated by adopting a WTT approach (CONCAWE, 2007) in order to consider the supply network operating impact on global warming from the biomass production all along toward fuel distribution to customers. Issues such as potential differences in vehicle conversion efficiency (fuel energy to mechanical energy) as well as in vehicle

technology related to the substitution of gasoline, the so called Tank-to-Wheel (TTW) contribution to the overall impact, were not dealt with in accordance to two assumptions: i) in a novel biofuel system the new fuel should be used in blends that do not need specific engines or equipment; ii) carbon dioxide emissions resulting from the combustion of the biofuel are assumed to trade-off part of the carbon dioxide captured during crop growth and are therefore not included in the total count.

The bioethanol production system layout depicted in Figure 3.1 must be now extended to include the biomass drying and storage stage (previously counted as part of the conversion process) within the set of LC stages. Accordingly, the extended set (represented in Figure 3.9) considered in evaluating the environmental performance of bioethanol production system is:

$$s \in S \equiv \{bc, bds, bt, fp, ft\}$$

where *bds* stands for biomass drying and storage stage.

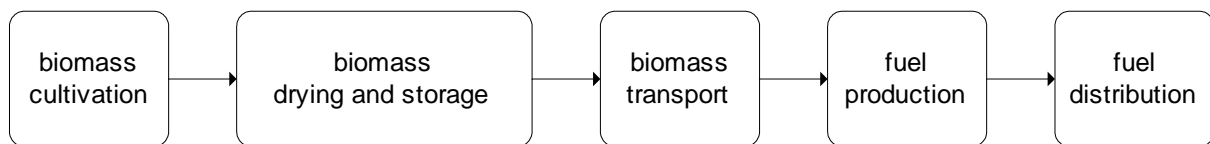


Figure 3.9 Life cycle stage of a biomass-based fuel SC: Well-to-Tank approach.

The last step in outlining the general features of the LCA analysis is the *emissions inventory*. Here we list the set of environmental burdens to be counted for evaluating the total ecological damage associated to the SC operation within the boundaries previously defined. In particular, the GHG contribution on global warming was captured by inventorying the following set of burdens:

$$b \in B \equiv \{\text{CO}_2, \text{CH}_4, \text{N}_2\text{O}\}$$

which were grouped together in a single indicator in terms of carbon dioxide equivalent emissions (CO₂-eq). The derivation of carbon dioxide equivalent emissions is based on the concept of 100-year global warming potentials (GWP) as specified by the International Panel on Climate Change (IPCC, 2001).

The global emission factors definition has been the crucial point of this part of the work: it is only through a rigorous set of parameters that the needs for accuracy and thoroughness required by the abovementioned exogenous comparison can be met. To comply with these requirements, it has been made the use of an interactive spreadsheet based tool specifically developed to investigate the GHG emission related to wheat-to-ethanol production in UK (Brown *et al.*, 2005). This rigorous tool uses default values based on a typical production

chain. The default input values have been modified and adapted in order to calculate the specific emission factors for corn-based ethanol production in Italy.

3.4.1 Biomass cultivation

Actual data regarding the Italian corn cultivation practice and, in particular, crop yields, mineral (N, K and P) and organic (cattle manure) fertilizers requirements, seeds and pesticides usage, and diesel fuel for irrigation were retrieved from both literature and Governmental institution databases (Grignani and Zavattaro, 2000; Grignani *et al.*, 2007; Guerini *et al.*, 2006; Locatelli, 2007; Marchetti *et al.*, 2004; Sacco *et al.*, 2003). As important differences exist between wheat and corn cultivation practices, the actual values of the global emission factors for corn cultivation ($f_{bp,g}$) were calculated adopting the equations recommended by the IPCC guidelines (IPCC, 2006).

Global emission factors are calculated with reference to one hectare of cultivated land. In order to match the needs of the mathematical formulation adopted, the set of $f_{bp,g}$ is assumed to be grid specific (and to refer to the units of biomass produced). This is not a trivial unit conversion exercise, because just a subset of the input parameters depends on the corn yield. As a consequence, the conversion was based on the following assumptions:

- i. mineral fertilizers usage was described³ as linearly dependent on the corn yield³: the larger the local yield the larger the amount of mineral fertilizers per unit of land (and the emissions due to fertilizers production);
- ii. organic fertilizer usage per unit of cultivated land was set constant: the larger the corn yield the lower the soil emissions due to manure usage;
- iii. diesel usage for irrigation per unit of cultivated land was set constant: the larger the corn yield the lower the emissions due to diesel usage.

As a result, a grid-dependent set of parameters was generated as illustrated in Figure 3.10, where every diamond represents the global emission factors $f_{bp,g}$ as a function of the crop yield. In this way, it was possible to represent the real situation adequately: the optimal impact per unit of biomass produced comes from a trade-off between usage of resources and effective corn yield.

The global emission factor identifying the foreign supplier ($g = 60$) was calculated by assuming a hypothetical corn yield that was set equal to the average CY_g value weighted on the Italian data. Under this assumption $f_{bp,60}$ turns out to be equal to 359.9 kg CO₂-eq/t. This approximation is needed to overcome the lack of actual data for the supplier countries

³ This is not generally true, but it is a reasonable compromise in the corn yield range considered in this study.

considered in the SC analysis. However, our analysis indicates that this assumption does not affect the quality of the results in a significant way.

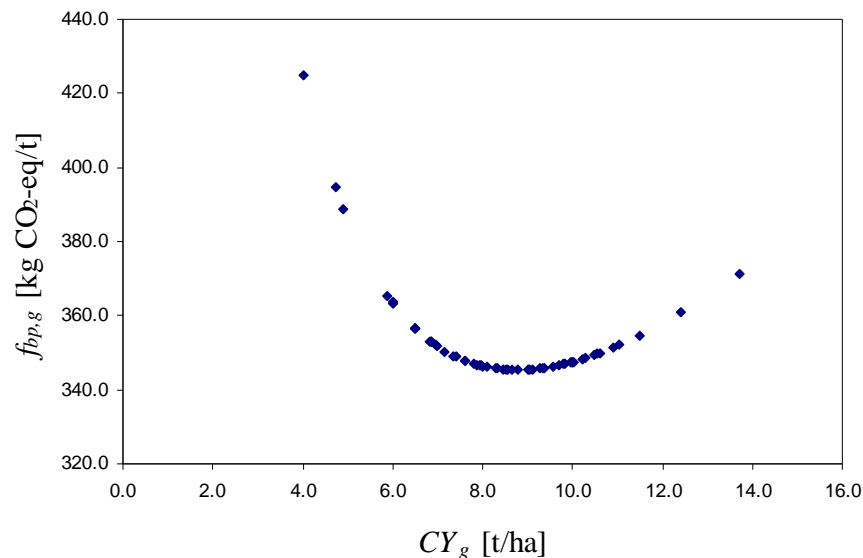


Figure 3.10 Global emission factors for corn cultivation ($f_{bp,g}$): the emission factor depends on the actual crop yield.

3.4.2 Biomass Drying and Storage

With respect to the GHG emissions related to biomass drying and storage, the set of parameters was derived from the spreadsheet results by implementing the model with country specific data. In particular, the emissions related to diesel and electricity usage in Italy were taken from DEFRA (2008) and EME (2003), respectively. Accordingly, the value of f_{bds} was set equal to 63.34 kg CO₂-eq/t.

3.4.3 Transport System

Global emission factors specific to each transport option were taken from DEFRA (2008). Table 3.10 reports the resulting transport related emission factors for biomass delivery and ethanol distribution ($f_{bt,i}$ and $f_{\hat{t},i}$, respectively).

3.4.4 Ethanol Production

Given the existing similarity between the wheat-based and the corn-based technology to convert starch into ethanol, also in this case the global emission factors have been directly calculated from the spreadsheet. Default values related to raw materials and utilities needs for wheat-based production have been replaced with those specific for corn-based production as evaluated in the previous section. Accordingly, the global emission factor for fuel production (f_{fp}) resulting from the spreadsheet calculation is equal to 1052.23 kg CO₂-eq/t.

Table 3.10 Global emission factors $f_{s,l}$ for different transport modes.

mean l	$f_{s,l}$ (kg CO ₂ -eq/t·km)
small truck	0.591
truck	0.123
rail	0.021
barge	0.009
ship	0.007
trans-ship	0.006

3.4.5 Emission Credits

In this work, according to Delucchi (2006), no credits have been assigned for land use. In fact, considering the conversion from crop-for-food to crop-for-fuel this raises a gap into the market that has to be filled by either buying corn from other markets (resulting in even higher impact) or cultivating other lands (resulting in less impact in case of set-aside land). Therefore, it makes sense to consider the average situation in which no credits come from land use.

Hence GHG emission credits are only associated to products displacement by using DDGS as valuable product for other markets. In particular, DDGS has value either as substitute of soy-meal as animal feed or as fuel in CHP generation. The formulation adopted in this stage of the project allows for the alternative choice between these two options on the use of DDGS, and then calculates credits for the GHG emissions avoided through product displacement.

In Italy soy-meal for animal feed is usually imported from Brazil. Unfortunately, limited data are available on life cycle emission from production and importation of Brazilian soy-meal to Italy. Therefore, the default data set regarding imported soy-meal from the USA has been used. They have been retrieved in CONCAWE (2003), where it is reported that each kilogram of DDGS is supposed to replace 0.78 kg of soy-meal, on the basis of relative protein content. Production in the USA and transport to EU of each kilogram of meal result in emissions of 0.46 kg CO₂-eq.

Concerning with DDGS used as fuel in CHP generation, credits have been calculated under the assumption (Morey *et al.*, 2006) that burning the all production of DDGS is enough to satisfy the production process utilities needs (in terms of both electricity and natural gas) plus a surplus of electricity that can be sold to the grid. This corresponds to a displacement of 12.3 GJ of natural gas and 5.2 GJ of electricity for each ton of ethanol produced (assuming a fixed yield of 0.954 kg_{DDGS}/kg_{EtOH}).

Chapter 4

Steady-State Design: Cost Minimisation

This Chapter¹ deals with the description of the steady-state spatially explicit MILP model devised for the strategic design of biofuels SCs under costs minimisation. A general description of the biofuels SC design issues is firstly presented. Next, the mathematical formulation of the main body of the model is drawn in details. The SC optimisation is then carried out referring to the case study presented in Chapter 3 and considering two instances: an unconstrained optimisation and a case where the current industrial plan for bioethanol production is taken into account. This is followed by a discussion of the results. Some final remarks on the model capabilities and shortcomings to be overcome conclude the Chapter and introduce the issues treated in the next one.

4.1 Problem statement

The design process involving a general biofuel SC usually entails a wide range of decisions relating to the best network configuration to be established in order to achieve the desired performance. Referring to bioethanol systems strategic design, decisions deal with geographical location of biomass cultivation sites, logistic definition of transport system and location as well as capacity assignment of production facilities. The design problem discussed here can be stated as follows. Given the following inputs:

- > geographical distribution of demand centres;
- > fuel demand over a fixed time horizon;
- > biofuel market characteristics;

¹ Portions of this Chapter have been published in Zamboni *et al.* (2008), Zamboni *et al.* (2009a) and Zamboni *et al.* (2009b).

- > biomass geographical availability;
- > biomass production costs;
- > biofuel production facilities capital and operating costs;
- > transport logistics (modes, capacities, distances, availability and costs),

the objective is to determine the optimal system configuration in terms of SC operating costs. Therefore, the key variables to be optimised are:

- > geographical location of biomass production sites;
- > biomass production for each site;
- > supply strategy for biomass to be delivered to production facilities;
- > biofuel production facilities location and scale;
- > distribution processes for biofuel to be sent to blending terminals;
- > SC management costs.

The general modelling framework has been formulated as an MILP problem and a spatially explicit approach (based on the grid introduced in Chapter 3) has been adopted so as to consider the well-known geographical dependence characterising any biofuel system. The model has been developed under steady-state conditions, therefore assuming all the parameters and variables invariant with time. Although biomass based systems are inherently dynamic, a static representation allows for a more detailed description and a lighter computational burden. As a result, biomass production (varying along the year) was averaged on a daily-based set. On the other hand, the time-variant nature of the product demand was addressed by formulating different demand scenarios representing the SC evolution pathway over the time horizon under investigation. A dynamic approach will be discussed in Chapter 6.

4.2 Mathematical formulation

The mathematical formulation of the proposed framework is based on the modelling approaches adopted in the strategic design of a multi-echelon SCs (Sahinidis *et al.*, 1989; Tsiakis *et al.*, 2001); it also embodies different features for spatially explicit facilities siting (Almansoori and Shah, 2006) and for capacity planning (Hugo and Pistikopoulos, 2005) of strategic fuel systems.

4.2.1 Objective function

The mathematical formulation of the MILP being investigated commences with the definition of the optimisation criterion upon which the system should be configured. The single objective considered here is the minimisation of the total daily costs TDC [€/d] in establishing and operating a biofuel supply chain. As a consequence, the TDC definition needs to embody the one-time investment to establish new production facilities as well as the overhead coming from the supply chain operation in terms of both biomass and fuel production costs along with transport expenses:

$$TDC = \frac{FCC}{\alpha} \cdot CCF + PC + TC \quad (4.1)$$

where the facilities capital costs FCC [€] is annualised through a capital charge factor CCF (0.333 y^{-1}) and divided by the network operating period α (340 d/y); the additional terms are the production costs PC [€/d], accounting for both biomass and fuel production, and the transport costs TC [€/d].

Once the optimisation criterion has been defined, all the terms included within the mathematical formulation have to be expressed as explicit functions of the design variables.

4.2.1.1 Facility capital costs

The FCC term accounts for the capital investment required to build up a new fuel conversion plant; this means that no other facilities (e.g., the biomass production related equipments or the product delivery transport means) are considered to contribute to the overall investment. The underlying assumption is that a biofuel system is not a completely ex-novo process but can be integrated to (part of) the existing production system. Therefore, FCC can be evaluated by simply summing up the capital cost PCC_p [€] of each single conversion plant size p in the territory, as expressed by the following equation:

$$FCC = \sum_{g,p} PCC_p \cdot Y_{p,g} \quad (4.2)$$

where $Y_{p,g}$ is the binary decision variable controlling whether to establish a production facility of size p in region g : a value of 1 allows the construction of a new production plant, otherwise 0 is assigned. It is worth stressing that this equation allows taking into account the plant scale effect on the capital costs as a discrete function of the production capacity (Gallagher *et al.*, 2005), as described in Chapter 3.

4.2.1.2 Production costs

Production costs PC relate to the net expenses required to operate fuel conversion plants as well as to manage biomass cultivations. Therefore, the final expression is given by:

$$PC = \sum_g \left(UPCb_g \cdot P_{biomass,g}^T + \sum_p UPCf_p \cdot Pf_{p,g} \right) \quad (4.3)$$

where $UPCb_g$ [€/t] is the local (in element g) biomass production cost, $P_{biomass,g}^T$ [t/d] is the local biomass production rate, $UPCf_p$ [€/t] is the biofuel production costs for plant size p , and $Pf_{p,g}$ [t/d] is the biofuel production rate from a plant of size p situated in g .

4.2.1.3 Transport costs

In this work, the transport system is treated as an additional service provided by existing actors already operating within the industrial/transport infrastructure. As a consequence, TC is evaluated as follows:

$$TC = \sum_{i,l} \left(UTC_{i,l} \cdot \sum_{g,g'} NTU_{i,g,l,g'} \cdot TCap_{l,i} \cdot ADD_{l,g,g'} \right) + UTC^* \sum_g NTU_l_g \cdot TCap^* \cdot LD_{g,g} \quad (4.4)$$

where $UTC_{i,l}$ [€/(tkm)] is the unit transport cost of product i via mode l , $NTU_{i,g,l,g'}$ is the number of transport units of mode l needed to transfer i between two elements g and g' , $TCap_{l,i}$ [t/trip] is the transport capacity for i via l , $ADD_{l,g,g'}$ [km] is the actual delivery distance for mode l between g and g' , UTC^* [€/(tkm)] is the unit transport cost for biomass transfer within g , NTU_l_g is the number of transport units (trucks of small capacity) for internal transfer within element g , $TCap^*$ [t/trip] is the internal transport capacity for biomass transfer, and $LD_{g,g}$ [km] is the average delivery distance within each element g .

The above formulation is very convenient as it acknowledges the modular nature of a transport system even without using time dependent variables. In fact, the product $NTU_{i,g,l,g'} \cdot TCap_{l,i}$ in Equation (4.4) forces the model to opt for a fully loaded transport unit for products delivery. Also, it can be observed that an analogous formulation is used to represent the costs related to the transfer of biomass within an element g ; that is necessary, for example, to account for the collection of corn before the delivery to other network elements or to supply the conversion plant sited within the same region.

Distance $ADD_{l,g,g'}$ is further decomposed as:

$$ADD_{l,g,g'} = LD_{g,g'} \cdot \tau_{l,g,g'} \quad (4.5)$$

where $LD_{g,g'}$ [km] is the local distance, resulting from the measurement of the straight route between the centre of each network element g , and $\tau_{l,g,g'}$ is the tortuosity factor depending on the different transport mode l .

Here, we also introduce two constraints:

$$NTU_{i,g,l,g'} \geq \frac{Q_{i,g,l,g'}}{TCap_{i,l}} \quad (4.6)$$

and

$$NTU_l \geq \frac{P_{biomass,g}^T}{TCap^*} \quad (4.7)$$

with $Q_{i,g,l,g'}$ [t/d] the flow rate of i via l between two grid elements g and g' . They simply impose that the number of transport units must be sufficient to transfer all of the product to be delivered.

4.2.2 Logical constraints and mass balances

All the cost terms in the objective function (4.1) depend on the design variables related to the fuel and biomass production, the product demand and the mass fluxes between grid points. The SC behaviour is then captured through the definition of mass balances as well as logical constraints that must be satisfied in each of the supply chain nodes.

4.2.2.1 Demand constraints

As usual in SC management, the driver of the design process of a biofuel supply network can be identified in the system capabilities of satisfying the product demand imposed by markets. Therefore, the superstructure capturing process has to be initiated through the biofuel demand definition in terms of the logical relation to the other main variables. According to this, it can be stated that the product demand $D_{i,g}^T$ [t/d] must be satisfied either by local production or by importing the commodity from other regions. This is defined by the following condition:

$$D_{i,g}^T = D_{i,g}^I + D_{i,g}^L \quad \forall i, g \quad (4.8)$$

where $D_{i,g}^I$ [t/d] identifies the amount imported in g to fulfil the demand of product i , and $D_{i,g}^L$ [t/d] the demand obtained through local production. Furthermore, the following constraints must hold:

$$D_{i,g}^L \leq P_{i,g}^T \quad \forall i, g \quad (4.9)$$

$$D_{i,g}^I \leq \sum_{l,g'} Q_{i,g,l,g'} \quad \forall i, g \quad (4.10)$$

i.e., the actual local production $P_{i,g}^T$ has to be at least equal to $D_{i,g}^L$, and $D_{i,g}^I$ cannot exceed the mass fluxes entering the region.

Biomass demand is bounded by the technological limits deriving from capacity of the production facilities to convert raw materials into fuel. Therefore, the local demand of biomass can be determined by applying a conversion factor γ (set equal to 0.324 kg_{EtOH}/kg_{biomass}) to the fuel production rate, as shown by the following equation:

$$D_{biomass,g}^T = P_{fuel,g}^T / \gamma \quad \forall g \quad (4.11)$$

Finally, a global constraint is placed on the supply network capabilities to satisfy the market requirements. This means that total production should cover the overall demand of commodity, as defined by the following equation:

$$TP_i \geq TD_i \quad \forall i \quad (4.12)$$

where total production TP_i [t/d] and total demand TD_i [t/d] of product i are obtained by adding up the local production and demands, respectively:

$$TD_i = \sum_g D_{i,g}^T \quad \forall i \quad (4.13)$$

$$TP_i = \sum_g P_{i,g}^T \quad \forall i \quad (4.14)$$

4.2.2.2 Production constraints

A new set of relations is formulated to constrain the commodity production rate. In particular, a global mass balance needs to be written for each product i and element g :

$$P_{i,g}^T = D_{i,g}^T + \sum_{l,g'} (Q_{i,g,l,g'} - Q_{i,g',l,g}) \quad \forall i, g \quad (4.15)$$

Fuel production can be achieved through conversion plants of different sizes. Therefore, the total amount of fuel produced in each element g results from the sum of the production rate of all plants of size p established in that same region:

$$P_{fuel,g}^T = \sum_p Pf_{p,g} \quad \forall g \quad (4.16)$$

Furthermore, $Pf_{p,g}$ must fall within certain limits ($PCap_p^{\max}$ and $PCap_p^{\min}$ [t/d]) defined respectively as the maximum and minimum production rate allowed:

$$Y_{p,g} \cdot PCap_p^{\min} \leq Pf_{p,g} \leq Y_{p,g} \cdot PCap_p^{\max} \quad \forall p, g \quad (5.17)$$

It is also assumed that only one conversion facility can be established within the territorial element and, therefore, we have that:

$$\sum_p Y_{p,g} \leq 1 \quad \forall g \quad (4.18)$$

Condition (4.18) reduces the model complexity without affecting the optimisation results significantly: in fact, note that a single large plant represents a less costly option than two or more smaller plants adding up to the same overall size.

Biomass production, too, cannot exceed the limits imposed by the effective regional production capability, which depends on agronomic-related factors such as maximum and minimum biomass cultivation fractions BCD_g^{\max} and BCD_g^{\min} of cultivated land over arable land in element g , and the cultivation yield CY_g [t/(d·km)]; additionally, the geographical characteristics such as the actual surface in an element GS_g [km²] and the related percentage of arable land AD_g contribute to define the biomass productivity. Thus, the following condition must hold:

$$GS_g \cdot CY_g \cdot AD_g \cdot BCD_g^{\min} \leq P_{biomass,g}^T \leq GS_g \cdot CY_g \cdot AD_g \cdot BCD_g^{\max} \quad \forall g \quad (4.19)$$

In order to avoid the potential risk of a local conflict between “biomass-for-food” and “biomass-for-fuel”, a maximum biomass utilization quota should be assumed to limit the total domestic production and is formulated as an utilisation factor ($SusP$) to be applied to the overall potential domestic biomass production $TPot$ [t/d]:

$$TP_{biomass} \leq SusP \cdot TPot \quad (4.20)$$

where:

$$TPot = \sum_g GS_g \cdot CY_g \cdot AD_g \cdot BCD_g^{\max} \cdot CF_g \quad (4.21)$$

with CF_g the binary parameter for the domestic biomass cultivation sites (a value of 1 identifies domestic regions; otherwise 0 is assigned).

4.2.2.3 Transport constraints

The last set of variables to be constrained is related to the transport system. First of all, it must be ensured that:

$$Q_{i,l}^{\min} \cdot X_{i,g,l,g'} \leq Q_{i,g,l,g'} \leq Q_{i,l}^{\max} \cdot X_{i,g,l,g'} \quad \forall i, l, g, g' \quad (4.22)$$

where $Q_{i,l}^{\min}$ and $Q_{i,l}^{\max}$ [t/d] represent the logical capacity limitations needed to justify the establishment of a transport link between elements: for instance, considering the case of transport via railways, the minimum and maximum flow rate allowed through a single route have been set equal to four and sixteen railcars respectively, according to common practice in the Italian rail system; $X_{i,g,l,g'}$ is the decision variable: its value is 1 if the transfer of product i between g and g' via mode l is allowed, and 0 otherwise.

The flow rate of a specific product i between adjacent elements is expected to occur only in one direction, either to satisfy the local demand or to cross an element towards a further destination. Accordingly, we have:

$$\sum_l X_{i,g,l,g'} + \sum_l X_{i,g',l,g} \leq 1 \quad \forall i, g, g': g \neq g' \quad (4.23)$$

The following condition:

$$\sum_i \sum_l X_{i,g,l,g} \quad \forall g \quad (4.24)$$

is added to avoid internal loops of product within the region itself (which may occur because of numerical issues).

Finally, the representation of the logistics behaviour is completed by a transport feasibility condition (e.g., transport by barges cannot be allowed if a waterway is not available):

$$\sum_{i,l,g,g'} X_{i,g,l,g'} = 0 \quad \forall i, g, l, g' \neq Total_{i,g,l,g} \quad (4.25)$$

4.2.2.4 Non-negativity constraints

The last constraints simply impose that a number of variables should maintain a physical meaning, i.e. they must be non-negative:

$$D_{i,g}^I \geq 0 \quad \forall i, g \quad (4.26)$$

$$D_{i,g}^L \geq 0 \quad \forall i, g \quad (4.27)$$

$$P_{i,g}^T \geq 0 \quad \forall i, g \quad (4.28)$$

$$P_{p,g}^f \geq 0 \quad \forall p, g \quad (4.29)$$

$$Q_{i,l,g,g'} \geq 0 \quad \forall i, l, g, g': g \neq g' \quad (4.30)$$

4.3 Case study

The case study described in Chapter 3 has been used to assess the modelling framework and to demonstrate the applicability as well as the potential capabilities of the proposed approach in steering the strategic design of energy systems such as biofuels supply networks.

Two demand scenarios (derived from the ethanol market penetration imposed by the current Governmental policy) have been considered:

A 3% penetration by energy content for 2009;

B 5.75% penetration by energy content for 2010.

The related bioethanol demand has been calculated by applying the methodology described in Chapter 3. Table 4.1 shows the ethanol demand values for each blending terminal in the two scenarios.

The Italian industrial plan (involving the establishment of four plants, as described in Chapter 3) was compared to the best SC design obtainable without imposing any constraints on plant location or capacity. Accordingly, for each scenario, two optimisation instances were carried out:

- 1 optimisation by fixing plant locations and capacities according to the Italian Industrial plan;
- 2 optimisation without plant location and capacity constraints.

An additional analysis has been performed to assess the effective implications entailed in the use of domestic biomass rather than imported one. The possibility to import ethanol was not considered in this work, following the national policy (common in most EU countries) aiming at supporting an energy security objective through local fuel production. Note that importing

corn does not affect such goals substantially, as there exists an internal corn production (which, if needed, may substitute imports).

Table 4.1 Bioethanol demand values (D_g^T) assigned to the blending centres of Northern Italy.

scenario A 3%		scenario B 5.75%	
region g	D_g^T (t/d)	region g	D_g^T (t/d)
22	65.10	22	120.53
25	87.12	25	179.35
27	185.56	27	348.02
32	87.73	32	179.64
37	43.04	37	57.2
39	92.73	39	178.88
41	61.68	41	123.23
46	64.74	46	112.69
52	94.56	52	148.86

4.4 Results and discussion

The developed modelling framework has been used to perform a SC optimisation of the emerging bioethanol Italian production system. The MILP models were solved through the CPLEX solver in the GAMS[®] modelling tool (Rosenthal, 2006).

As abovementioned, two demand scenarios defined according to the market penetration imposed by the biofuels regulation have been compared. Initially, Italian corn only was considered as suitable raw material.

Instance A.1 fixes the plant location according to the most likely industrial plan, i.e. two production plants sited in Venice ($p = 1$ and $g = 32$) and Porto Viro ($p = 2$ and $g = 43$). Figure 4.1 shows the graphical representation of the optimisation results. Truck delivery is the preferred transport option for high-density products (e.g. ethanol) and for short distances; rail is chosen when large amounts of product need to be transported (corn from crop fields to production plants or ethanol from plants to truck distribution nodes).

Instance A.2 does not impose any constraints on the system configuration. Plant locations and capacity assignments are optimised to define the best trade-off between production costs (favouring high capacity centralised plants) and transport costs (reduced by a more distributed system). Two production plants are situated in elements $g = 32$ and $g = 27$ (Figure 4.2).

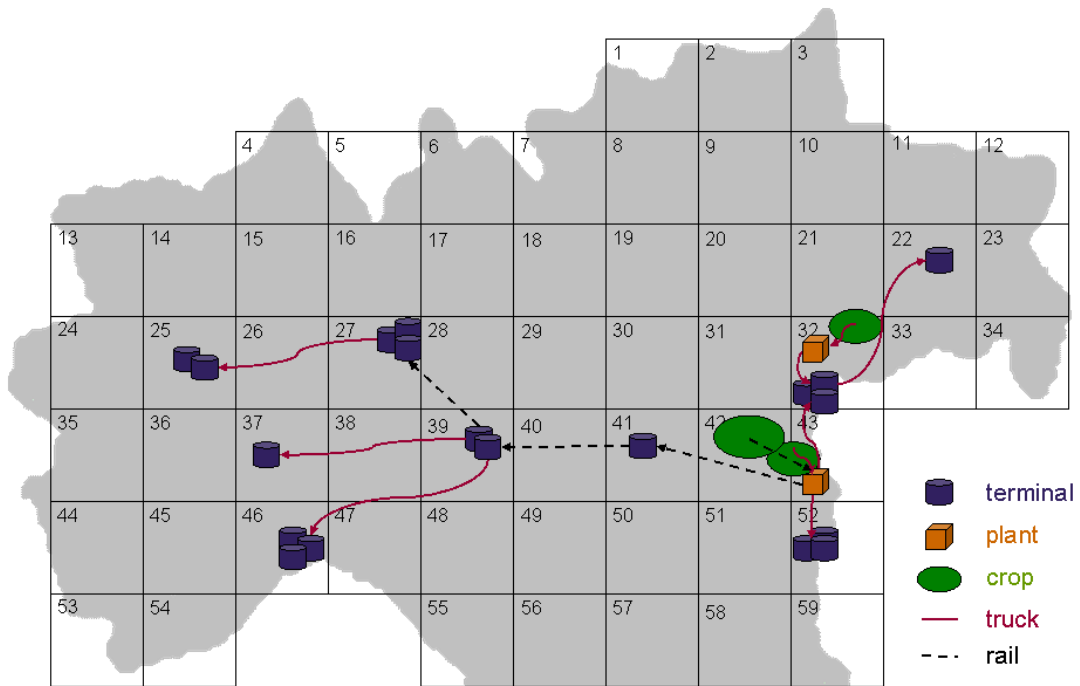


Figure 4.1 Optimal network configuration with fixed plant location: instance A.1.

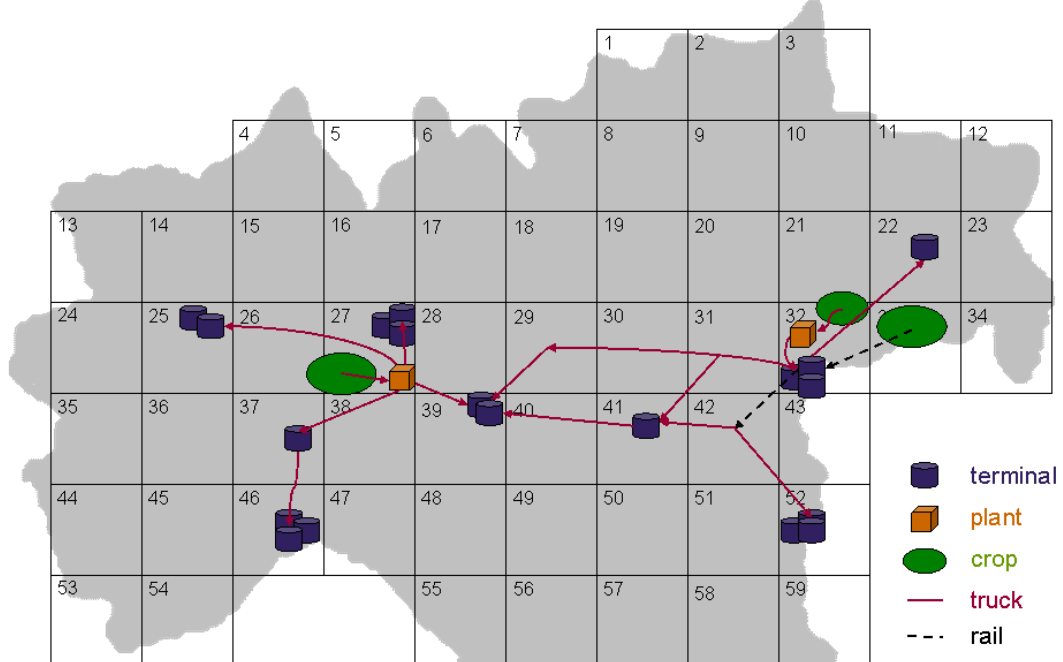


Figure 4.2 Optimal network configuration without constraints: instance A.2.

The first facility matches exactly with both the location and the capacity planned for the plant under construction in Venice (110,000 t/y). The second one is set at a capacity of 160,000 t/y and is placed in a more central area. From the results summarised in Table 4.2, it is evident that instance A.1 is a suboptimal solution: the total operating costs increase by about 4% mainly as a direct result of the transportation costs that are 35% higher than in instance A.2. The non-optimised plant location also results in a slight worsening of the biomass production site locations (accounting for a 1.1% increase in the facilities operating costs).

Instance B.1 requires all the four plants envisaged in the Italian industrial perspective. The unconstrained instance B.2 proposes two plants of large capacity ($p = 4$) in regions $g = 26$ and $g = 32$. Given the contiguity of elements $g = 26$ and $g = 27$, a nearly optimal solution could be obtained by considering only two of the facilities currently envisaged ($g = 32$ and $g = 27$) and making them larger.

Table 4.2 Demand scenario A: results of the SC cost minimisation. The third column indicated the difference (Δ) of costs in the A.1 constrained instance with respect to the A.2 unconstrained instance.

demand scenario A	instance A.1 (€/d)	instance A.2 (€/d)	Δ (%)
total daily costs (TDC)	671,255	648,056	3.6%
facilities capital costs (FCC)	157,827	157,827	0.0%
facilities operating costs (FOC)	442,894	437,873	1.1%
biomass production costs	320,355	315,430	1.6%
ethanol production costs	122,539	122,443	0.1%
transport costs (TC)	70,534	52,356	34.7%
marginal costs (€/GJ _{EiOH})	25.5	24.6	3.6%

Table 4.3 Demand scenario B: results of the SC cost minimisation. The third column indicated the difference (Δ) of costs in the B.1 constrained instance with respect to the B.2 unconstrained instance.

demand scenario B	instance B.1 (€/d)	instance B.2 (€/d)	Δ (%)
total daily costs (TDC)	1,256,672	1,161,580	8.2%
facilities capital costs (FCC)	315,655	272,522	15.8%
facilities operating costs (FOC)	817,331	802,543	1.8%
biomass production costs	590,594	586,732	0.7%
ethanol production costs	226,737	215,812	5.1%
transport costs (TC)	123,686	86,515	43.0%
marginal costs (€/GJ _{EiOH})	25.7	23.8	8.2%

Results for scenario B are summarised in Table 4.3. Smaller plant capacities (B.1) cause a significant increase in both capital and operating costs (corresponding to an ethanol production costs increase of about 5%); note that transport costs rise by about 43%. An overall increase of more than 8% in the SC operating costs occurs when instance B.1 is chosen instead of instance B.2.

Additional discussion can be based on the marginal costs evaluated from the entire supply system operating costs. Instances A.1 and B.1 determine a marginal cost for operating the whole system equal to 25.5 €/G_{EIOH} and 25.7 €/G_{EIOH}, respectively; the breakeven with gasoline production costs occurs with the oil price at about 100 \$/bbl (the breakeven value represents the oil price determining a gasoline production cost per energy unit equivalent to the bioethanol one). In scenarios A.2 and B.2, the marginal values turn out to be 24.6 €/G_{EIOH} and 23.8 €/G_{EIOH}, respectively (corresponding to a breakeven point of about 97 \$/bbl and 94 \$/bbl). Thus, as long as the oil price stays below such thresholds, the ethanol industry would need a substantial government intervention to enable the penetration of ethanol in the automotive fuels market. The Italian Government is keen on issuing a regulation imposing a minimum ethanol content in the gasoline blend. However, this kind of policy is likely to cause an increase in the fuel price. Alternatively, a different form of subsidy might be the reductions on renewable fuel taxation (Solomon *et al.*, 2007). The current regulations set the inland duties for biofuels at 13.5 €/GJ against the quota of 17.7 €/GJ applied to gasoline. This produces the obvious outcome to reduce the gap between gasoline and ethanol production costs (the breakeven point is for an oil price of 84 €/bbl considering instance A.1 and B.1, whereas it results equal to 80 \$/bbl and 78 \$/bbl in instance A.2 and B.2), but with the social effect of using financial resources.

A possible alternative aiming at the reduction of the overall SC operating costs is to allow foreign suppliers to provide the required biomass. The effect of external imports was assessed for all previous instances. Results are summarised in Table 4.4 and Table 4.5.

The results clearly show the economic convenience in availing of foreign suppliers: despite the higher transport costs due to the corn shipping as well as to the consequent distribution to conversion plants, the lower purchase cost entails an overall operating costs reduction of about 4% in instance A.1 and 5% in instance B.1. The marginal costs lower down to 24.5 €/G_{EIOH} for both cases, and that corresponds to a breakeven point with gasoline at about 96 \$/bbl (80 \$/bbl considering the mentioned subsidies). If the model were optimised without any plant location constraints, the economic benefit of importing biomass from a foreign country would increase even further: if instance B.2 is considered, the breakeven point would be about at 90 \$/bbl (74 \$/bbl if the subsidies were considered).

Table 4.4 Demand scenario A.1 with biomass importation: results of the SC cost minimisation. The third column indicated the difference (Δ) of costs in the A.1 instance without importation (Table 4.2) with respect to the A.1 instance with importation.

scenario A.1	with importation (€/d)	Δ (%)
total daily costs (TDC)	645,065	4%
facilities capital costs (FCC)	157,827	0.0%
facilities operating costs (FOC)	399,190	10.9%
biomass production costs	276,688	15.8%
ethanol production costs	122,502	0.0%
transport costs (TC)	88,047	-19.9%
marginal costs (€/GJ _{E_{EtOH}})	24.5	4%

Table 4.5 Demand scenario B.1 with biomass importation: results of the SC cost minimisation. The third column indicated the difference (Δ) of costs in the B.1 instance without importation (Table 4.3) with respect to the B.1 instance with importation.

scenario B.1	with importation (€/d)	Δ (%)
total daily costs (TDC)	1,197,056	4.9%
facilities capital costs (FCC)	315,655	0.0%
facilities operating costs (FOC)	739,650	10.5%
biomass production costs	512,913	15.1%
ethanol production costs	226,737	0.0%
transport costs (TC)	141,751	-12.7%
marginal costs (€/GJ _{E_{EtOH}})	24.5	4.9%

4.5 Conclusions

The results show that to meet the Government requirement for 2009 the best solution is to establish ethanol plants in Venice and in the industrial area of Milan with a production capacity respectively of 120,000 t/y and 150,000 t/y. For the 2010 perspective, the optimal supply network configuration suggests a capacity increase for the plant in Venice up to 240,000 t/y, and the construction of a similar capacity plant east of Milan. This solution would allow about an 8% saving on the total daily operating costs when compared to the likely planned scenario. The modelling tool can be used to provide consistent results in order to drive political decisions about energy policies for the future biofuels industry. For instance, the representation of production costs in terms of costs per unit of service provided by a fuel can be a consistent indicator to assess the actual fuel performance. These metrics have been

used as terms of comparison between different suitable options: in particular, the domestic corn supply has been compared with the imported one. Results show that as long as the oil price follows the current trend (in October 2009 price was about 87 \$/bbl (Data 360: www.data360.org)) the economic performance measured for the Italian bioethanol industry do not seems to be competitive within the fuel market. However, biomass importation may allow mitigation of the social cost of a biofuel system and supporting market penetration. Furthermore, this seems to be the only viable option if the production target is to be increased (unless second generation technologies were available for industrial production). On the other hand, importing corn from Eastern European Countries to meet biomass demand poses the question on the effective environmental performance of the system as conceived.

Another important conclusion, which can be drawn from the abovementioned results, is that the economic feasibility of the business under assessment tightly depends on the cost allocation assigned to DDGS when used as animal feed substitute due to its effect on operating costs reduction.

Notwithstanding the fairly acceptable economic performance of the system under these conditions, we still do not have any guaranty about the environmental behaviour of the bioethanol SC. This is though a foremost issue it is worth to be investigated, especially when bioethanol acts within the EU market requiring for quite strict GHG emissions saving (set to a minimum quota of 35%).

According to this, the next Chapter will deal with the environmental features which have been embodied within the modelling framework here described. The main aim is to investigate on the best trade-off between economic and environmental needs so as to evaluate the systems capabilities to comply with the EU regulation.

Chapter 5

Steady-State Design: Multi-objective Optimisation

The core of this Chapter¹ is to address the development of an environmentally conscious decision making tool for the strategic design level of biofuels systems. The steady-state spatially explicit MILP model described in Chapter 4 has been enhanced by embodying environmental issues to the optimisation criteria considered. A general description of the new design issues is firstly presented. Next, the additional mathematical features associated with the MoMILP part of model are presented in detail. In the successive section, the multi-objective SC optimisation is then carried out to further assess the main issues ensuing from the discussion on the economic optimisation results. Different suitable biomass supply options are compared relating to the 2010 demand scenario. In addition, the use of valuable sub-products (specifically the DDGS coming from the corn conversion into ethanol) is investigated as a suitable alternative to improve the environmental performance of the system. Some final remarks on the model capabilities and shortcomings conclude the Chapter.

5.1 Problem statement

Chapter 4 addressed the development of a spatially explicit MILP model for the strategic design of biofuels production systems. The integrated management of the whole SC including agricultural practice, biomass supply, fuel production and logistics of transport was taken into account. Costs minimisation was adopted as the optimisation criterion to configure the system according to the traditional approach assuming the economic benefits as main drivers to motivate and drive the design process. However, the economics of the system should not be the only issue to focus on in pursuing a detailed assessment of biofuel SCs where conflicting aspects may concur in determining the optimal configuration of the network: the latest EU

¹ Portions of this Chapter have been published in Zamboni *et al.* (2009c) and Zamboni *et al.* (2009d).

regulation, indeed, requires the biofuels usage to perform a minimum GHG emission savings of 35% (quota that should increase up to 50% in 2017).

Accordingly, the design process of bioethanol SCs should be conceived as an optimisation problem in which the production system is required to comply with both costs and GHG emissions minimisation criteria.

Therefore, the design problem is here reformulated as follows. Given the following inputs:

- > geographical distribution of demand centres;
- > fuel demand over a fixed time horizon;
- > biofuel market characteristics;
- > biomass geographical availability;
- > biomass production costs;
- > biofuel production facilities capital and operating costs;
- > transport logistics (modes, capacities, distances, availability, costs);
- > environmental burden of biomass production;
- > environmental burden of biofuel production;
- > transport means emissions,

the global objective is now to determine the set of optimal system configurations resulting from the trade-off between operating costs and GHG emission for the entire SC. Therefore, the key variables to be optimised are:

- > geographical location of biomass production sites;
- > biomass production for each site;
- > supply strategy for biomass to be delivered to production facilities;
- > biofuel production facilities location and scale;
- > distribution processes for biofuel to be sent to blending terminals;
- > supply chain management costs;
- > supply chain impact on global warming.

5.2 Mathematical formulation

The new modelling framework builds on the spatially explicit MILP problem addressed in the previous Chapter. The model has been developed by enhancing the previous mathematical formulation according to the new core drivers. The additional environmental frame as well as the MoMILP solution algorithm are based on the approach proposed by Hugo and Pistikopoulos (2005) following the works by Papalexandri and Dimkou (1998) and Dua and Pistikopoulos (2000).

5.2.1 Objective function

The mathematical formulation of the MoMP problem commences with the definition of the environmental criterion to be coupled with the economic one. The objective is the minimisation of the total daily impact TDI [kg CO₂-eq/d] resulting from the operation of the biofuel SC. Thus, the definition of TDI needs considering each life cycle stage contribution, as expressed by the following equation:

$$TDI = \sum_s I_s \quad (5.1)$$

The environmental impact I_s [kg CO₂-eq/d] resulting from the operation of the single stage s is calculated as follow:

$$I_s = \sum_b d_b \cdot c_{b,s} \cdot F_s \quad \forall s \in S \quad (5.2)$$

where the reference flow F_s [units/d], specific for each life cycle stage s , is multiplied by the emission coefficient c_{bs} , representing the quantity of substance b emitted at stage s per unit of reference flow, and by the damage factor d_b , characterising the contribution of each burden b to the global warming in terms of carbon dioxide emissions equivalent per unit of burden emitted, namely the GWPs.

This formulation, although broadly acknowledged as a rigorous and comprehensive practice, may nonetheless turn out to be too onerous in terms of both calculation effort and data collection. For this reason, the mathematical formulation was simplified by grouping the emission coefficient, c_{bs} , together with the damage factor, d_b , thus devising a global emission factor f_s , which represents the carbon dioxide emissions equivalent at stage s per unit of reference flow. Accordingly, Equation (5.2) takes the form:

$$I_s = f_s \cdot F_s \quad \forall s \in S \quad (5.3)$$

As will be further detailed in the following sections, both f_s and F_s might be either grid- or transport-dependent according to the specific life cycle stage s they refer to. As a consequence, Equation (5.3) can be expressed either as:

$$I_s = \sum_g f_{s,g} \cdot F_{s,g} \quad \forall s \in \{bc, bds, fp\} \quad (5.3a)$$

or as:

$$I_s = \sum_t f_{s,t} \cdot F_{s,t} \quad \forall s \in \{bt, ft\} \quad (5.3b)$$

5.2.2 Life cycle stages impact

The stage-related environmental impacts as represented in Equation (5.3) are generally defined for the entire set of life cycle stages. However, the reference flows as well as the impact factors may depend either on the specific location (grid element g) or on the transport mode l . Thus, it is necessary to uniquely define the reference flows for each individual life cycle stage and express them explicitly as a function of the design variable controlling the optimisation problem.

5.2.2.1 Biomass production

GHG emissions resulting from the production of biomass notoriously depend on the cultivation practice adopted as well as on the geographical region in which the biomass crop has been established (Romero Hernández *et al.*, 2008). In particular, the actual environmental performance is affected by fertiliser and pesticides usage, irrigation techniques and soil characteristics. The factor may differ strongly from one production region to another. Accordingly, the form of Equation (5.3) for the biomass production stage is defined as follows:

$$I_{bc} = \sum_g f_{bc,g} \cdot F_{bc,g} \quad (5.4)$$

where $f_{bc,g}$ is the carbon dioxide emissions equivalent per unit of biomass produced in element g [kg CO₂-eq/t] and $F_{bc,g}$ is the daily biomass production in element g , i.e. $P_{biomass,g}^T$ [t/d].

5.2.2.2 Biomass drying and storage

The environmental performance of this stage has no relation with the geographical location of the dedicated facilities but rather depends on the technology adopted to process the biomass. This last issue was simplified by considering an average emission factor, f_{bds} [kg CO₂-eq/t],

estimated with reference to the performance of the most common practices adopted. Therefore, the total emission of the drying and storage stage is only influenced by the amount of biomass processed:

$$I_{bds} = f_{bds} \cdot \sum_g F_{bds,g} \quad (5.5)$$

5.2.2.3 Transport system

The global warming impact related to both biomass supply and product distribution is due to the use of different transport means fuelled with fossil energy, typically either conventional oil-based fuels or electricity. The resulting GHG emissions of each transport option depend both on the distance run by the specific means and on the freight load delivered. As a consequence, the emission factor $f_{s,l}$ represents the total carbon dioxide emissions equivalent released by transport unit l per km driven and ton carried. Thus, I_s is evaluated as follows:

$$I_s = \sum_l f_{s,l} \cdot F_{s,l} \quad \forall s \in \{bt, ft\} \quad (5.6)$$

with the reference flow $F_{s,l}$ now representative of the delivery distance ($ADD_{l,g,g'}$) and the load of goods transported ($Q_{i,g,l,g'}$), as defined by the equation:

$$F_{s,l} = \sum_g \sum_{g'} Q_{i,g,l,g'} \cdot ADD_{l,g,g'} \quad \forall s \in \{bt, ft\} \quad (5.7)$$

5.2.2.3 Fuel production

The environmental impact of the biofuel production stage is related to raw materials (other than biomass) and utilities required in operating the conversion facilities. Accordingly, the GHG emissions resulting from this life cycle stage were assumed proportional to the total daily amount of biofuel produced, $P_{fuel,g}^T$ [t/d] (taken as reference flow $F_{fp,g}$) and independent of location, as shown in the following expression:

$$I_{fp} = f_{fp} \cdot \sum_g F_{fp,g} \quad (5.8)$$

5.2.2.3 Emission credits

The effect of by-products, some of which are valuable products in other markets, is essential to allocate the total impact associated with a particular production chain. Currently, there is no accepted best method to cope with this issue. In this work, allocation by substitution was chosen following the recommendations of Rickeard *et al.* (2004): this method assigns to the

primary product the total GHG emissions minus the credits derived by the emissions avoided due to displacements of alternative goods by the by-products.

In first generation bioethanol systems based on grains, the main by-product is a high-protein meal coming from the solid fraction of the post-process residues (DDGS). This is a valuable substitute for cattle feed, and may also be used as a fuel for CHP generation (Morey *et al.*, 2006). The modelling framework was developed so as to take into account these two alternative options in order to calculate credits for emissions avoided through displacement of equivalent amounts of cattle feed production (*sm*) or electricity and heat generation (*en*). Following Delucchi (2006) no credits were assigned for land usage. In fact, the conversion from crop-for-food to crop-for-fuel generates a gap in the market that has to be filled either by importing corn (resulting in a higher impact) or by cultivating other lands (resulting in a lower impact in the case of set-aside land). Therefore, it is advised to consider an average situation in which no credits arise from changes in the land usage.

The by-product credits allocation was included in the mathematical formulation by considering the emission credits as a negative contribution to the life cycle stage impact calculation. This means that the sum on the right side of Equation (5.1) needs to comprise one more competitive contribution that can be alternatively:

$$I_{sm} = -f_{sm} \cdot \sum_g F_{sm,g} \quad (5.9)$$

where f_{sm} is the carbon dioxide emissions equivalent credit assigned to cattle feed displacement per unit of fuel produced and $F_{sm,g}$ is the daily fuel production in element g , $P_{fuel,g}^T$ [t/d]; or:

$$I_{en} = -f_{en} \cdot \sum_g F_{en,g} \quad (5.10)$$

with f_{en} representing the CO₂ equivalent emission assigned to energy production displacement per unit of fuel produced and $F_{en,g}$ still indicating the daily fuel production in element g .

Note that according to the formulation adopted in this work the two alternatives are assessed independently as a pseudo life cycle stage set $C \equiv \{sm, ec\}$. Accordingly, Equation (5.3) is reformulated as follows:

$$I_s = f_s \cdot F_s \quad \forall s \in S \cup C \quad (5.11)$$

5.3 Case study

Results reported in Chapter 4, showed that importing corn allowed for a more economical design of the overall SC. However, biomass importation from Eastern European Countries poses the question on the effective environmental performance of the system as conceived. In fact, one may ask how the best design in terms of cost reduction performs from an environmental standpoint. Thus, the case study allowing for corn importation described in Chapter 4 was taken as reference to formulate a new case study for the multi-objective modelling framework addressed here. The ethanol market penetration imposed by current Italian regulations for 2010 was assumed as the only demand scenario to design the corn-based ethanol SC considering both operating costs and GHG emission minimisation criteria. As a first instance, we considered that the DDGS would be used as animal feed with the corresponding allocation of SC operating costs and GHG emissions. Results were compared to a second instance where DDGS is assumed to fuel a CHP station providing the utility requirements of the conversion facilities.

5.4 Results and discussion

The two objective functions problem is solved through the CPLEX solver in the GAMS[®] modelling tool (Rosenthal, 2006).

Figure 5.1 shows the resulting trade-off set of non-inferior solutions. The shape of the curve reveals the expected conflict existing between environmental and economic performance. The optimum in terms of economic performance (case A as reported in Figure 5.1) involves a marginal operating cost value of 23.03 €/G_{J,EtOH} against an overall environmental impact of 79.15 kg CO₂-eq/G_{J,EtOH} corresponding to a GHG emissions reduction of about 8% compared to gasoline (the GHG emissions factor for gasoline was assumed equal to 85.8 kg CO₂-eq/GJ, according to Brown *et al.* (2005)). Table 5.1 resumes the details of the optimisation outcomes of case A, whilst Figure 5.2 shows the corresponding network configuration. The graphical representation reveals the SC general structure. Biomass demand is met by importing corn from Eastern European Countries. Corn is directly shipped to the two production plants of the maximum capacity (about 250 kt/y) and located within the industrial areas close to the main ports of Venice ($g = 32$) and Genoa ($g = 46$). This configuration allows for the best economic performance in terms of both biomass supply costs, due to the lower price of the imported corn, and of ethanol production costs, positively affected by the scale factor.

In terms of environmental performance, an 8% of GHG reduction in the emissions is not enough to meet the latest EU standards which require biofuels to have a minimum of 35% of GHG emissions savings. However, even minimising the impact (point B of Figure 5.1) the resulting GHG emissions are still too high to meet the minimum requirements, albeit the substantial economic effort required to reach the target: reducing the marginal impact down to

74.88 kg CO₂-eq/GJ_{E_{EtOH}} (equal to 13% of GHG reduction) results in an increase of the overall operating costs up to 25.80 €/GJ_{E_{EtOH}}.

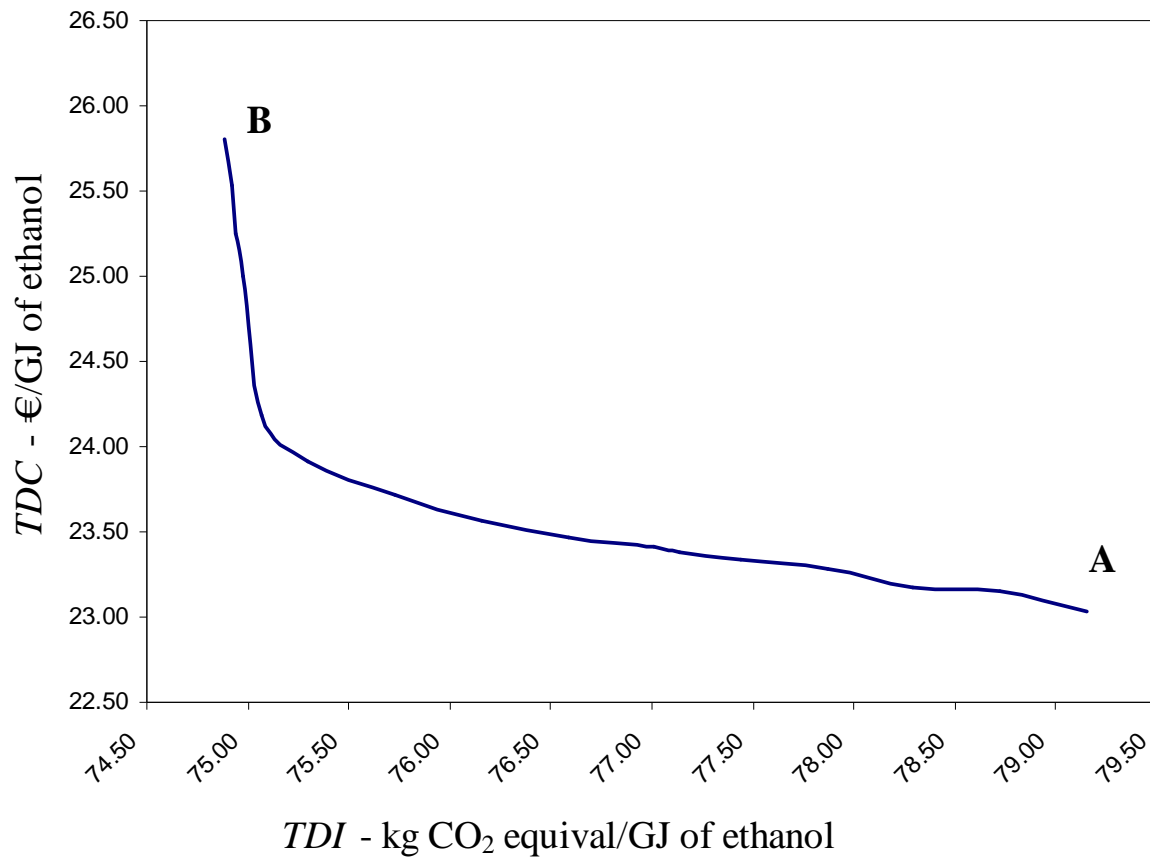


Figure 5.1 Pareto curve: simultaneous optimisation under operating costs and GHG emissions minimisation criteria.

Table 5.1 Costs-optimal solution: results of the SC optimisation. Case A: cost minimisation.

	operating costs €/GJ	GHG emissions kg CO ₂ -eq/GJ
biomass production	13.12	41.21
biomass drying and storage	-	7.25
transport system	3.16	4.34
fuel production	12.51	39.04
allocation credits	5.76	12.70
total	23.03	79.15

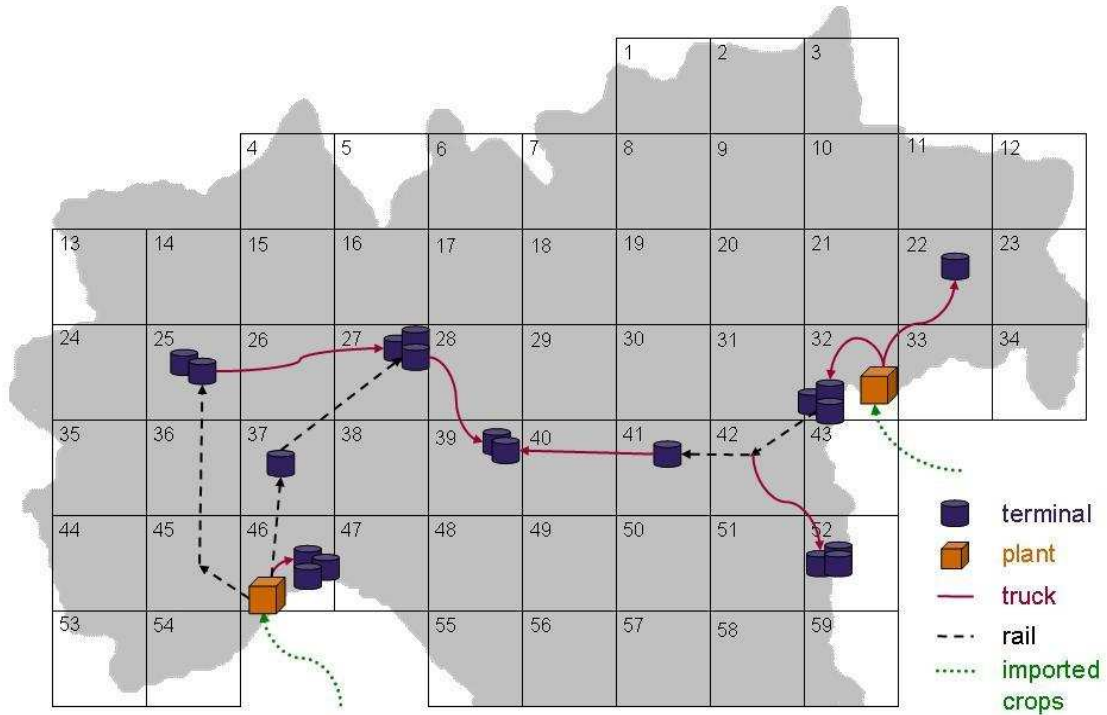


Figure 5.2 Costs-optimal solution: supply network configuration. Case A: cost minimisation.

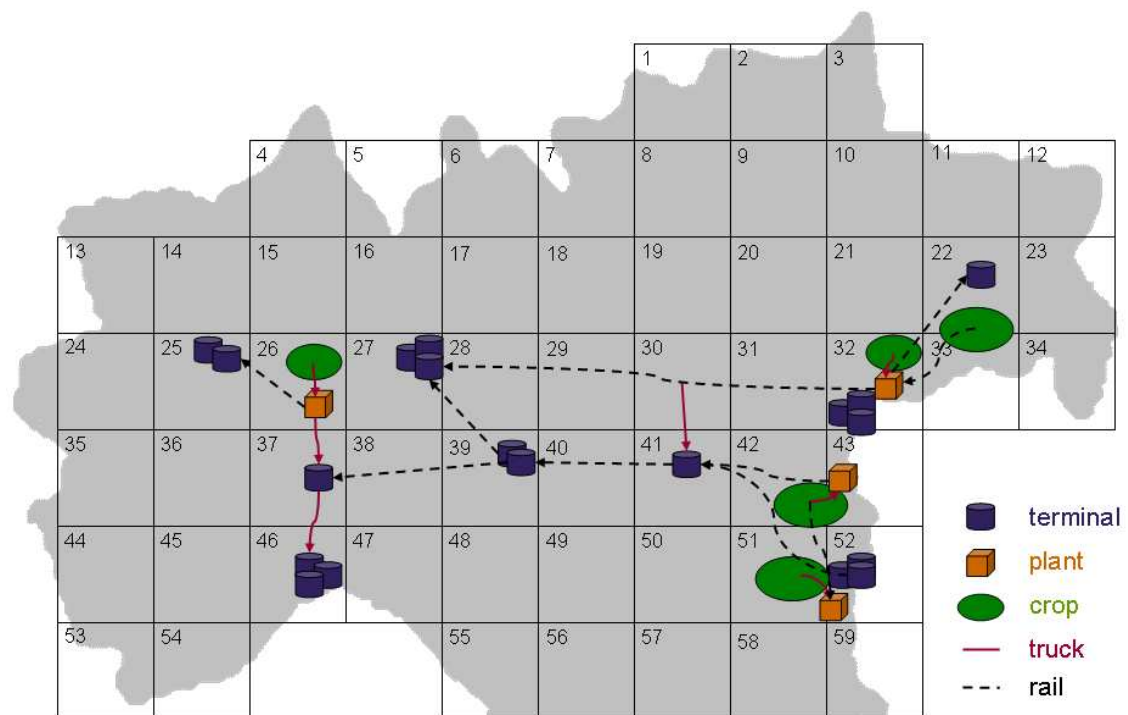


Figure 5.3 Emissions-optimal solution: supply network configuration. Case B: environmental optimisation.

In fact, when moving along the Pareto curve (Figure 5.1) from point A to point B, we see a gradual transition towards a network configuration (illustrated in Figure 5.3) proposing a more decentralized fuel production system that requires the establishment of four conversion plants: one of large capacity ($p = 4$) located in the neighbourhood of Venice ($g = 32$) and three other plants of smaller size ($p = 1$) sited in the most convenient area in relation to the domestic biomass production ($g = 26, 43$ and 52).

Comparing the related costs details reported in Table 5.2 with those of case A, it is evident that the supply solution outlined in case B would ensure a better environmental performance in terms of biomass distribution and corn production impact, but also a clear deterioration of the system economics due to the negative scale factor on ethanol production costs as well as to the unprofitable biomass supply conditions. Furthermore, even achieving a more sustainable supply system does not satisfy the EU standard requirements in terms of GHG emissions saving.

Table 5.2 Emissions-optimal solution: optimisation results. Case B: environmental optimisation.

	operating costs €/GJ	GHG emissions kg CO ₂ -eq/GJ
biomass production	15.21	39.64
biomass drying and storage	-	7.25
transport system	3.84	1.64
fuel production	13.20	39.04
allocation credits	6.45	12.70
total	25.80	74.88

The second instance considers DDGS as a fuel for CHP stations. This alternative use of DDGS would entails a production costs reduction, due to substantial savings on utilities supply costs, but also a considerable capital investment for the power station installation. The surplus of electricity production (globally amounting to 3.2 MJ for each ton of ethanol produced) can be sold to the national grid so as to gain some emission credits assigned for electricity displacement. The Pareto curve is similar to the one in Figure 5.1 and is not reported here. In fact, the optimal network configuration defined by the costs optimisation is identical to the one illustrated in Figure 5.2: this is quite expected, as cost minimisation would still favour low cost corn (imported from abroad) and large plants. However, the marginal operating costs value is now lower and equal to 22.40 €/G_{EIOH} against an overall environmental impact of 38.85 kg CO₂-eq/G_{EIOH}. As reported in Table 5.3, this reduction on the entire SC overheads is due to the decrease in ethanol production costs, notwithstanding a slight reduction in the allocation credits (now accounting for the 15% of the overall SC

operating costs). On the other hand, the substantially improved environmental performance occurring with this system configuration is attributable to the larger emission credits coming from the alternative use of by-products. This solution, indeed, would allow for a GHG reduction of about 55% compared to gasoline.

Table 5.3 Costs-optimal solution: results of the SC optimisation considering DDGS as CHP fuel.

	operating costs €/GJ	GHG emissions kg CO₂-eq/GJ
biomass production	13.12	41.21
biomass drying and storage	-	7.25
transport system	3.18	4.30
fuel production	10.05	39.04
allocation credits	3.95	52.96
total	22.40	38.85

If the optimisation is forced toward the minimisation of the environmental impact, the SC performance in terms of GHG emissions is even more promising. As reported in Table 5.4, the optimisation results in an estimated environmental burden reduction of about 60% (corresponding to a marginal value of 34.58 kg CO₂-eq/GJ_{EtOH}). However, in this situation the marginal operating costs increase up to 26.81 €/GJ_{EtOH}, thus exceeding the value calculated in the first instance. This depends on the lower costs allocation that is not balanced by the utilities supply costs reduction.

Table 5.4 Emissions-optimal solution: results of the SC optimisation considering DDGS as CHP fuel.

	operating costs €/GJ	GHG emissions kg CO₂-eq/GJ
biomass production	15.17	39.63
biomass drying and storage	-	7.25
transport system	3.44	1.62
fuel production	12.93	39.04
allocation credits	4.73	52.96
total	26.81	34.58

Additional remarks are drawn by analyzing the social costs of bioethanol production. As mentioned in Chapter 4, Italian regulation provides for a taxation discount on inland duties amounting to 4.2 €/GJ with respect to other conventional automotive fuels. This involves a

reduction of the breakeven point with gasoline down to 74 \$/bbl. However, if the objective is to promote maximum GHG mitigation, then either additional subsidies would be needed or a higher breakeven point is to be expected. The cost to bridge this gap amounts to about 3 €/G_{EIOH} (0.10 €/L_{EIOH}) when DDGS is used as animal feed substitute. If DDGS is used CHP fuel the difference is about 4 €/G_{EIOH} (0.12 €/L_{EIOH}). However, note the second instance allows for a breakeven point of about 72 \$/bbl when optimised under costs minimisation.

This last situation would allow for a better use of financial resources: the system might be supported with the same amount of subsidies so as to ease the market penetration and still it would be possible to match the EU regulation in terms of GHG reduction for biofuels production processes. Therefore, in the particular case of the Italian corn-based ethanol production a well-advised strategy would address the design process under economic criteria, especially adopting a system configuration in which by-products are used to provide the energy needs of the production facilities.

5.5 Conclusions

The non-inferior set of viable solutions indicates that the most interesting alternative proposes: i) the design of the bioethanol supply system under costs minimisation, and ii) the usage of DDGS as fuel to produce the heat and power required by the production facilities. The optimisation outcomes demonstrate the system's effectiveness in reaching the GHG mitigation (by 55%) necessary to meet the EU standards.

However, although our assumptions of the GHG emissions concerning corn in Eastern European countries appears to be sensible enough, it is important to note that importing corn from countries characterised by uncertain environmental standards in cropping practice may significantly affect the environmental results and put at risk the achievement of the EU goals (albeit through an improvement of the overall economics).

It is also noteworthy that, in this study, the economic performance of the system has been defined in terms of the ethanol production costs, only. As a consequence, the effect of using DDGS as animal fodder or CHP fuel has been discussed (and optimised) without assessing the potential variations in terms of the production profitability (e.g., in terms of Net Present Value, NPV). However, the great uncertainty on the DDGS selling price as well as on the subsidies (Green Credits) deriving from selling "renewable" electricity to the national grid, suggested that a first evaluation tool should be based on costs. The next Chapter will be dedicated to a more comprehensive financial analysis. The aim is to evaluate the effective impact of DDGS end-use on the financial performance of the system. The effects of market uncertainty on the financial behaviour will be taken into account, too, so as to provide a more conscious planning strategy.

Chapter 6

Dynamic Planning under Uncertainty

The objective of this Chapter¹ is to describe an enhancement of the modelling framework previously developed which has been modified in order to take into account both the capacity planning dynamics and the effect of market uncertainty.

A general description of the new modelling issues is presented together with some remarks on the financial indexes adopted to evaluate the performance of the system. The case study along with the probabilistic analysis on the modelling parameters is described, and the results of the stochastic optimisation are shown and discussed.

6.1 Problem statement

The steady-state optimisation model, addressed in Chapter 4 and Chapter 5, provided good insight on the economic and environmental performance of bioethanol production systems. The modelling outcomes envisaged that in establishing a new bioethanol production network good economic performance would be achieved when the system is configured involving biomass importation to provide corn needs as well as adopting a DDGS end-use as animal fodder substitute. However, the modelling design as conceived does not allow for any conclusion about a proper assessment of the financial performance of the system and of its sensitivity to uncertainty on market conditions.

Accordingly, the steady-state formulation previously adopted should be replaced by a dynamic one aiming at a planning tool capable of taking into account the market volatility over a long-term horizon.

The problem addressed in this Chapter deals with the strategic design and planning of a general biofuel SC over a 10-years horizon. The problem is formulated as a spatially explicit time dynamic modelling framework devised for the strategic design and investment planning of multi-echelon supply networks operating under uncertainty. Strategic decisions in designing a biofuel production network still deal with the geographical location of biomass

¹ Portions of this Chapter have been published in Dal Mas *et al.* (2009a) and submitted for publication in Dal Mas *et al.* (2009b).

cultivation sites, logistic definition of transport system and supply chain node location. On the other hand, planning decisions relates to the capacity assignment of production facilities and the demand satisfaction along the time steps composing the time horizon. Accordingly, the optimisation problem discussed here can be stated as follows. Given the following inputs:

- > geographical distribution of demand centres;
- > fuel demand over a the entire time horizon;
- > biofuel market characteristics in terms of prices distribution;
- > biomass geographical availability;
- > biomass purchase costs;
- > biofuel production facilities capital and operating costs;
- > transport logistics (modes, capacities, distances, availability, and costs),

the objective is to determine the optimal system configuration in terms of SC profitability and financial risk on investment. Therefore, the key variables to be optimised over the planning time horizon are:

- > geographical location of biomass production sites;
- > biomass production for each site;
- > supply strategy for biomass to be delivered to production facilities;
- > biofuel production facilities location and scale;
- > biofuel market demand satisfaction rate;
- > distribution processes for biofuel to be sent to blending terminals;
- > SC profit;
- > financial risk under uncertainty.

An important assumption (and a critical difference with respect to the steady-state assessment previously addressed) is that the satisfaction of bioethanol demand is not set, but represents an upper bound. In other words, the optimiser is free to choose how much ethanol should be produced up to the quota set by the EU directive (EC, 2003), representing the maximum market demand. The underlying assumption is that an investor would enter the bioethanol

market if there is a chance for profitability and not because there is a production quota to be fulfilled (at least without subsidies).

Finally, it is important to notice that the investment analysis has been assessed by formulating the optimisation problem through two alternative financial criteria in terms of economic indicators such as the expected net present value (eNPV) as formulated by Bagajewicz (2008) and the conditional value-at-risk (CVaR) (Rockafellar and Uryasev, 2000): the eNPV maximisation is oriented to optimise the financial profitability of the system; whilst the CVaR maximisation allows for a reduction on the risk on investment.

6.2 Mathematical formulation

The time dynamic MILP model builds on the steady-state frame addressed in the previous Chapters and the new improvements are based on the approaches applied to the multi-echelon SC optimisation under uncertainty (Sahinidis *et al.*, 1989; Tsiakis *et al.*, 2001; Guillén-Gosálbez and Grossmann, 2009). It embodies different features for spatially explicit siting of supply networks nodes (Almansoori and Shah, 2009) and capacity planning of strategic fuel systems (Hugo and Pistikopoulos, 2005). A stochastic formulation is implemented to handle the effect of uncertainty (Tsang *et al.*, 2007a; Tsang *et al.*, 2007b).

6.2.1 Objective functions

According to the common rules of optimisation problems, the mathematical formulation commences with the definition of the objective function to be minimised in configuring the system. The first objective considered here is the expected net present value (Obj_{eNPV} [€]). Given the financial nature of the problem, that imposes the maximisation of profit-related indexes, the Obj_{eNPV} value is required to be written in its negative form, as stated by the following equation:

$$Obj_{eNPV} = -\sum_{q,r} NPV_{q,r} \cdot \pi_{q,r} \quad \forall q,r \quad (6.1)$$

where $NPV_{q,r}$ is the Net Present Value and $\pi_{q,r}$ the event probability both related to each scenario deriving from the combination of corn purchase cost q and ethanol market price r .

Alternatively, the objective function to be minimised is given by the negative value of the CVaR index. This financial indicator represents the NPV evaluated within a scenario of maximum potential economic losses due to market fluctuation on an investment in a certain time interval and with a specific confidence level. It directly derives from the VaR index (Rockafellar and Uryasev, 2000): with respect to a specified confidence β -level, the β -VaR of an investment is the lowest amount α such that, with probability β , the loss will not exceed α ,

whereas the β -CVaR is the expectation that losses are above that amount α . Here, the worst potential market scenarios with a 10% occurrence probability are taken into account. Accordingly, the second objective function can be formulated as follows:

$$Obj_{CVaR} = -\frac{\sum_{q,r} NPV_{q,r} \cdot \pi_{q,r}}{\sum_{q,r} \pi_{q,r}} \quad \forall q, r = worst_{q,r} \quad (6.2)$$

The NPV for each scenario is defined as the discounted profits minus the discounted costs:

$$NPV_{q,r} = \sum_t (PBT_{t,q,r} \cdot \varepsilon Cap_t - FCC_t \cdot \varepsilon FCC_t) \quad \forall q, r \quad (6.3)$$

where $PBT_{t,q,r}$ [€/y] represents the profit before taxes, FCC_t are the facility capital costs [€/y] for time period t and scenario (q,r) . Both terms are discounted through factors collected in two different arrays εCap_t and εFCC_t , since capital costs are allocated at the beginning of each year and are yearly discounted, while revenues are received at the end of the year and discounted every two-year period. Thus, they are defined as (Douglas, 1988):

$$\varepsilon Cap_t = \frac{2 + \zeta}{(1 + \zeta)^{2t}} \quad (6.4)$$

$$\varepsilon FCC_t = \frac{1}{(1 + \zeta)^{2(t-1)}} \quad (6.5)$$

where ζ is the future interest rate. The value of this index is meant to vary with time. However, to reduce the computational burden, here ζ has been assumed to be a constant (Tsang *et al.*, 2007a). The value has been set equal to the Minimum Accepted Rate of Return (MARR, 15% according to Peters *et al.* (2003)), considerably higher than the standard risk-free interest rate (8%); that is quite a typical assumption in the preliminary evaluation of investment decisions.

6.2.1.1 Gross profits

The profit before taxes $PBT_{t,q,r}$ represents the gross profits and has been defined as the difference between the total annual revenues $TAR_{t,q,r}$ [€/y] and the total operating costs $TOC_{t,q,r}$ [€/y] for period t at the scenario (q,r) :

$$PBT_{t,q,r} = TAR_{t,q,r} - TOC_{t,q,r} \quad \forall t, q, r \quad (6.6)$$

Depreciation charges are neglected for computational issues. $TAR_{t,q,r}$ are annual revenues and depend on both ethanol and DDGS sales:

$$TAR_{t,q,r} = 12 \cdot \sum_g \left[P_{fuel,g,t,q,r}^{tot} \cdot (MPe_r + \sigma \cdot MPd) \right] \quad \forall t, q, r \quad (6.7)$$

where $P_{fuel,g,t,q,r}^{tot}$ is the monthly ethanol production rate [t/month] in region g at period t and scenario (q,r) ; MPe_r is the ethanol market price [€/t] relating to scenario r ; σ is a constant representing the rate of DDGS per unit of ethanol produced in a standard dry-grind ethanol plant and has been set equal to $0.7288 \text{ t}_{DDGS}/\text{t}_{EtOH}$ (Morey *et al.*, 2006) and MPd is the DDGS market price [€/t].

$TOC_{t,q,r}$ are evaluated by summing up the transport costs $TC_{t,q,r}$ [€/month] and the facilities operating costs $FOC_{t,q,r}$ [€/month] at time period t and scenario (q,r) :

$$TOC_{t,q,r} = 12 \cdot (TC_{t,q,r} + FOC_{t,q,r}) \quad \forall t, q, r \quad (6.8)$$

$FOC_{t,s,r}$ [€/month] are evaluated as:

$$FOC_{t,q,r} = \sum_g \left(UPCc_q \cdot P_{biomass,g,t,q,r}^{tot} + \sum_p UPCe_p \cdot Pf_{p,g,t,q,r} \right) \quad \forall t, q, r \quad (6.9)$$

where $UPCc_q$ [€/t] is the unit purchase cost of corn in scenario q , and is multiplied by the biomass production rate $P_{biomass,g,t,q,r}^{tot}$ [t/month] in region g at period t and scenario (q,r) . $UPCe_p$ [€/t] is the unit production cost of ethanol for the plant of size p , and is multiplied by the ethanol production rate $Pf_{p,g,t,q,r}$ [t/month] in region g at period t for the plant of size p and scenario (q,r) .

As in the previous Chapters, the transport system is treated as an additional service provided by existing actors already operating within the industrial/transport infrastructure. As a consequence, $TC_{t,q,r}$ is evaluated as follows:

$$TC_{t,q,r} = \sum_{i,l} \left(UTC_{i,l} \cdot \sum_{g,g'} NTU_{i,g,l,g',t,q,r} \cdot TCap_{l,i} \cdot ADD_{l,g,g'} \right) + UTC^* \sum_g NTU_{g,t,q,r} \cdot TCap^* \cdot LD_{g,g} \quad \forall t, q, r \quad (6.10)$$

where $NTU_{i,g,l,g',t,q,r}$ is the number of transport units of mode l needed to transfer i between two elements g and g' at time period t in the scenario (q,r) ; $NTU_{g,t,q,r}$ is the number of

transport units (trucks of small capacity) for internal transfer within element g at time period t in the scenario (q,r) ; $UTC_{i,l}$ [€/t(km)], $TCap_{l,i}$ [t/trip], UTC^* [€/t(km)], $TCap^*$ [t/trip], $ADD_{l,g,g'}$ [km] and $LD_{g,g}$ [km] are defined as in Chapter 4.

Here, we also introduce two constraints:

$$NTU_{i,g,l,g',t,q,r} \geq \frac{Q_{i,g,l,g',t,q,r}}{TCap_{i,l}} \quad \forall i, g, l, g', t, q, r \quad (6.11)$$

and

$$NTU_{g,t,q,r} \geq \frac{P_{biomass,g,t,q,r}^{tot}}{TCap^*} \quad \forall g, t, q, r \quad (6.12)$$

with $Q_{i,g,t,g',t,q,r}$ [t/month] the flow rate of i via mode l between two grid elements g and g' at period t and scenario (q,r) . They simply impose that the number of transport units must be sufficient to transfer all of the product to be delivered.

6.2.1.2 Facility capital costs

The FCC_t term in Equation (6.3) accounts for the capital investment required to establish the entire supply network along the whole time horizon. FCC_t can be evaluated by summing up the capital cost PCC_p [€] of each single conversion plant size p in the territory.

$$FCC_t = \sum_{p,g} \left(Y_{p,g}^{start} \cdot PCC_p \cdot inY_t + Y_{p,g,t}^{plan} \cdot PCC_p \right) \quad \forall t \quad (6.13)$$

where $Y_{p,g}^{start}$ is the binary decision variable that initialises the problem starting from the supply chain configuration already established at the time $t = 1$ (given by the static model of Chapter 4). $Y_{p,g,t}^{plan}$ is the Boolean variable, evaluated at the beginning of time period t and controlling if a new production facility of size p in region g is established in that time period (a value of 1 means that the construction of a new production plant is allowed, otherwise 0 is assigned).

Finally, inY_t is a binary array specifically devised to initialise the problem by assigning the capital costs of the starting SC configuration to the first time period $t = 1$ (thus assuming zero values $\forall t \neq 1$).

6.2.2 Logical constraints and mass balances

The network behaviour needs to be subjected to mass balances as well as logical constraints in each of the supply chain nodes.

6.2.2.1 Demand constraints

Demand $D_{i,g,t,q,r}^{tot}$ [t/month] of product i in region g at period t and scenario (q,r) is satisfied by local production or by importing the commodity from other regions. Accordingly:

$$D_{i,g,t,q,r}^{tot} = D_{i,g,t,q,r}^{loc} + D_{i,g,t,q,r}^{imp} \quad \forall i, g, t, q, r \quad (6.14)$$

where $D_{i,g,t,q,r}^{imp}$ [t/month] identifies the amount imported in g to fulfil the demand of product i , and $D_{i,g,t,q,r}^{loc}$ [t/month] is the demand satisfied through local production.

Furthermore, the following constraints must hold:

$$D_{i,g,t,q,r}^{loc} \leq D_{i,g,t,q,r}^{tot} \quad \forall i, g, t, q, r \quad (6.15)$$

$$D_{i,g,t,q,r}^{imp} \leq \sum_{l,g'} Q_{i,g',l,g,t,q,r} \quad \forall i, g, t, q, r \quad (6.16)$$

i.e. the local production $P_{i,g,t,q,r}^{tot}$ has to be at least equal to $D_{i,g,t,q,r}^{loc}$ and $D_{i,g,t,q,r}^{imp}$ cannot exceed the mass fluxes $Q_{i,g',l,g,t,q,r}$ entering the region g .

The local biomass demand necessary to supply the production plant sited within the same region g , is determined by applying the corn-to-ethanol conversion factor γ (as defined in Chapter 4) to the fuel production rate, as shown by the following equation:

$$D_{biomass,g,t,q,r}^{tot} = \frac{P_{fuel,g,t,q,r}^{tot}}{\gamma} \quad \forall g, t, q, r \quad (6.17)$$

Finally, the supply network production capabilities should satisfy the market requirements according to which the total production of i should equal the overall demand of this commodity. Accordingly:

$$TD_{i,t,q,r} = TP_{i,t,q,r} \quad \forall i, t, q, r \quad (6.18)$$

Total goods production $TP_{i,t,q,r}$ [t/month] and total demand $TD_{i,t,q,r}$ [t/month] are obtained by adding up the local variables:

$$TD_{i,t,q,r} = \sum_g D_{i,t,q,r}^{tot} \quad \forall i, t, q, r \quad (6.19)$$

$$TP_{i,t,q,r} = \sum_g P_{i,t,q,r}^{tot} \quad \forall i, t, q, r \quad (6.20)$$

6.2.2.2 Production constraints

The following set of relations is formulated to constrain the commodity production rate. First, a global mass balance has to be fulfilled:

$$P_{i,g,t,q,r}^{tot} = D_{i,g}^{tot} + \sum_{l,g'} (Q_{i,g,l,g',t,q,r} - Q_{i,g',l,g,t,q,r}) \quad \forall i,t,q,r \quad (6.21)$$

The total amount of fuel produced in each element g results from the sum of the production rate of all plants of size p $Pf_{p,g,t,q,r}$ [t/month] established in the same region at period t and scenario (q,r) :

$$P_{fuel,g,t,q,r}^{tot} = \sum_p Pf_{p,g,t,q,r} \quad \forall g,t,q,r \quad (6.22)$$

Furthermore, $Pf_{p,g,t,q,r}$ is upper- and lower-bounded according to the maximum and the minimum capacity of a plant of size p : $PCap_p^{\max}$ and $PCap_p^{\min}$ [t/month] are the maximum and minimum production rates allowed for the plant of size p . Thus:

$$Y_{p,g,t} \cdot PCap_p^{\min} \leq Pf_{p,g,t,q,r} \leq Y_{p,g,t} \cdot PCap_p^{\max} \quad \forall p,g,t,q,r \quad (6.23)$$

where $Y_{p,g,t}$ is a Boolean variable: a value of 1 means that at the time t , a plant of size p is present in the region g ; its value is set to 0 if no plant exists. It is also assumed that only one conversion facility can be established within one territorial element (as stated by Equation (4.18)):

$$\sum_p Y_{p,g,t} \leq 1 \quad \forall g,t \quad (6.24)$$

Also, it is assumed that once a production facility has been built, it will be operating for the remaining time frame. This is ensured by the following recursive definition on $Y_{p,g,t}$:

$$Y_{p,g,t+1} = Y_{p,g,t} + Y_{p,g,t}^{plan} \quad \forall p,g,t \quad (6.25)$$

Note that in a region g , $Y_{p,g,t}^{plan}$ and $Y_{p,g,t}$ cannot be equal to 1, simultaneously: as soon as a new plant is planned at time $t = t^*$ ($Y_{p,g,t=t^*}^{plan} = 1$), then $Y_{p,g,t=t^*+1}$ becomes equal to 1, too. Thus, for the successive time periods, relations (6.24) and (6.25), imposes $Y_{p,g,t>t^*}^{plan} = 0$.

The first year configuration is set by initialising $Y_{p,g,t}$ as:

$$Y_{p,g,1} = Y_{p,g}^{start} \quad \forall p,g \quad (6.26)$$

Biomass production, too, cannot exceed the limits imposed by the effective regional production capability, which depends on agronomic-related factors such as maximum and minimum biomass cultivation fractions BCD_g^{\max} and BCD_g^{\min} of cultivated land over arable land in element g , and the cultivation yield CY_g [t/(d·km)]; additionally, the geographical characteristics such as the actual surface in an element GS_g [km²] and the related percentage of arable land AD_g contribute to define the biomass productivity. Thus, the following condition must hold:

$$GS_g \cdot CY_g \cdot AD_g \cdot BCD_g^{\min} \leq P_{biomass,g,t,q,r}^{tot} \leq GS_g \cdot CY_g \cdot AD_g \cdot BCD_g^{\max} \quad \forall g \quad (6.27)$$

To ensure a sustainable biomass to biofuel purposes, a maximum biomass utilization quota should be set to limit the total corn domestic crop to biofuel production: the utilization factor $SusP$ defined in Chapter 3 is applied to the overall potential domestic biomass production $TPot_t$ [t/month]:

$$TP_{biomass,t,s,r} \leq SusP \cdot TPot_t \quad \forall t, s, r \quad (6.28)$$

where:

$$TPot_t = \sum_g GS_g \cdot CY_g \cdot AD_g \cdot BCD_g^{\max} \cdot CF_g \quad \forall t \quad (6.29)$$

6.2.2.3 Transport constraints

A further set of constrains is devoted to transport logistics. First of all, it must be ensured that:

$$Q_{i,g,l,g',t,q,r} \leq Q_{l,i}^{\max} \cdot X_{i,g,l,g',t,q,r} \quad \forall i, l, g, g', t, q, r \quad (6.30)$$

where $Q_{l,i}^{\max}$ [t/month] represents the flow-rate limitations due to the transport mode delivery capacities and the related maximum tolerable monthly trips; $X_{i,g,l,g',t,q,r}$ is the decision variable whose value is 1 if the transfer of product i between g and g' via mode l is allowed, and 0 otherwise.

The flow rate of a specific product i between adjacent elements is expected to occur only in one direction:

$$X_{i,g,l,g',t,q,r} + X_{i,g',l,g,t,q,r} \leq 1 \quad \forall i, g, l, g', t, q, r : g \neq g' \quad (6.31)$$

Furthermore, internal loop trips of product are not allowed:

$$\sum_{l,g} X_{i,g,l,g',t,q,r} = 0 \quad \forall i, g, l, g', t, q, r : g \neq g' \quad (6.32)$$

Finally, the representation of the logistics behaviour is completed by a transport feasibility condition (for instance, transport by barges is not allowed if a waterway is not available):

$$\sum_{i,l,g,g'} X_{i,g,l,g',t,q,r} = 0 \quad \forall i, g, l, g', t, r, q : (i, g, l, g') \neq Total_{i,g,l,g'} \quad (6.33)$$

6.2.2.4 Non-negativity constraints

The last constraints simply impose that a number of variables should retain a physical meaning and be non-negative:

$$P_{i,g,t,q,r}^{tot} \geq 0 \quad \forall i, g, t, q, r \quad (6.34)$$

$$P_{p,g}^f \geq 0 \quad \forall p, g \quad (6.35)$$

$$Q_{i,g,l,g',t,q,r} \geq 0 \quad \forall i, l, g, g', t, q, r \quad (6.36)$$

$$D_{i,g,t,q,r}^{loc} \geq 0 \quad \forall i, g, t, q, r \quad (6.37)$$

$$D_{i,g,t,q,r}^{imp} \geq 0 \quad \forall i, g, t, q, r \quad (6.38)$$

6.3 Case study

Results reported in Chapters 4 and 5 evidenced the high economic sustainability of the bioethanol production system when biomass is imported and DDGS is used as animal fodder substitute to be sold within the market. However, the inherent design of the problem as previously conceive does not enable to produce any results about the effective financial profitability of the optimal solution. This issue should be assessed by considering not only the operating costs of the system but also the revenues coming from both the ethanol business and the DDGS marketing. Also, the financial assessment should take into account the market price variation of goods over a defined time horizon. This has involved the formulation of a case study considering 16 scenarios of combined average values of ethanol market price (r) and corn purchase cost (q). The optimisation problem is addressed by formulating two alternative case studies referring to two likewise objectives. Accordingly, two cases (corresponding to the financial indicators adopted as optimisation criteria) are considered:

A eNPV maximisation;

B CVaR maximisation.

Moreover, the sensitivity on the optimisation results to three different options for DDGS prices is assessed. Note that the fluctuations on DDGS price were not included in the probability functions as there is not sufficient information to build up a reliable probability curve. As a consequence, for each case study, three optimisation instances were carried out:

1. optimisation fixing MPd equal to 300 €/t;
2. optimisation fixing MPd equal to 200 €/t;
3. optimisation considering a progressive DDGS devaluation over the time; the DDGS price is supposed to vary as follows: 300 €/t since 2009 to 2012, 200 €/t since 2013 to 2016 and 100 €/t since 2017 to 2019 (the hypothesis is reasonably supported by a potential excess of production).

6.3.1 Demand centres

As already mentioned in Chapter 3, bioethanol is assumed to be sent to blending terminals existing at given locations. Their gasoline delivery rates (satisfying the regional demand centres) are supposed to be constant all over the time horizon. The overall gasoline demand is set equal to 455,979 t/y. Location, number and actual gasoline delivery rate of each terminal are defined as discussed in Chapter 3. Bioethanol demand is set to vary along the 10-years time horizon, starting from 2009 to 2019. In accordance to the EU Directive, the bioethanol quota is set equal to 3% for 2009, 5.75% by 2010 and from 2010 to 2019 minimum increments of bioethanol percentages are provided in order to achieve 2020 EU target of 10% (all these percentages are set on energetic basis). The overall time horizon has been divided into couples of years, in order to reduce the computational burden (accordingly, each blending percentage is an average value over a period of two years' time). Table 6.1 shows the varying blending quota (represented by the $etperc$ parameter) for the 5 time periods (t as appear in the mathematical formulation). In the $etperc$ array, the blending percentages (on a mass basis) are averaged over couples of years (corresponding to one time period t). Constant increments are used in the range 5.75-10%_E.

Table 6.1 The $etperc$ array with ethanol blending percentages on mass basis over the years.

period t	1	2	3	4	5
$etperc[\%_w]$	6.87	9.45	11.21	12.47	13.71

As mentioned in a previous section, the problem is conceived so as to keep the ethanol demand as a free variable which the problem solution aims at optimising according to the maximisation of the financial performance of the system. This means that is not compulsory for the production system to fulfil the market demand of ethanol whenever it resulted unprofitable from an economic point of view. The actual market demand represents an upper bound parameter defined by imposing the minimum blending quota to the gasoline market demand values. Accordingly, the new constraint:

$$D_{fuel,g,t,q,r}^{tot} \leq DEM_{fuel,g,t,q,r} \quad \forall i, g, t, q, r \quad (6.39)$$

must be added to the equation list reported in the previous section. This fix a ceiling (represented by the actual market demand for ethanol in region g at period t and scenario (q, r) , $DEM_{fuel,g,t,q,r}$) for the range within which $D_{fuel,g,t,q,r}^{tot}$ is allowed to vary.

6.3.2 Definition of price scenarios

Each scenario is a particular combination of ethanol market price and corn purchase cost. The analysis of historical data concerning the biomass purchase cost in Italy for the time period 1993-2008 (Frascarelli, 2008) and the bioethanol market price in Southern Europe for the period 2005-2008 (Agra Informa, 2009) has allowed fitting the following two distribution functions for biomass and ethanol, respectively:

$$pdf(UPCc) = 18.4240 \cdot \Gamma[UPCc, 87.6592, 1.4964] + 10.5057 \cdot [UPCc, 57.0740, 3.0429] \quad (6.40)$$

$$pdf(MPe) = 83.8326 \cdot \Gamma[MPe, 362.6378, 2.0258] \quad (6.41)$$

where $UPCc$ [€/t] is the corn purchase cost and MPe [€/t] is the ethanol market price, as previously stated. Γ represents the price trend function related to each product subjected to market uncertainty. The compound probability density function is represented in Figure 6.1. The probability functions are discretised into the vectors of scenarios $q \in Q = [127.75, 159.25, 190.75, 222.25]^T$ and $r \in R = [645, 695, 745, 795]$ of corn purchase costs and ethanol market prices, respectively. The two vectors are combined into a 4×4 matrix (q, r) of 16 scenarios, whose probabilities is summarised in Table 6.2. Note that according to this approach, each scenario q or r is assumed to represent an average cost or price for all the 10 years' period. This represents quite a simplification with respect to a most rigorous approach recombining all the 16 realizations at each time period t (and producing 1,048,576 scenarios!).

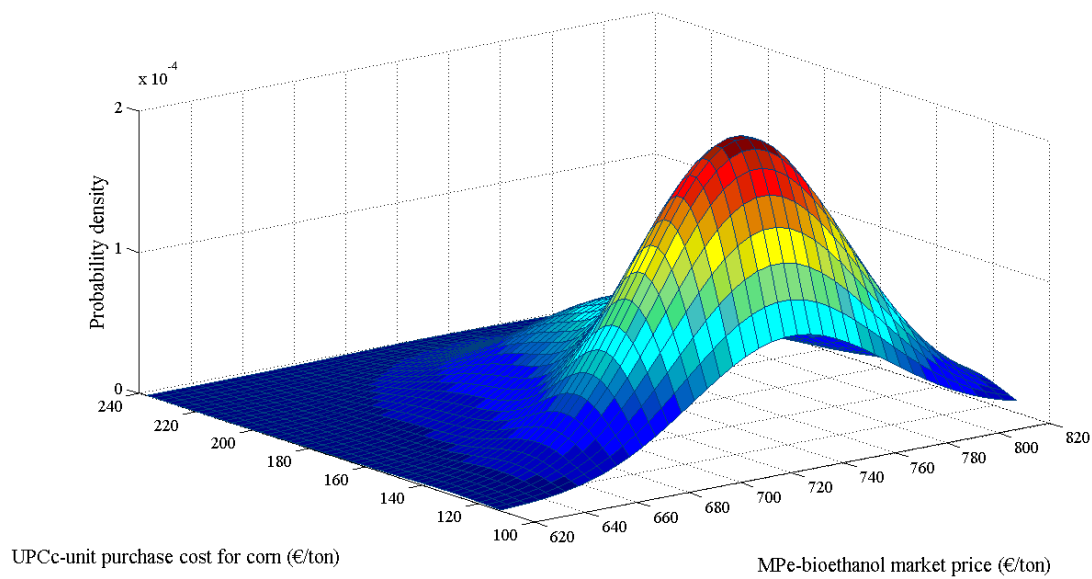


Figure 6.1 Compound probability density functions for corn production cost and ethanol market price.

Table 6.2 Medium scenario probabilities.

$q \backslash r$	1	2	3	4
1	0.0229	0.1682	0.2481	0.0873
2	0.0130	0.0952	0.1404	0.0494
3	0.0064	0.0467	0.0688	0.0242
4	0.0013	0.0094	0.0139	0.0049

In order to maintain a reasonable computational complexity, we have preferred to retain a detailed description of the structure of the bioethanol SC and simplify the probabilistic representation. In fact, the 16 scenarios do belong to the more complex probability space and can be exploited for a preliminary analysis capable of incorporating price uncertainty in the SC design.

6.3.3 eNPV evaluation

The expected NPV is evaluated by adding up the discounted and weighted cash flows, each of them performed for one of the combinations of purchase corn cost and ethanol market price and added up by a weighting factor given by the corresponding scenario probability. Thus, FCFs are evaluated employing the same average corn cost and bioethanol price all over the time horizon. The discounted cumulative cash position is attained by multiplying each FCF by

the discount factors previously defined (see Equation (6.4) and (6.5)). Table 6.3 reports the discount factors values for each time period t .

Table 6.3 Values of the εCap_t and εFCC_t arrays.

period t	1	2	3	4	5
εCap_t	1.626	1.230	0.930	0.703	0.531
εFCC_t	1.000	0.756	0.572	0.432	0.327

6.3.4 CVaR evaluation

The CVaR-based optimisation criterion mirrors risk-averse investors' decisions. The optimisation framework is led toward the design of an SC configuration minimising economic losses and rejecting the worst market scenarios that are verified with a 10% confidence level. The worst scenarios are represented by (q,r) couples (2,1), (3,2), (4,3), (3,1), (4,1) and (4,2) composing the $worst_{q,r}$ subset in Equation (6.2).

6.3.5 Taxes and depreciations

Net discounted FCFs for each year are evaluated offline by means of an Excel spreadsheet. They are derived from the $TAR_{t,q,r}$, $TOC_{t,q,r}$ and FCC_t resulting in the optimal SC configuration, setting a 43% taxation rate of positive gross FCFs. The taxation framework provides constant depreciation charges for the FCC over 8 years.

6.4 Results and discussion

The two financial indicators adopted as optimisation criteria (i.e. the eNPV (case A) and the CVaR (case B)) define two SC configurations and discounted cumulative cash position layouts. The MILP modelling framework was solved through the CPLEX solver of the GAMS[®] tool (Rosenthal, 2006).

6.4.1 Case A: planning under profit maximisation

Three different instances are assessed according to the eNPV optimisation criterion by varying the DDGS market price. The modelling outcomes are reported in terms of SC graphical topology as well as in terms of production planning over the 10 years time horizon. The results show the high reliance for the business profitability on revenues coming from the side production of DDGS. In particular high market price values lead to high business profitability as indicated by a greater ROI value and a lower payback time. This also reduces the importance of the economy of scale in planning the ethanol production capacity, thus allowing for a more distributed SC configuration in which smaller production plants are still

profitable. Table 6.4 shows that when the DDGS price is 300 €/t (instance A.1) no large-size plants ($p = 4$) are established. It is also worth noting that the ROI index, evaluated on a medium basis over the business horizon, is equal to 33.0%, significantly higher than the minimum acceptable threshold for a new product entering an established markets (usually set at 24% (Peters *et al.*, 2003)).

Table 6.4 SC configuration when $MPd = 300$ €/t through the eNPV optimisation (instance A.1).

period t	new plants establishment ($Y_{p,g,t}^{plan}$)
1	$[p = 2; g = 46]; [p = 3; g = 52]$
2	$[p = 2; g = 27]$
3	$[p = 2; g = 32]$
4	-
5	-

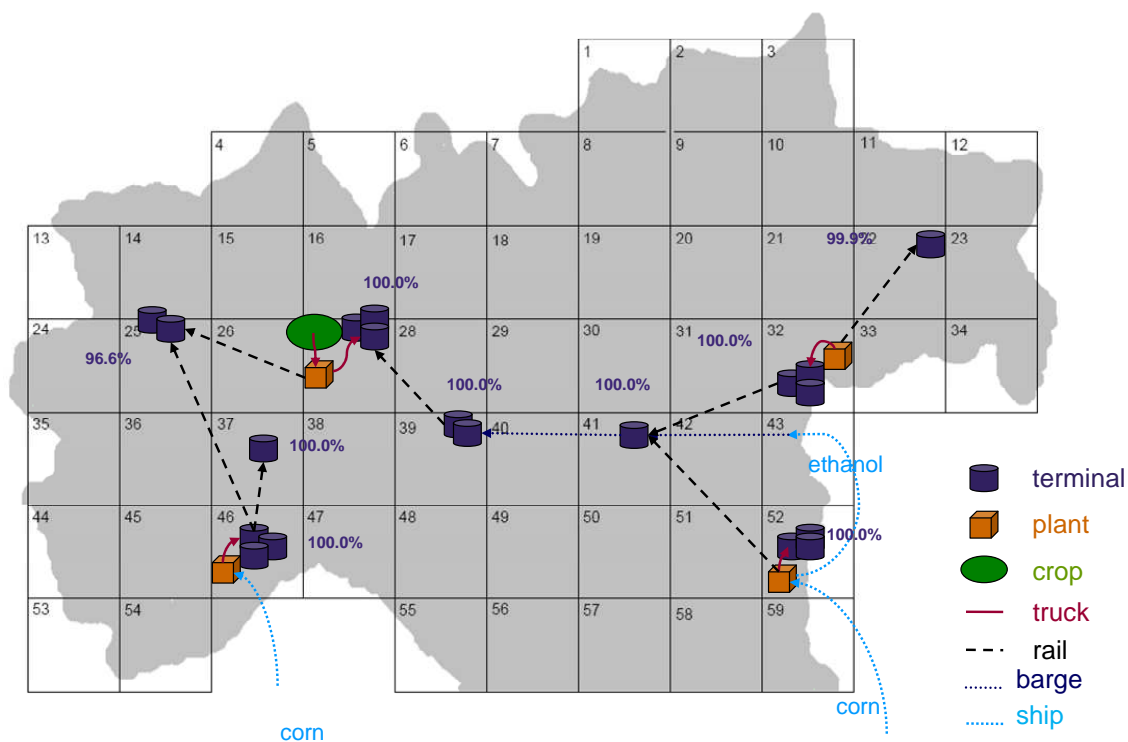


Figure 6.2 Optimal SC configuration for instance A.1.

Figure 6.2 illustrates the optimal SC configuration as planned at the end of the network lifetime for instance A.1: plant sites are located in Milan ($g = 27$), Venice harbour ($g = 32$), Genova ($g = 46$) and Ravenna ($g = 52$). It also shows that biomass importation is mostly preferred to domestic production. Truck delivery is selected only for local transport of high-

density product (ethanol from plants to blending terminals), whereas for long distances bulkier transport means, such as barges or train, are preferred (as they result in a more economical solution for the delivery of low-density biomass).

As the DDGS market price decreases, the economy of scale becomes more important. If the DDGS price is set equal to 200 €/t (instance A.2), three plants of greater average sizes are planned to be built by 2011 (Table 6.5). In particular, plants are established in Venice harbour ($g = 32$), Genova ($g = 46$) and Porto Viro ($g = 43$). This indicates that the payback time is not short enough to suggest the construction of production plants at a later time. Also the average ROI index decreasing to 28.1% reveals the global worsening on the business profitability, which nonetheless remains substantially good. The eNPV moves from 250 M€ for instance A.1 down to 137 M€ for instance A.2 and the NPV best scenario translates from 447 M€ to 327 M€. In Instance A.2 the NPV for the worst scenario becomes -432 M€ (instead of -295 M€ for instance A.1).

Table 6.5 SC configuration when $MPd = 200$ €/t through the eNPV optimisation (instance A.2).

period t	new plants establishment ($Y_{p,g,t}^{plan}$)
1	$[p = 1; g = 32]; [p = 4; g = 46]$
2	$[p = 3; g = 43]$
3	-
4	-
5	-

It is now interesting to compare the demand satisfaction rate for the instances A.1 and A.2. As reported in Table 6.6, bioethanol demand is not completely satisfied in instance A.2, because of a diminution in the business profitability. In other words, the optimal solution does not propose the complete fulfilment of the available quota for biofuel blending. Although the possibility to import ethanol is not considered in this study, which aims at analyzing the possibility of an internal production of biofuels, this is clearly a case for which a different solution is suggested in order to match the market demand: either by allowing for ethanol importation or by introducing some kind of government subsidies.

Finally, the case with a DDGS market price progressively decreasing (instance A.3) is assessed. The planning table reported in Table 6.7 shows a situation very similar to instance A.2 (as demonstrated by the ROI index, which is now equal to 28.7%). Long-term payback times pushes towards an early realization of the bioethanol plant sites.

Table 6.6 Percentages of bioethanol demand fulfilment: comparison between instances A.1 and A.2.

period t	Instance A.1	Instance A.2
1	100.0%	99.7%
2	100.0%	99.9%
3	100.0%	99.7%
4	100.0%	91.2%
5	99.5%	83.0%

Table 6.7 SC configuration when DDGS devaluates over the time through the eNPV optimisation (instance A.3).

period t	new plants establishment ($Y_{p,g,t}^{plan}$)
1	$[p = 1; g = 46]; [p = 4; g = 43]$
2	$[p = 3; g = 27]$
3	-
4	-
5	-

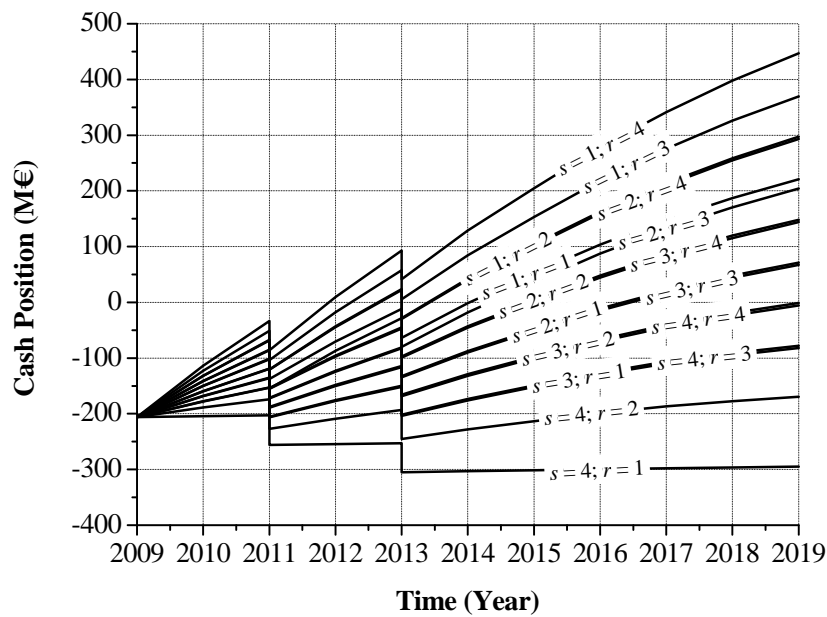


Figure 6.3 Cumulative and discounted cash position chart: instance A.1.

Figure 6.3 shows the discounted cumulative cash position chart for Instance A.1. The discontinuities denote the investments into new plants (in chronological order: Genova and Ravenna by 2009, Milan by 2011 and finally Venice harbour by 2013). It also shows that in the most propitious situation $((q,r) = (1,4))$ the NPV reaches 450 M€ and the investment is

paid back in about three years (with a probability of about 9%). If a maximum payback time of 5 years is considered as an acceptable limit, still a good probability of success is granted (the event probability to have a payback time lower than 5 years is around 69%). On the contrary, the probability not to pay back the investment by the end of the lifetime of the production system (set to 10 years) is about 8%. Figure 6.3, shows that in the optimal solution most possible configurations determine positive NPV values, indicating an NPV distribution shifted toward favourable scenarios.

6.4.2 Case B: planning under risk minimisation

The eNPV optimisation can steer decision makers toward investments aiming at the maximum profit, but it cannot guarantee to prevent economic losses in case of very adverse market conditions. Thus, a risk-averse investor would be more interested at optimising the less favourable situations and other indicators, such as the CVaR, are more suitable than eNPV. The SC planning under CVaR optimisation has the objective to determine the best SC configuration that may diminish the expected economic losses when market conditions are unfavourable. The optimisation shows that when DDGS price goes below 200 €/t the discounted cumulative cash position is never positive even after 10 years. Consequently, the best solution is not to invest on any businesses at all and, accordingly, for instances B.2 and B.3 the proposed solution are not to enter the market. With reference to instance B.1 and as shown in Table 6.8, a few plants of the bigger size are planned according to an economy of scale approach. However, the average ROI index is still not supporting such an investment decision, showing a return on the capital expenditures of 18.8%. Finally, it is also worth noting that the demand satisfaction rate from 2013 onwards is never exceeding the 73.6% of the market requirement: this is clearly representative of a situation in which risk prevention is considered a better solution than meeting the market needs.

Table 6.8 SC configuration when $MPd = 300$ €/t through the CVaR optimisation (instance B.1).

period t	new plants establishment ($Y_{p,g,t}^{plan}$)
1	[$p = 4$; $g = 43$]
2	[$p = 4$; $g = 46$]
3	-
4	-
5	-

Finally, in Figure 6.4 the cumulative and discounted cash position for the scenarios considered in the CVaR optimisation is illustrated. The discontinuities (representing an investment decision) are now occurring only at the very beginning of the time horizon, so

confirming the more adverse financial environment that suggests a less risky investment strategy. This more cautionary behaviour allows for a partial mitigation of the economic losses: for example, the business profitability now falls in the positive region for both scenarios (2,1) and (3,2), while they did not within instance A.1 (as shown in Figure 6.3), although the payback time does not seem high enough to make the investment reasonable. The cautionary approach of the CVaR optimisation can also be observed by comparing the worst scenario ($q = 4; r = 1$) of instances A.1 and B.1 (referring to Figure 6.3 and 6.4, respectively): the NPV is -294.9 M€ for instance A.1 and -222.7 M€ for instance B.1, thus demonstrating a remarkable reduction in the economic losses in planning the production capacity of a supply system.

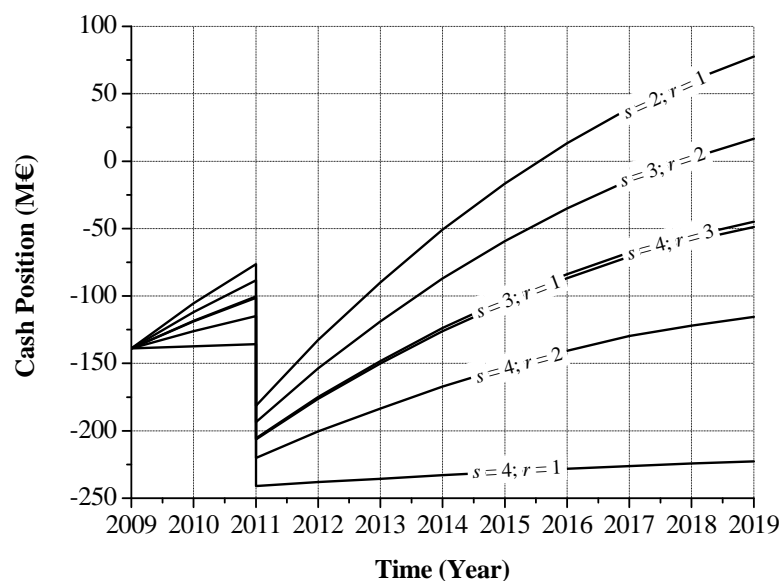


Figure 6.4 Cumulative and discount cash position maximising the CVaR criterion: instance B.1.

6.5 Conclusions

The design of the bioethanol SC through eNPV maximisation suggests that there is always a reasonable probability to obtain profitable results even when it is assumed that the DDGS price may decrease along the years (the average ROI index is about 28% in such a situation). The optimisation results support distributed SC configurations with more plants of smaller size in case of favourable market conditions (instance A.1).

On the other hand, if only the worst market scenarios are considered through the CVaR optimisation, the results show that only a high DDGS selling price (300 €/t) allows for a

profitable configuration (a ROI value of 18.8% is obtained); in the other cases the best solution is not to enter the business.

What we may conclude from the whole set of results presented so far, is that both the economic feasibility and environmental sustainability of bioethanol production in Northern Italy rely on the end-use option for DDGS as valuable product for other applications. In particular, selling DDGS as animal fodder substitute would allow for good performance in terms of both production costs and financial profitability. On the other hand, that reveals an extreme dependence on market conditions. In particular, DDGS price volatility would potentially expose the business to excessive risks as the market value decreases below a limit of about 200 €/ton. Furthermore, this solution would not allow reaching the EU targets in terms of GHG emissions saving: to the scope, it would better perform a technical solution envisaging DDGS as fuel to produce the energy needs of the production plants as showed in Chapter 5. Hence, this option should be further assessed by simultaneously considering the financial performance of the systems as well as its capabilities in mitigating GHG emissions. However, the environmental impact in operating such a production system not only depends on the DDGS end-use solution adopted, it also undergoes the effect of cultivation practices in the biomass production stage of the SC. With concerns to this, an important role is played by fertiliser application to the soil at the crops management level. The next Chapter will be dedicated to the combined financial and environmental analysis of the bioethanol production system by simultaneously optimising DDGS end-use destination and agricultural practices in terms of fertiliser dosage.

Chapter 7

Towards an Overall GHG Emissions Minimisation

The core of the work presented in this Chapter aims at devising a design tool capable of improving the environmental performance of biofuels production so as to reach the mandatory EU standards on GHG emissions. An MILP modelling framework has been developed to optimise the crops management as well as the DDGS end-use technologic choice by simultaneously considering financial and environmental criteria. A general description of the problem issues is firstly presented. Next, the mathematical formulation of the optimisation model is drawn in details. The subsequent section outlines the assessment of the system response to different fertiliser dosages in terms of economic, technological as well as environmental parameters variation trends. Finally, the multi-objective optimisation of the system is carried out according to both profit maximisation and GHG emission minimisation criteria. Some final remarks on the modelling outcomes conclude the Chapter.

7.1 Introduction

The work addressed so far has been dealing with the development of an optimisation tool specifically devised for the simultaneous minimisation of costs and GHG emissions which occur in operating biofuels supply networks as well as for the maximisation of the financial performance of biofuels business. The application of such a strategic tool to assess the oncoming Northern Italy corn-based ethanol production system evidenced that the economic feasibility and financial sustainability strongly rely on the ultimate use of valuable by-products such as DDGS. The analysis also highlighted the high sensitivity of the environmental performance to the biomass cultivation features: in fact, as reported in Chapter 5, biomass production is responsible for about 45% of the overall GHG emissions. In particular, mineral fertilisers (mainly nitrogen-based ones) are deemed as the foremost factor affecting the global warming mitigation potential of biofuels production (especially when first generation technologies are considered). In fact, the extensive application of fixed nitrogen in agriculture is broadly acknowledged to be the primary source of polluting by-products such as

nitrous oxide (N_2O). N_2O is a GHG with an average GWP about 300 times larger than CO_2 . As a source for NO_x , it also plays a major role in stratospheric ozone chemistry (Crutzen, 1970). As a consequence, the increasing production of biofuels to replace fossil fuels might not bring the intended climate cooling due to the accompanying emissions of N_2O (Crutzen et al., 2008). Moreover, nitrogen fertilisers application, together with other crop management practices such as irrigation and planting date, directly affect the net energy value (NEV)¹ and thereby the effective sustainability of the entire production chain (Persson *et al.*, 2009).

The global effect of nitrogen dosage variation in the biomass cultivation stage of bioethanol would entail certain *direct effects* on biomass production parameters and, as a consequence, *indirect effects* on the following stages of the network itself. Hence, increasing the nitrogen inputs per unit of cultivated hectare would:

- 1 directly increase corn yield (*CY*), and, indirectly, ethanol yield (*EY*);
- 2 directly increase the yield in protein (*PY*) to the detriment of starch content of corn grains (*SY*), and, indirectly, improve DDGS yield (*DDGSY*) as well as penalise ethanol yield;
- 3 directly increase costs related to fertilisers, but also reduce operating overheads as an indirect consequence of the potential increase in the products yield (*EY*, *DDGSY*);
- 4 indirectly increase the total impact on global warming (*TDI*) due to greater GHG emissions coming from both fertilisers production and N_2O release from soil, but also increase emission credits coming from products displacement (direct consequence of DDGS overproduction).

All these issues evidence a conflicting situation which cannot be cleared by means of a mere heuristic evaluation of the pros and cons of fertiliser application. Thus, it raises the obvious need for a specific and quantitative tool to steer the crop management toward the best nitrogen dosage ensuring best performance in terms of both costs and GHG emissions.

In light of this, the development of a design tool aiming at a more conscious management of nitrogen application might be effective to tune the environmental performance of bioethanol production so as achieving sensible reduction of GHG emissions. In addition to this, there cannot be found in literature any attempt to assess the bioethanol production through an optimisation tool capable of simultaneously optimising both conversion technology features

¹ The NEV represents the ethanol and co-product output energy minus non-renewable input energy requirements in the production chain, and constitutes a well-defined and established measurement of the energy gain and sustainability of bio-ethanol (Shapouri *et al.*, 2002) and other biofuels (Kim and Dale, 2005a; Pradhan *et al.*, 2008).

and crop management practices. Thus, the ultimate step of the work will be dealing with the inclusion within an MILP framework of nitrogen fertilisers usage and DDGS end-use choice as SC design variables: profit maximisation as well as emissions minimisation will be considered.

7.2 Problem statement

In this Chapter, a general modelling framework is developed to optimise the fertilisers application within the biomass production stage of the bioethanol SC. In particular, the model is conceived as an optimisation problem in which the production chain is required to comply with both NPV maximisation and GHG emissions minimisation criteria.

The optimisation problem can be stated as follows. Given the following inputs:

- > biomass production response to nitrogen dosage (yields, costs, etc);
- > biofuel production facilities capital and operating costs as a function of biomass characteristics;
- > transport logistics costs;
- > environmental burdens of biomass production as a function of nitrogen dosage;
- > environmental burdens of biofuel production as a function of nitrogen dosage as well as of the DDGS end-use options;
- > transport logistics emissions;
- > energy market features (energy purchase prices and green credits),

the objective is to determine the optimal system configuration in terms of financial profitability and GHG emissions. Therefore, the key variables to be optimised are:

- > nitrogen dosage over the biomass crop field;
- > DDGS end-use solution;
- > system financial performance over a 10 years horizon;
- > system impact on global warming.

The problem is referred to a fixed land surface (30,000 ha) fully cultivated to supply the biomass needs of a unique production plant of flexible capacity, anyway ranging within a consistent interval, namely 80–120 kt/y. This represents a conversion plant of small size (corresponding to category $p = 1$, according to Chapter 3 notations). Although the plant size is

meant to affect both the economic performance (due to the economy of scale effect, lowering down the operating cost as much as the size increases) and the financial ones (bigger size entails higher capital investments), this issue should not tamper with the effective consistency of the analysis which indeed relies on more dominant factors, i.e. technological choices and crop management.

The same motivation can stand to justify the simplifications introduced to evaluate the transport system impact on the economic and environmental performance. Accordingly, delivery distances and transport option parameters, for both biomass supply and ethanol distribution, have been averaged on the basis of heuristic considerations (according to the analysis conducted in Chapters 4 and 5), as will be further detailed in a following section.

Finally, the linearity constraints of the MILP mathematical formulation imposed to discretise the nitrogen application domain into 12 intervals n (25 kg_N/ha of extension).

7.3 Mathematical formulation

The mathematical formulation of the proposed framework is based on the modelling approaches adopted in the design of multi-echelon SCs (Sahinidis *et al.*, 1989; Tsiakis *et al.*, 2001), by also introducing dynamic features to address the financial analysis. On the other hand, no features related to capacity allocation and spatially explicit siting of production facilities have been considered. The simplification here introduced is justified by the goal of the optimisation problem under assessment: as the scope of the analysis is to optimise crop management practices and technological choices in terms of DDGS final destination, there is no reason to weigh down the model by adopting a spatially explicit formulation.

7.3.1 Objective functions

The mathematical formulation commences with the definition of the objective functions to be minimised in configuring the system. The first objective considered is the NPV (Obj_{NPV} [€]) of the business to be established. This imposes the maximisation of profit-related indexes, and hence the Obj_{NPV} value is required to be written in its negative form:

$$Obj_{NPV} = FCC - DNI \quad (7.1)$$

where FCC [€] are the facility capital costs and DNI [€] represents the discounted net incomes.

On the other hand, the second objective is to minimise the total daily impact (Obj_{TDI} [kg CO₂-eq/d]) resulting from the operation of the biofuel SC. Thus, the definition of Obj_{TDI} needs considering each life cycle stage contribution, as expressed by Equation (5.1).

Once the optimisation criteria have been defined, all the terms included within the mathematical formulation have to be expressed as explicit functions of the design variables.

7.3.1.1 Facility capital costs

The *FCC* term accounts for the capital investment required to establish a new fuel conversion facility. However, this model allows for the choice between two different technological options according to the two mentioned solution proposed for DDGS use: this requires to distinguish between the possibility to adopt either the standard conversion technology ($k = 1$), in which DDGS is processed as a simple by-product to be sold to the animal fodder market, or an alternative one ($k = 2$) envisaging the construction of a CHP station fuelled by DDGS to produce heat and electricity. The latter option entails additional capital expenditures as shown by the parameters value reported in Table 7.1.

According to this, *FCC* can be calculated by alternatively assigning the capital investment value (CI_k [€]) corresponding to the technological features adopted, as expressed by:

$$FCC = \sum_{n,k} CI_k \cdot W_{n,k} \quad (7.2)$$

where $W_{n,k}$ is the binary decision variable controlling whether to establish a production facility of type k when a nitrogen dosage n is applied: a value of 1 allows for the construction of the plant type k , otherwise 0 is assigned.

Table 7.1 Facilities capital investment (CI_k) of technological option k .

technology k	CI_k
1	75,320,000
2	97,110,000

7.3.1.2 Discounted net incomes

The discounted net incomes *DNI* is defined as the sum over the 10 year operating period of the annual profit before taxes (PBT_t [€/y]) plus the annual depreciation charge related to the capital investment (D [€/y]) minus the taxation charge for each year t (TAX_t [€/y]), as expressed by the following equation:

$$DNI = \sum_t (PBT - TAX_t + D) \cdot \varepsilon_t \quad (7.3)$$

All the terms on the right hand side of Equation (7.3) have been discounted through the application of a discount factor (ε_t) defined as (Douglas, 1988):

$$\varepsilon_t = \frac{1}{(1 + \zeta)^t} \quad (7.4)$$

The profit before taxes PBT represents the gross annual profit and has been defined as the difference between the total annual revenues TAR [€/y] and the total operating costs OC [€/y] for year t minus the depreciation charge D . Accordingly:

$$PBT = TAR - OC - D \quad (7.5)$$

TAR represents the annual incomes which depend on both ethanol and DDGS sales:

$$TAR = MPE \cdot \sum_{n,k} Pe_{n,k} + \sum_{n,k} Pd_{n,k} \cdot MPd_{n,k} \cdot \omega_k \quad (7.6)$$

where MPE is the bioethanol market price (set equal to 709 €/t according to the latest trends for Southern Europe market, (Agra Informa, 2009)); $Pe_{n,k}$ [t/y] and $Pd_{n,k}$ represent, respectively, the ethanol and DDGS production rate related to plant technology k when a nitrogen dosage n is applied to crop biomass; $MPd_{n,k}$ is the DDGS market value and depends on the DDGS end-use solution k . When DDGS is used as soy-meal substitute in the animal fodder market ($k = 1$), $MPd_{n,1}$ is the market price that also depends on the nitrogen dosage n and has been estimated following the detailed procedure that will be later discussed. On the other hand, if power generation is chosen as end-use solution ($k = 2$), $MPd_{n,2}$ identifies the market price per unit of electric energy sold to the grid. This is equal to 91.34 €/MWh_e concerning with the conventional electricity production, although it might be 180 €/MWh_e if green credits are considered (GSE, 2009) and does not depend on the nitrogen dosage n in any case (this is based on the assumption that the variation in the protein content does not affect the DDGS heating value significantly). This modelling solution also requires the application of a conversion factor, ω_k , to quantify the amount of by-product produced per unit of DDGS. Thus, when power generation is chosen as end-use solution ($k = 2$), $\omega_{n,2}$ [kWh_e/t_{10%_m}] identifies the amount of energy that can be sold to the grid per unit of DDGS produced. This conversion factor has been estimated using the process model described in Chapter 3 following the detailed procedure that will be later discussed. On the other hand, when DDGS is used as soy-meal substitute in the animal feed market ($k = 1$), the amount of by-product to be sold should be equal to the overall DDGS production. Therefore, in order to comply with Equation (7.6), $\omega_{n,1}$ [t/t] has been set equal to 1.

OC is given by the sum of the annual operating costs over the entire supply chain. Accordingly:

$$OC = BPC + EPC + TC - BC \quad (7.7)$$

where BPC [€/y] represents the biomass production costs, EPC [€/y] are the ethanol production costs (also embodying the DDGS production overheads), TC [€/y] the transport costs for both biomass supply and ethanol distribution and BC [€/y] defines the by-products allocation credits.

All these terms are defined by the following equations:

$$BPC = \sum_{n,k} Pb_{n,k} \cdot UPCb_n \quad (7.8)$$

$$EPC = \sum_{n,k} Pe_{n,k} \cdot UPCe_n \quad (7.9)$$

$$TC = UTCb \cdot \sum_{n,k} Pb_{n,k} + UTCe \cdot \sum_{n,k} Pe_{n,k} \quad (7.10)$$

$$BC = \sum_{n,k} Pe_{n,k} \cdot UCRd_{n,k} \quad (7.11)$$

where $Pb_{n,k}$ represents the biomass production rate supplying a conversion plant of type k when a nitrogen dosage n is applied to crop fields, $UPCb_n$ [€/t_{DM}] and $UPCe_n$ [€/t] are respectively the unit production costs for biomass and ethanol, $UTCb$ [€/t_{DM}] and $UTCe$ [€/t] define the unit transport costs for biomass and ethanol respectively, and $UCRd_{n,k}$ is the costs reduction per unit of DDGS used as a valuable alternative k and produced when a nitrogen dosage n is applied. This last parameter mainly depends on the DDGS end-use solution k . When DDGS is used as soy-meal substitute in the animal fodder market ($k = 1$), $UCRd_{n,1}$ is set equal to 0, because no costs reductions come from this business. Whilst, if the power generation is chosen as end-use solution ($k = 2$), $UCRd_{n,2}$ identifies the costs reduction coming from the gas and electricity saving due to CHP self-generation. The savings also depend on the nitrogen dosage n and have been estimated using the process model described in Chapter 3 following the detailed procedure that will be later discussed.

The last factor defining PBT in Equation (7.5) is the depreciation charge D evaluated by simply dividing the total capital investment by 10 (thus assuming a constant depreciation strategy) expressed by the following equation:

$$D = \frac{TCI}{10} \quad (7.12)$$

Finally, with concerns to TAX_t , this variable could not be defined through a unique equation. Indeed, the taxation charge should be applied only when a positive annual gross profit is obtained, otherwise it must be avoided. Moreover, TAX_t is a function of PBT and thereby

Equation (7.3) would be in conflict with the linearity needs imposed by the MILP formulation. Hence, the problem was overcome through the introduction of an indicator variable (as suggested by Williams (1985) to keep the conventional MILP formulation when this kind of problems occurs), V_t , so that if PBT results positive V_t takes a value of 1, otherwise 0 is assigned. This results by the imposition of the following set of constraints:

$$TAX_t \geq 0 \quad (7.13)$$

$$TAX_t \geq Trate \cdot PBT - V_t \cdot M \quad (7.14)$$

$$M \cdot (1 - V_t) \geq PBT \quad (7.15)$$

$$-M \cdot V_t \leq PBT \quad (7.16)$$

where $Trate$ is the taxation rate (set equal to 43% according to Peters *et al.* (2003)) and M is a constant coefficient representing a known upper bound for PBT . Accordingly, if PBT is positive Equation (7.15) imposes V_t equal to 0, and thus, as Equation (7.14) holds, TAX_t is minimised and lowered down to the minimum value allowed (that is $Trate \cdot PBT$); otherwise, if PBT is negative, V_t is set equal to 1 by Equation (7.16), and hence, according to Equations (7.13) and (7.14), TAX_t is set equal to 0.

7.3.1.3 Environmental impact

The definition of stage-related environmental impacts represented by Equation (5.3) still holds for the entire set of life cycle stages here considered. The reference flows as well as the impact factors depend both on the nitrogen dosage n and on the technology k adopted for biomass processing. Accordingly, Equation (5.3) now takes the form:

$$I_s = \sum_{n,k} f_{s,n,k} \cdot F_{n,k} \quad (7.17)$$

Thus, it is necessary to uniquely define the reference flows for each individual life cycle stage and express them explicitly as a function of the design variable controlling the optimisation problem. Table 7.2 summarises the reference flow assignment to each life cycle stage.

7.3.2 Logical constraints and mass balances

All the cost terms in the objective function (7.1) and the reference flows of Equation (7.17) depend on the SC design variables related to fuel, biomass and DDGS production rates as well as on the decision variables characterising the technological and crop management

choices. All these variables are then linked to the specific SC features through the definition a set of constraints that must be satisfied in each of the SC stage.

Table 7.2 Reference flows F_s , as assigned to each life cycle stage.

stage s	F_s
bp	$Pb_{n,k}$
bt	$Pb_{n,k}$
ep	$Pe_{n,k}$
ed	$Pe_{n,k}$
bc	$Pd_{n,k}$

7.3.2.1 Constraints

A set of relations is formulated to constrain the goods production rate together with the binary variables. In particular, $Pb_{n,k}$ is the dominant production variable and is defined as follows:

$$Pb_{n,k} = LA \cdot GY_n \cdot W_{n,k} \quad (7.18)$$

where LA [ha] is the land availability (set equal to about 30,000 ha, as declared in the previous section) and GY_n [t_{DM}/ha] the grain yield per hectare when a nitrogen dosage n is applied.

Once the biomass production is quantified, the ethanol and DDGS production rates can be derived by simply applying a specific conversion factor. Accordingly:

$$Pe_{n,k} = Pb_{n,k} \cdot \gamma_n \quad (7.19)$$

$$Pd_{n,k} = Pb_{n,k} \cdot \delta_n \quad (7.20)$$

where γ_n [t_{biofuel}/t_{biomass}] and δ_n [t_{10%DM}/t_{biomass}] are respectively the alcohol and DDGS yields when biomass is cropped by applying a nitrogen dosage n .

Variable $W_{n,k}$ (Equation (7.2)) involves decisions about whether to apply a nitrogen dosage n and whether to adopt a production technology k . In addition, we assumed the operation of a unique production plant that is supplied by a hypothetical crop field of 30,000 ha of surface. Consequently, the crop management choice as well as the technological option to be defined through the optimisation problem has to be unique. Therefore, we have that:

$$\sum_{n,k} W_{n,k} = 1 \quad (7.21)$$

Finally, the last constraints simply impose that a number of variables should maintain a physical meaning, i.e. they must be non-negative:

$$Pb_{n,k} \geq 0 \quad (7.22)$$

$$Pe_{n,k} \geq 0 \quad (7.23)$$

$$Pd_{n,k} \geq 0 \quad (7.24)$$

7.4 Modelling assumptions

This section presents the description of the procedure that has been followed in defining the set of modelling parameters with reference to the case study so far considered. The methodology adopted in this Chapter still refers to the classical SCA (for economic evaluations) and LCA techniques (in relation to environmental analysis).

It is noteworthy to declare here an important assumption that was made at the preliminary step of the study: after an unprofitable literature review specifically focussed on corn cultivation in the geographical region of study and on the related issue of nitrogen fertiliser application, no consistent and/or complete set of data has been found so as to carry out the corn-based analysis thoroughly. Thus, it was decided to base the parameters definition onto detailed data sources broadly available for wheat and subsequently to tune up the wheat data set to corn cultivation. Notwithstanding this simplification, it is our belief that the existing similarities between corn and wheat cropping systems still allow for a rigorous assessment.

7.4.1 Response curves

Kindred *et al.* (2008) in assessing the difference between hard- and soft-endosperm wheat varieties response to nitrogen application evidenced the consistent effect of fertilisation on grain yield, grain protein content and alcohol yield. They also assessed the optimal nitrogen application in achieving the maximum alcohol yield under cost minimisation and emission savings criteria, although they did not use a proper optimisation-based framework, but rather a heuristic approach, to carry out the analysis. The reference data set comes from the experimental work conducted by different groups and, in particular, refers to the work by Smith *et al.* (2006) which is here taken as the reference benchmark. Data and diagrams reported in the cited work have been used to define both the graphical and mathematical dependence of grain yield (*GY*), grain protein content (*PC*) and alcohol yield (*EY*) on nitrogen dosage (*ND*), i.e. the primary response curves. Figure 7.1 shows the trends of the response

curves, whereas in Table 7.3 the parameters of the polynomial fittings², which describe the mathematical dependency, are reported.

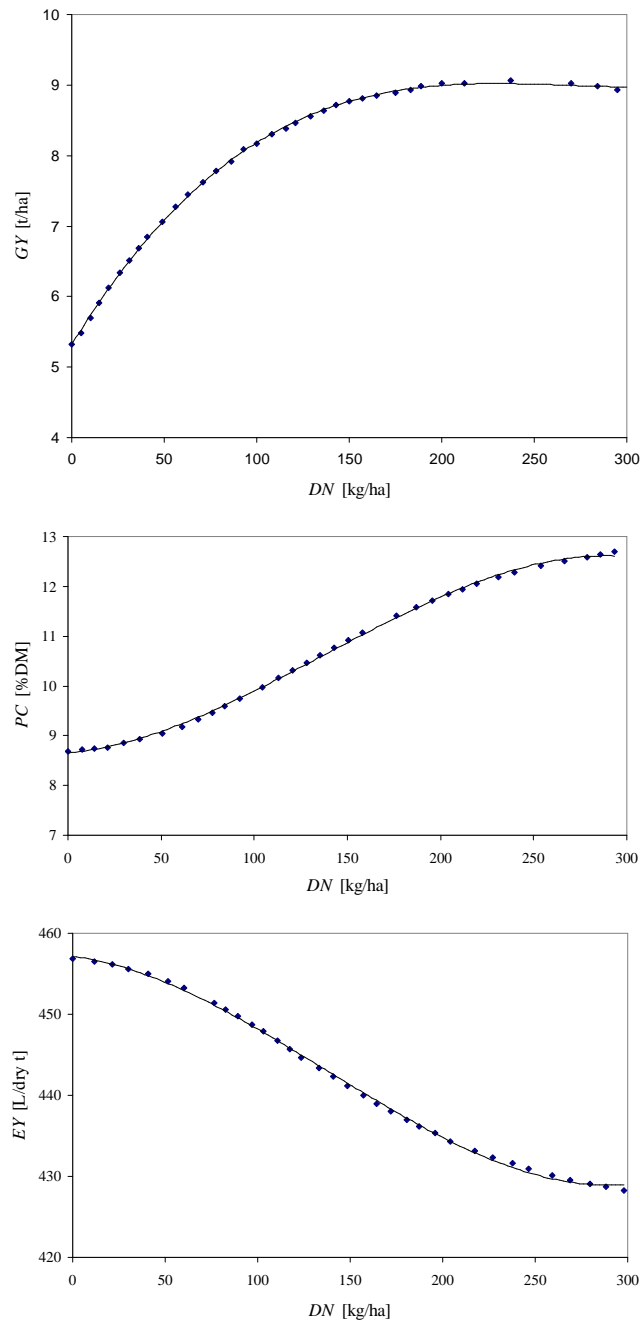


Figure 7.1 Primary response curves for wheat as derived from Smith et al. (2006).

²The polynomial relations can be generally expressed by the formulation:

$$Y = A \cdot DN^3 + B \cdot DN^2 + C \cdot DN + D \quad (7.25)$$

where Y is representative of GY , PC and EY .

Table 7.3 Primary response curves polynomial coefficients.

	A	B	C	D
GY	2.0×10^{-7}	-1.6×10^{-4}	0.0430	5.32
PC	3.0×10^{-7}	1.2×10^{-4}	0.0034	8.65
EY	1.9×10^{-6}	8.0×10^{-4}	0.0282	457.15

Once the fundamental relations have been defined, the secondary response curves can be estimated. The detailed procedure is reported in Appendix C. Then the wheat response curves have been adapted to corn cultivation and subsequently discretised as discussed in details in Appendix D.

7.4.2 Modelling parameters

The entire set of model parameters and their inherent dependence on nitrogen application have been estimated on the basis of the response curves previously defined.

7.4.2.1 Technological analysis

Starting with the technological related parameters, GY_n , δ_n , γ_n and μ_n (this is the soy-meal replacement capacity factor expressed in t of soy-meal that can be replaced by a t of DDGS according to the relative protein content) have been directly obtained by assigning for each nitrogen dosage value (DN_n) the corresponding response function value, respectively GY , $DDGSY$, EY and $SMrepl$. The resulting technological parameters are summarised in Table 7.4.

Table 7.4 Model parameters for corn cultivation: technological analysis.

dosage n	DN_n (kg/ha)	GY_n (t_{DM}/ha)	δ_n (t_{10%_m}/t_{DM})	γ_n (t/t_{DM})	μ_n (t_{SM}/t_{10%_m})
1	12.5	8.62	0.345	0.374	0.69
2	37.5	9.13	0.346	0.373	0.71
3	62.5	10.01	0.347	0.372	0.72
4	87.5	10.72	0.349	0.370	0.74
5	112.5	11.27	0.352	0.368	0.77
6	137.5	11.68	0.355	0.365	0.80
7	162.5	11.97	0.358	0.363	0.84
8	187.5	12.16	0.361	0.360	0.87
9	212.5	12.27	0.364	0.357	0.90
10	237.5	12.32	0.367	0.355	0.93
11	262.5	12.32	0.368	0.353	0.95
12	287.5	12.30	0.370	0.352	0.96

7.4.2.2 Economic analysis

With concerns to the economic parameter definition, the unit production costs for biomass cropping ($UPCb_n$) have been calculated using a data sheet reporting the detailed costs list (CRPV, 2007) for corn production in Northern Italy and varying the nitrogen fertiliser costs according to N_n . The procedure results in a hectare dependent data set that has been converted into a “dry matter” weight basis by dividing by the grain yield (GY_n). Unit production costs for ethanol ($UPCe_n$) have been estimated using the purpose-designed financial model described in Chapter 3. The model has been hence adapted to take into account different operating conditions in terms of corn grain composition, ethanol yield and DDGS yield. This went through the formulation of the following assumptions:

- 1 capital costs do not change with the feed flow variation: this should not affect the results reliability because the ethanol production rates lay within the production plant flexibility.
- 2 the drying-house gas requirements, depending on the DDGS yield, and the steam production gas requirement, depending on biomass inputs, have been separated to derive respectively the “heat requirement per unit of DDGS” and “heat requirement per unit of corn” factors to apply in estimating the production costs for the entire set of n dosage intervals.
- 3 electricity as well as process and cooling water needs have been entirely allocated to ethanol production and set proportional to the corn input rate.
- 4 capital charge expenditures as well as biomass supply costs have been discounted from the overall cost estimation because they have been already accounted in the main model formulation.
- 5 no costs allocation has been taken into account because DDGS is considered as a source of revenues in the objective function.

Unit costs reduction ($UCRd_{n,k}$) coming from DDGS use as valuable product for other scopes depends on the end-use solution k adopted to capitalise on the by-product. As already mentioned, when DDGS is used as soy-meal substitute in the animal fodder market ($k = 1$), $UCRd_{n,1}$ is set equal to 0 because no costs reductions come from this business. However, if the power generation is chosen as end-use solution ($k = 2$), $UCRd_{n,2}$ identify the costs reduction coming from the gas and electricity saving due to CHP generation within the system itself. The nitrogen dosage dependent set of value has been obtained as the difference between $UPCe_n$ and the unit production costs calculated through the financial model neglecting all the utilities costs. This involves the assumption that the DDGS-fuelled CHP station always provides a sufficient amount of energy to supply the energy needs in operating the ethanol plant (Morey *et al.*, 2006).

Also the DDGS market price ($MPd_{n,k}$) depends on the DDGS end-use solution k and on the nitrogen application n due to the variation in soy-meal replacement capabilities (represented by the μ_n parameter). When DDGS is used as soy-meal substitute in the animal feed market ($k = 1$), $MPd_{n,1}$ is the market price mentioned in the previous section. This has been set equal to 300 €/t for the standard DDGS characteristics (corresponding to $n = 4$) and then scaled depending on the DDGS protein content as a function of nitrogen dosage. If the power generation is chosen as end-use solution ($k = 2$), $MPd_{n,2}$ identifies the price per unit of electric energy sold to the grid.

The resulting economic parameters are summarised in Table 7.5.

Table 7.5 Model parameters for corn cultivation: economic analysis.

dosage n	DN_n (kg/ha)	$UPCb_n$ (€/t _{DM})	$UPCe_n$ (€/t)	$UPCd_{n,k}$ (€/t _{0%_m)}		$MPd_{n,k}$	
				$k = 1$	$k = 2$	$k = 1$ (€/t _{0%_m)}	$k = 2$ (€/MWh)
1	12.5	151.2	195.6	0	112.7	264.6	91.3 or 180.0
2	37.5	139.7	193.8	0	120.4	272.4	91.3 or 180.0
3	62.5	132.1	191.4	0	114.2	276.9	91.3 or 180.0
4	87.5	127.3	190.3	0	115.2	282.9	91.3 or 180.0
5	112.5	124.3	190.1	0	116.4	295.3	91.3 or 180.0
6	137.5	122.8	190.4	0	117.5	308.8	91.3 or 180.0
7	162.5	122.3	191.2	0	118.7	322.6	91.3 or 180.0
8	187.5	122.6	192.3	0	119.8	335.9	91.3 or 180.0
9	212.5	123.6	193.5	0	120.9	348.0	91.3 or 180.0
10	237.5	125.0	194.7	0	121.8	358.0	91.3 or 180.0
11	262.5	126.7	195.7	0	122.6	365.2	91.3 or 180.0
12	287.5	128.5	196.5	0	123.1	368.8	91.3 or 180.0

Finally, the transport related unit costs for biomass supply ($UTCb$) and ethanol distribution ($UTCe$) have been estimated by multiplying the average delivery distance (assumed equal to 50 km for biomass delivery and 75 km for ethanol distribution) by the average between train, trucks and small trucks transport costs. This results in a constant value of about 15.5 €/t for biomass delivery and of about 24.4 €/t for ethanol distribution).

7.4.2.3 Environmental analysis

The environmental analysis implemented to evaluate the impact factors (f_s) response to nitrogen dosage has been carried out according to the LCA principles and features as described in Chapter 3.

Accordingly, the global emission factor for biomass cultivation ($f_{bp,n}$) has been defined by using an interactive spreadsheet based tool specifically developed to investigate the GHG emission related to wheat-to-ethanol production in the UK (Brown *et al.* 2005) and adapted to corn cultivation: the input parameters have been changed according to the case study under assessment; in particular, hectare specific impact factors depending on nitrogen application (DN_n) have been calculated assigning the nitrogen dosage specific for each interval n and then converted into a grain production rate basis by dividing by the grain yield (GY_n). It is important to notice that in this model the drying and storage stage (and thus the related emissions) has been included within the biomass production one.

The transport related emission factors for biomass delivery (f_{bt}) and ethanol distribution (f_{et}), expressed as kgCO₂-eq per ton delivered, have been estimated by multiplying the average delivery distance previously mentioned by the average emission factors between train and truck means (resulting in a constant value of about 3.59 kgCO₂-eq/t for biomass delivery and of 5.38 kgCO₂-eq/t for ethanol distribution).

Similarly to $f_{bp,n}$, the global emission factor for ethanol production ($f_{ep,n}$) has been estimated by using the mentioned spreadsheet: this tool has been adapted by changing time by time the DN_n specific input parameters and, in particular, biomass feeding composition, ethanol yield and DDGS yield (it is worth to remind that energy needs and utilities consumption mainly depend on these parameters).

Finally, according to what addressed in Chapter 3, also in this analysis a certain amount of emission savings have been assigned to DDGS end-use options. The so called emission credits ($f_{ec,n,k}$) depend on the DDGS end-use solution k as well as on the nitrogen dosage n and are expressed as kg of CO₂-eq avoided per unit of DDGS (at 10% of moisture) produced. When DDGS is used as soy-meal substitute in the animal feed market ($k = 1$), $f_{ec,n,1}$ has to account for the emissions avoided to produce and import from US an equivalent amount of soy-meal: this globally results in emissions of 0.46 kgCO₂-eq (Brown *et al.* 2005) for each kilogram of soy-meal produced and transported; this value has been then multiplied by the soy-meal replacement factor (μ_n) so as to obtain the DN_n depended parameter. On the other hand, if the power generation is chosen as end-use solution ($k = 2$), $f_{ec,n,2}$ identifies the emission credits coming from the gas and electricity saving due to CHP generation with DDGS as fuel. The nitrogen dependent set of value has been obtained by summing two contributes:

- 1 natural gas (heat needs) saved per unit of DDGS at 10% of moisture (a value obtained by dividing the natural gas needs per unit of ethanol by the DDGS yield per unit of ethanol produced, both DN_n dependent) multiplied by the natural gas combustion emission factor (60.8 kgCO₂-eq/GJ, see DEFRA (2008)).

- 2 electric energy produced (accounting for both the plants needs and the energy sold to the grid) per unit of DDGS at 10% of moisture (corresponding to the CHP station energy production rate) multiplied by the electric energy emission factor (130.05 kgCO₂-eq/GJ, see EME (2003)).

The set of parameters is reported in Table 7.6.

Table 7.6 Model parameters for corn cultivation: environmental analysis.

dosage n	DN_n (kg/ha)	$f_{bp,n}$ (kgCO ₂ -eq/t _{DM})	$f_{ep,n}$ (kgCO ₂ -eq/t)	$f_{ec,n,k}$ (kgCO ₂ -eq/t _{10%_m)}	
				$k = 1$	$k = 2$
1	12.5	272.73	1052.10	316.41	1532.65
2	37.5	291.14	1052.55	325.77	1531.46
3	62.5	296.25	1054.18	331.21	1527.23
4	87.5	305.45	1056.63	338.34	1521.02
5	112.5	317.88	1059.71	353.16	1513.39
6	137.5	333.03	1063.23	369.29	1504.92
7	162.5	350.61	1066.99	385.81	1496.14
8	187.5	370.39	1070.80	401.76	1487.54
9	212.5	392.14	1074.43	416.21	1479.61
10	237.5	415.62	1077.64	428.21	1472.77
11	262.5	440.49	1080.21	436.83	1467.44
12	287.5	466.30	1081.88	441.12	1464.03

7.5 Results and discussion

The developed modelling framework has been used to perform the crop management and DDGS end-use choice optimisation for the bioethanol production system of study. The MILP models were solved through the CPLEX solver in the GAMS[®] modelling tool (Rosenthal, 2006).

The model has been firstly applied to optimise the system by assuming standard market conditions for the electric energy vending ($MPd_{n,2} = 91.34$ €/MWh).

The sub-optimal set of solutions coming from the trade-off between the environmental (total impact, TI, expressed in kt CO₂-eq) and the financial (Net Present Value, NPV, expressed in M€) criteria is reported in Figure 7.2.

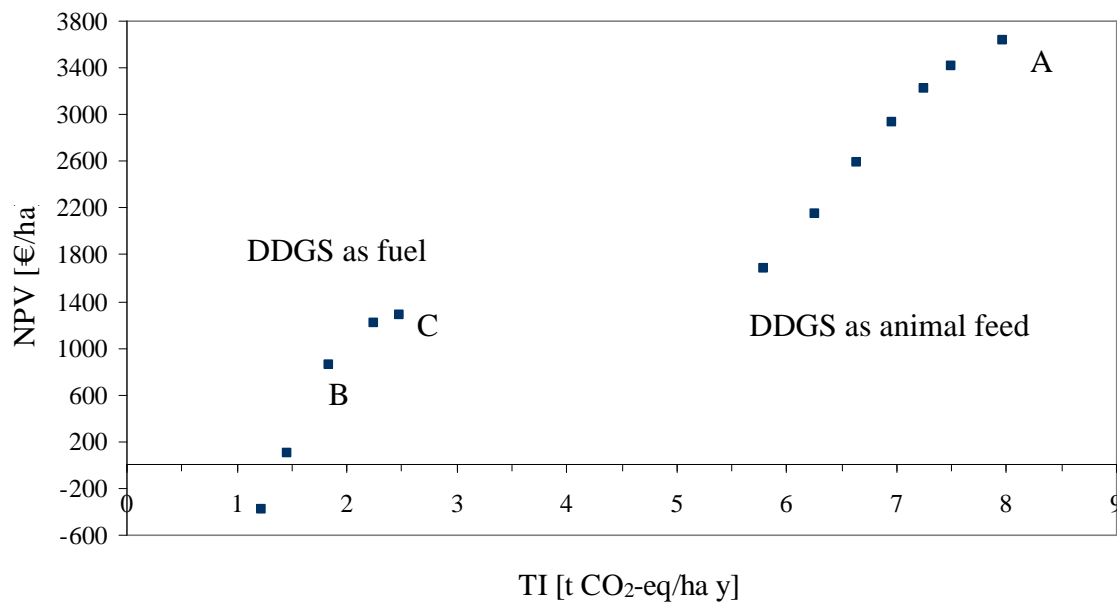


Figure 7.2 Pareto curve for the simultaneous optimisation under NPV maximisation and GHG emissions minimisation criteria when $MPd_{n,2} = 91.34 \text{ €/MWh}_e$.

Point A on the diagram represents the best optimum in terms of economic performance that can be obtained by applying a nitrogen dosage of $237.5 \text{ kg}_N/\text{ha}$ and using DDGS as animal fodder substitute. However, this is not a feasible solution if we consider the EU target of 35% of emission savings: point A, indeed, corresponds to a GHG emissions reduction of about 21% that totally amount to $238.9 \text{ kt CO}_2\text{-eq}$ (about $67.6 \text{ kg CO}_2\text{-eq/GJ}_{\text{EtOH}}$). The mentioned target is never met if we keep using the DDGS as animal feed substitute. Thus, it is worth to investigate on the other alternative, namely the use of DDGS to fuel a CHP station. In this case, we assist to a sensible GHG emissions reduction by still remaining within the economic feasibility region. It is possible to obtain payback times lower than 6 years from point B up to point C. The environmental optima (that also assures feasible economic conditions) involves a nitrogen dosage of $87.5 \text{ kg}_N/\text{ha}$ (point B) so allowing for a GHG emissions reduction of about 80% ($17.1 \text{ kg CO}_2\text{-eq/GJ}_{\text{EtOH}}$) with respect to gasoline and realising an NPV of about 25.7 M€ (the payback time is still reasonable and amounting to about 6 years, as it is shown in Figure 7.3). On the other hand, the financial optima (still assuring feasible environmental performance) involves a greater nitrogen dosage ($162.5 \text{ kg}_N/\text{ha}$, point B) so resulting in higher GHG emissions, although still more than acceptable ($21.2 \text{ kg CO}_2\text{-eq/GJ}_{\text{EtOH}}$, corresponding to 75% of emissions savings with respect to gasoline), and realises an NPV of about 38.5 M€ (the payback time is now 5.5 years, as it is shown in Figure 7.4).

The situation might be even more profitable if the bioethanol business would be supported by governmental subsidies, as it is actually envisaged according to the latest Italian regulation on renewable energy: accordingly the electric energy produced from renewable energy sources can be sold at a price of 180 €/MWh_e .

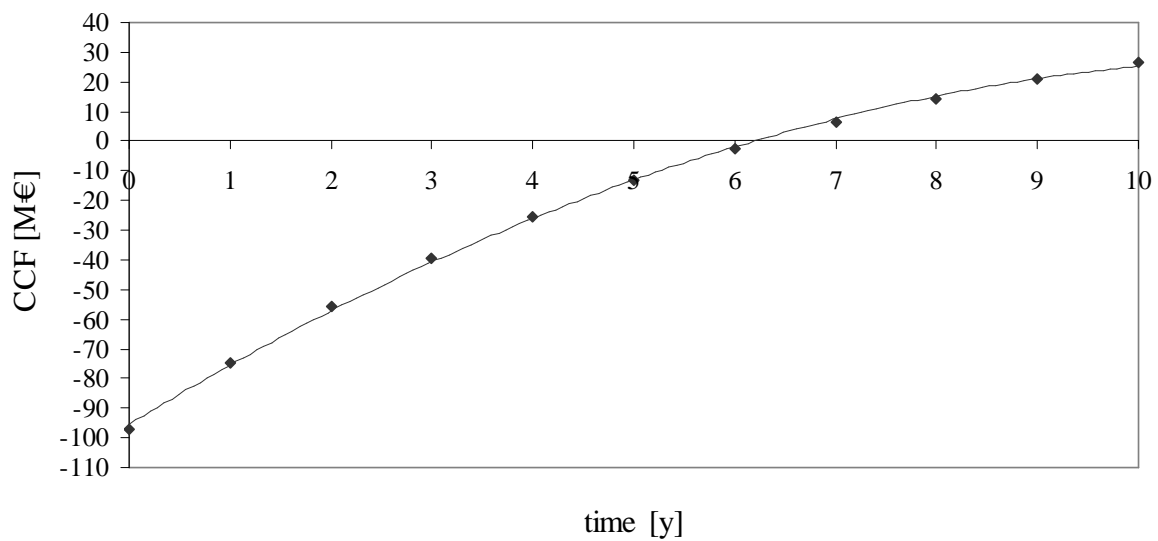


Figure 7.3 Actualised Cumulative Cash Flow: financial performance when a nitrogen dosage of 87.5 kg_N/ha (point B) is applied and DDGS is used to fuel a CHP station.

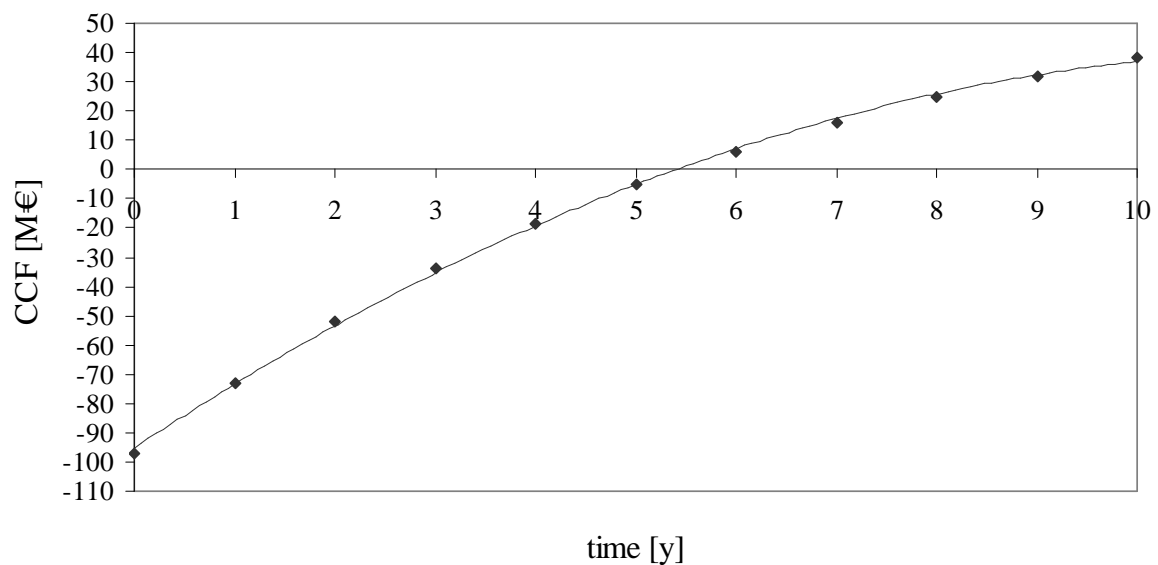


Figure 7.4 Actualised Cumulative Cash Flow: financial performance when a nitrogen dosage of 162.5 kg_N/ha (point C) is applied and DDGS is used to fuel a CHP station.

The positive effect of these subsidies is evident from the set of sub-optimal solutions reported in Figure 7.5. Considering the solution involving DDGS as animal feed substitute, the situation does not change because green credits do not affect the financial features of this option. On the other hand, the financial performance is actually enhanced if DDGS is used to fuel a CHP station: as evidenced in the graph depicted in Figure 7.5 the points between D and E represent feasible options in terms of both economic and environmental criteria. For instance, by applying a nitrogen dosage of 37.5 kg_N/ha (point D) the environmental optima entails a GHG emissions reduction amounting to about 82% (15.8 kg CO₂-eq/GJ_{EIOH}) with an

economic profit of about 27 M€ over a 10 years horizon (the payback time is about 6 years, still). However, if the profit maximisation is preferred, it is possible to apply up to 162.5 kg_N/ha (point E) so as to keep within the environmental feasibility region (the GHG emissions reduction would be 75% with respect to gasoline) and realising excellent financial performance: as shown in Figure 7.6, the NPV now amounts to 68.4 M€ so allowing for the lowest payback time (4 years).

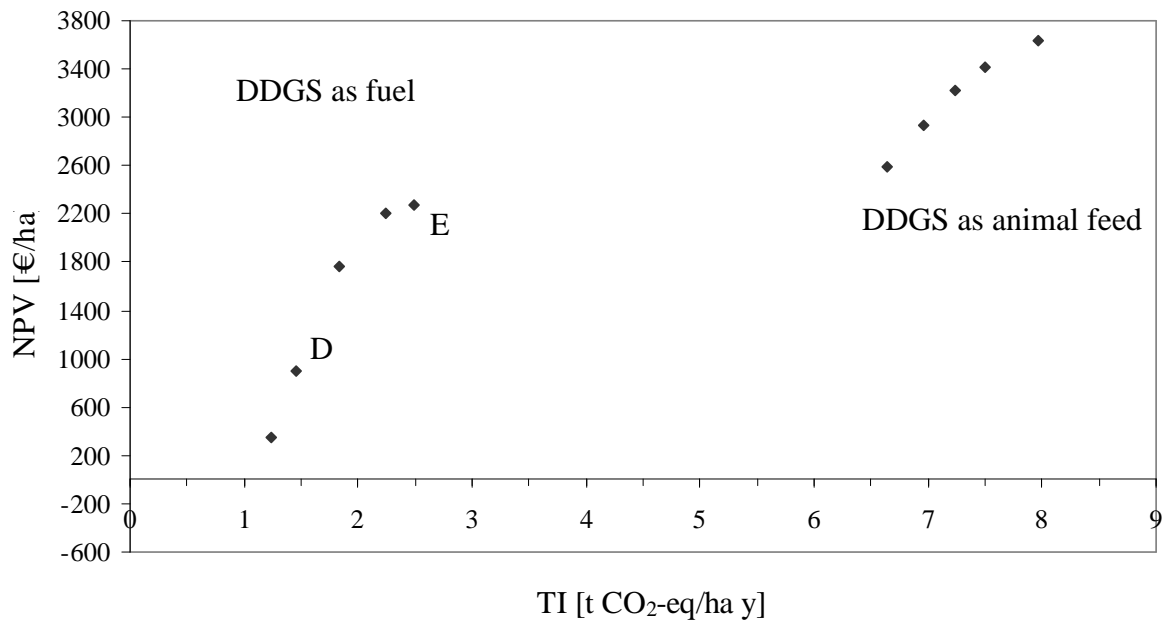


Figure 7.5 Pareto curve: simultaneous optimisation under NPV maximisation and GHG emissions minimisation criteria by considering the green credits effect.

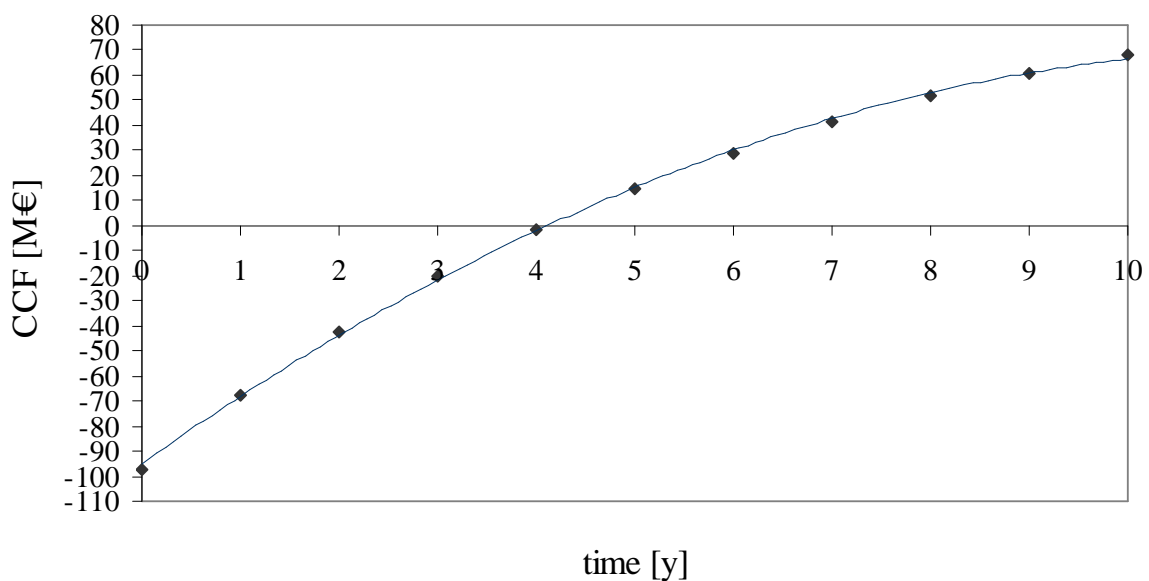


Figure 7.6 Actualised Cumulative Cash Flow: financial performance when a nitrogen dosage of 162.5 kg_N/ha (point E) is applied and DDGS is used to fuel a CHP station.

7.6 Conclusions

The analysis conducted in this Chapter has considered crop management and DDGS end-use choice as design features to be optimised under both financial and environmental criteria. NPV maximisation and the simultaneous GHG emission minimisation suggest that the only way to meet both financial feasibility (referred to a payback time threshold of about 6 years) and the EU standards on biofuels (namely the 35% of emission savings) is to adopt a technological solution envisaging the construction of a CHP station to be fuelled with DDGS. This would allow to provide the energy needs of the biofuel production plant and, at the same time, to perform an electricity overproduction that would grant consistent incomes to make the business financially feasible. On the other hand, the crop management practices would be more sustainable, too: the technological option adopted would allow for more sustainable agricultural practices involving very low nitrogen dosage as mineral fertiliser (about 87.5 kg_N/ha) so as to reach GHG emission savings of about 80% with respect to gasoline production.

The situation would be even more sustainable if the ethanol production is promoted by deploying governmental subsidies on renewable energy generation. Given the Italian regulation perspectives, they would entail a selling price for electric energy produced by renewable sources of about 180 €/MWh: at these conditions the same financial performance would be reached by penalising the biomass yield (thus reducing the nitrogen fertiliser application down to about 37.5 kg_N/ha) so as enhancing the GHG emissions savings (now accounting for 82% of reduction with respect to gasoline). It is also worth mentioning that a more thoughtful use of mineral fertiliser would also reduce other environmental impacts coming from fixed nitrogen application to agricultural soils like, for instance, eutrophication and acidification of the ecosystem.

If we look at the problem by the investors point of view, the system should be designed under profit maximisation. This can be realised by pushing the fertiliser application toward the maximum allowed by the environmental feasibility conditions. Accordingly, it results in a nitrogen dosage of about 162.5 kg_N/ha, condition that would involve an NPV equal to 38.5 M€ (value which might increase up to 68.4 M€ if governmental subsidies are considered).

Finally, it is important to mention that a similar assessment has been conducted for wheat-based ethanol production and it led to similar conclusions. However, we preferred showing the results related to corn-based production because they lay on the same logic strand of the rest of the Thesis, referring to corn-based ethanol in Northern Italy.

Chapter 8

Final Remarks and Future Work

In this Chapter, the main research achievements are finally outlined. Besides, some of the most relevant issues to focus on in the future will be discussed as potential directions toward a further enhancement of the modelling framework described in this Thesis.

8.1 Conclusive overview

In the previous Chapters, we have found that the establishment of novel biofuels productions poses several challenges mainly related to the economic feasibility of the business and the environmental sustainability of the system. The deriving question cannot be faced through the traditional approaches mainly based on heuristic or simulation methods and limited to a narrow view of the problem often focussed on the mere design of the production process.

Thus, the objective of the project was to develop a decision-making tool to support strategic policies on biofuels production systems. The proposed modelling framework was based on an MILP mathematical formulation and adopted a SCM approach. The model application and capabilities were illustrated outlining the optimal configuration of a real world case study, namely the bioethanol supply chain for automotive vehicle use in Northern Italy.

The geographical and technological features of the case study were firstly assessed through the economic and environmental evaluation of the network nodes. These issues, along with the detailed characterisation of the SC nodes categories in terms of modelling parameters through SCA and LCA techniques were reported in Chapter 3.

Once the case study definition was completed, the optimisation of the bioethanol SC was carried out through the modelling framework formulation and application. This step of the study has gone through two main logic strands. Bioethanol production were assessed considering a wide range of inherent questions, i.e. costs minimisation, global warming mitigation and profit maximisation, which have been step by step faced and discussed. This resulted in the formulation of four distinct models to describe specific issues related to the SC assessment.

The first model consisted in a spatially explicit steady-state MILP addressing the design of the bioethanol SC under costs minimisation. Key decisions to be taken involved (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 and (v) distribution processes for biofuel to be sent to blending terminals. The system was assessed considering two ethanol demand scenarios inferring from the ethanol market penetration imposed by the current Governmental policy. For each scenario, two optimisation instances were carried out to compare the present Italian industrial plan to the best SC design obtainable without imposing any constraints on plant location or capacity. An additional analysis was performed to assess the effective implications entailed in the use of domestic biomass rather than imported one. The results reported in Chapter 4 evidenced that the industrial plan as conceived does not represent the best SC design choice: it differs from the optimal network configuration for what concerns both the location and the capacity assignment of the production plants. It was also showed the economic convenience in availing of biomass importation from Eastern European Countries: despite the higher transport costs due to corn shipping and the consequent distribution to conversion plants, the lower purchase cost entails a consistent operating costs reduction. Another important conclusion, which can be drawn from the static model implementation, is that the economic feasibility of the business under assessment tightly depends on the cost allocation assigned to DDGS when used as animal feed substitute due to its effect on operating costs reduction. The proposed modelling framework is capable of analysing and optimising some of the crucial factors underpinning the design of a biofuel SC. However, there are still a number of open issues concerning the system environmental impact and its financial performance in a long-term and uncertain market scenario.

Chapter 5 aimed at analysing both the environmental and economic questions through an MoMILP model based on the steady-state spatially explicit MILP described in Chapter 4. This model was enhanced by embodying environmental objectives to the optimisation criteria previously considered. Stating the same key decisions to be taken, the bioethanol SC was designed by simultaneously accounting for costs and GHG emissions minimisation. The case study allowing for corn importation described in Chapter 4 was taken as reference to formulate a new case study for the multi-objective modelling framework addressed in Chapter 5. The ethanol market penetration imposed by the current Italian regulation for 2010 was assumed as the only demand scenario to design the corn-based ethanol SC. As a first instance, we considered that the DDGS would be used as animal feed with the corresponding allocation of SC operating costs and GHG emissions. The MoMILP model implementation resulted in a trade-off set of non-inferior (or Pareto optimal) solutions which confirmed the expected conflict existing between environmental and economic performance. The economic optima still involves biomass importation from Eastern European Countries and production plants of the maximum capacity. Although the system would perform well from the economic standpoint, this solution would not allow for feasible environmental performance since they

do not match the EU emissions limits. However, even by pushing the design toward the environmental optima, the supply system still does not satisfy the EU standards, although a sensible deterioration of the system economics. The second instance considered DDGS as a fuel for CHP stations. Interestingly, the usage of DDGS as fuel to produce heat and power would allow to reach the GHG mitigation necessary to meet the EU standards due to the higher amount of emission credits assigned to this solution.

The third step into the modelling framework development was dedicated to a more comprehensive analysis, also including financial features. Chapter 6 aimed at evaluating the effects of market uncertainty in terms of ethanol market price and corn purchase costs in order to evaluate the effective performance of the system from a financial risk standpoint. The steady-state formulation previously adopted was replaced by a dynamic one aiming at taking into account the market volatility over a long-term horizon. Key decisions to be taken in the design and planning under uncertain conditions involved (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) biofuel market demand satisfaction rate, (vi) distribution processes for biofuel to be sent to blending terminals. The optimisation problem were addressed by formulating two alternative case studies referring to two likewise objectives. On one hand, we considered the eNPV maximisation, oriented to optimise the financial profitability of the system as the best NPV over the whole set of scenarios; on the other hand, a CVaR maximisation was implemented, allowing for a reduction on the risk on investment through a maximisation of the NPV over the worst scenarios. The effect of DDGS price fluctuations were assessed by implementing a sensitivity analysis on the optimisation results of the two cases. The results show the high reliance for the business profitability on revenues coming from the side production of DDGS. The design through eNPV maximisation suggested that there is always a reasonable probability to obtain profitable results even when it is assumed that the DDGS price may decrease along the years. On the other hand, if only the worst market scenarios are considered (CVaR maximisation), the results show that only a high DDGS selling price allows for a profitable configuration, otherwise the best solution is not to enter the business.

What we may conclude from the whole set of results presented so far, is that both the economic feasibility and environmental sustainability of bioethanol production in Northern Italy tightly rely on the end-use option for DDGS as valuable product for other applications. In particular, selling DDGS as an animal fodder substitute would allow for good performance in terms of both production costs and financial profitability. However, it reveals an extreme dependence on market conditions and, as already evidenced in Chapter 5, it would not allow to reach the EU targets in terms of GHG emissions saving. Thus, the further step was to investigate whether a more comprehensive optimisation taking into account cultivation practices, too, might determine a better environmental performance.

Therefore, the final modelling approach, described in Chapter 7, was oriented to address the combined financial and environmental analysis of the bioethanol production system by simultaneously optimising DDGS end-use destination and agricultural practices in terms of fertiliser dosage. Key decisions to be taken to the scope are (i) fertiliser dosage over the biomass crop field, (ii) DDGS end-use solution, (iii) NPV over a 10 years horizon and (iv) GHG emissions. The problem was referred to a fixed land surface fully cultivated to supply the biomass needs of a unique production plant of flexible capacity. The multi-objective optimisation suggested that the only way to meet both financial feasibility and the EU standards on biofuels is to adopt a technological solution envisaging the construction of a CHP station to be fuelled with DDGS. On the other hand, the crop management practices would be more sustainable, too, involving very low nitrogen dosage as mineral fertiliser so as to reach acceptable GHG emission savings with respect to gasoline production. The situation would be even more sustainable if the ethanol production is promoted by deploying governmental subsidies on renewable energy generation. This more thoughtful use of mineral fertiliser would also reduce other environmental impacts coming from fixed nitrogen application to agricultural soils like, for instance, eutrophication and acidification of the ecosystem.

8.2 Contribution of this Thesis

The work addressed in this Dissertation may be labelled according to the two main topics covered along the dissertation, namely the optimisation of bioenergy systems and the SCM through mathematical modelling. The main contribution of the project to the concerning research area, however, would not lie within any of them if considered separately.

The major novelty of the project compared with other approaches is the methodology adopted to couple the SCM tools application within the optimisation of biofuels SC. As evidenced in the literature review outlined in Chapter 1, both simulation-based and MP SCM tools have been broadly applied to optimise the design of novel biomass-to-energy supply networks. However, very limited work was found addressing the use of MP optimisation models to design a bioethanol supply system. Moreover, these contributions seem to focus on logistic optimisation rather than on the strategic design of entire infrastructures.

Therefore, the research project was thought to cover this lack of knowledge so as developing a comprehensive decision-making tool capable of steering the strategic design of first generation bioethanol production systems through a full set of optimisation features.

The main original contributions that mark the value of this work can be summarised as follow:

- 1 *Relevance and broadness of the modelling applications*: as claimed by Henning (2009), a likely reason bounding the effective industrial success of SC optimisation through mathematical modelling is the very limited application of academic models to real world case studies; this is evident in the biofuels systems optimisation area: restricted views of the problems in terms of both supply system boundaries and optimisation issues as well as a lack of real-world applications characterise most of the approaches devised to date. It is our belief, that the systematic use of MP to assess broader infrastructural problems would for sure increase the appeal of different industrial stakeholders on SC optimisation packages and on their effective application to real-world problems. In light of this, we developed a SC modelling framework capable of assessing the design of emerging biofuels systems by adopting the extended view of SCM and tailoring the problem to real applications through the adoption of actual data sets. Spatially explicit and stochastic features were also added to improve the framework capabilities to capture the reality of these applications. Moreover, the optimisation models were devised so as to empower the analysis over a full range of strategic issues: combined economic and environmental SC optimisations and the analysis of the effect of market uncertainty on the financial sustainability over a long term horizon were thereby implemented to provide a specific answer to the most concerning issues related to biofuels production.
- 2 *Assessment of the DDGS end-use effect on the system behaviour*: the combined performance evaluation in terms of both financial and environmental performance, has never been carried out before, at least considering the by-product usage technical options as a key variable of the optimisation framework. Hence, a model enabling the assessment of the optimal technical solution to simultaneously achieve the best performance in terms of market penetration and global warming mitigation were developed.
- 3 *Optimisation of both crop management practices and conversion technology features*: this represents a relevant endeavour to tune up the environmental performance of bioethanol production so as to achieve sensible reduction of GHG emissions. Although some other works have been previously attempted on the same direction, they were heuristic evaluations focussed on wheat crops as suitable biomass for alcohol production, and limited to the cultivation stage of the production system without considering technological issues or other aspects of the SC. Thus, the final approach implemented dealt with the simultaneous optimisation of DDGS end-use and nitrogen fertiliser application on corn crops through quantitative models so as to achieve concrete GHG emissions reduction together with competitive financial performance.

8.3 Future work

In conclusion, we believe that the work presented has resulted in quantitative and valuable tools capable of supporting decision-making for strategic energy sectors. However, although this Thesis discussed several questions concerning with the bioethanol SC, there are still several open issues that need further investigations. These issues can be classified into two main categories: the first one is related to modelling, while the second class concerns with the energy systems analysis.

8.3.1 Modelling issues

The variety of the analysis shown in this work, fully demonstrate the MILP formulation capabilities to fit with different design needs and to provide an exhaustive modelling tool to represent the complex behaviour of biofuels SCs. However, as new features are added to the assessment and a more representative SC characterisation is pursued, the problem might become so time consuming and large as to hamper the model solution. The problem was quite clear when the steady-state formulation was replaced by a dynamic one and price scenarios were included to handle the uncertainty (Chapter 6). This problem has required drastic simplifications and a consistent scenarios reduction to be sorted. To overcome such difficulties, new types of modelling approaches, such as decomposition methods, should be adopted along with further modelling structure simplifications in order to speed up the solution time through a problem dimension reduction that would not affect the model precision (e.g., Guillén-Gosálbez and Grossmann (2009) and Li and Ierapetritou (2009)).

8.3.2 Energy systems analysis

Other open issues relate to the analysis carried out on bioethanol production, and on energy systems in general.

With concerns to the first-generation technology here considered, a further discussion should regard the future technological learning that might affect the entire system behaviour in terms of economic and environmental performance. Hence, some of the perspectives outlined by Hettinga *et al.* (2009) can be considered so as to implement a sensitivity analysis oriented toward the assessment of the likely technological evolution effect on the competitiveness of corn-based ethanol productions against second generation technologies.

However, this comparison should be performed on the basis of equal terms and hence requiring the formulation of an equivalent optimisation framework for second generation ethanol production (similar to the one developed by Dunnett *et al.* (2008)).

In relation to the environmental performance of the system, a new approach might be adopted to minimise the GHG emissions of the system. For instance, a “carbon tax” can be assumed to assign an economic value to GHG emissions so as to evaluate the effect of environmental

penalties on the economic performance of the production system. This would also allow to assess the problem through single-objective MILP models (instead of multi-objective formulations) which would result in smaller dimension problems.

However, the proposed approach imposes to take into account the complex market features characterising the emerging carbon trade, thus requiring the enlargement of the SCM boundaries. Accordingly, a broader approach might be adopted also accounting for other market issues, such as international regulations on goods trade and import/export taxation (e.g., for what concerns biomass and DDGS). This approach is referred to as Enterprise-wide Optimisation (EWO), as defined by Grossmann (2005b).

Finally, the last issue to consider for future research routes emerges from the consideration that a biofuel production network cannot be considered as a mere closed system. On the contrary, it clearly represents a complex environment in which dynamic interactions with different energy sectors exists. In other words, it should be assessed as one of the parts of a more global energy supply system. Accordingly, a more comprehensive optimisation framework must consider the influence of other interacting energy sectors as well as integrate them in a wider problem conception. This involves a broader range of strategic decisions such as, for instance, biomass type assignment to cultivation sites, biomass type allocation to conversion technologies, biofuel type assignment and sub- and by-products end-use applications for alternative biofuel production or heat and power generation.

Appendix A

Grid-dependent Parameters

This Appendix collects the Tables summarising the grid-dependent parameters defined in Chapter 3 and subsequently used as input for the modelling frameworks.

Table A.1 Values for the squared region surfaces (GS_g) in Northern Italy.

element g	GS_g (km^2)	element g	GS_g (km^2)	element g	GS_g (km^2)
1	1875	21	2500	41	2500
2	2500	22	2500	42	2500
3	1500	23	1250	43	1500
4	1250	24	2000	44	2500
5	1000	25	2500	45	2500
6	1250	26	2500	46	1750
7	2000	27	2500	47	2000
8	2500	28	2500	48	2500
9	2500	29	2500	49	2500
10	2500	30	2500	50	2500
11	2500	31	2500	51	2500
12	1250	32	1500	52	1000
13	2000	33	750	53	1000
14	2250	34	250	54	1500
15	2500	35	2500	55	1500
16	2000	36	2500	56	2500
17	2500	37	2500	57	2500
18	2500	38	2500	58	2500
19	2500	39	2500	59	1750
20	2500	40	2500	60	200000

Table A.2 Input values for blended fuel demand in each discrete region g (DEM_g).

element g	DEM_g (t/d)	element g	DEM_g (t/d)	element g	DEM_g (t/d)
1	64.85	21	287.67	41	314.40
2	86.47	22	257.65	42	291.45
3	51.88	23	323.54	43	153.72
4	49.47	24	334.87	44	105.36
5	161.49	25	316.99	45	148.70
6	43.71	26	249.91	46	286.78
7	131.44	27	1884.43	47	255.39
8	110.73	28	345.71	48	159.78
9	100.51	29	348.43	49	263.90
10	110.98	30	401.37	50	361.97
11	213.36	31	492.53	51	324.51
12	107.21	32	291.60	52	138.81
13	76.92	33	144.69	53	121.44
14	149.39	34	188.16	54	174.70
15	524.46	35	340.28	55	239.51
16	816.23	36	238.04	56	368.01
17	477.83	37	198.94	57	377.61
18	302.34	38	198.59	58	387.85
19	191.18	39	187.63	59	271.49
20	312.26	40	234.36	60	492.53

Table A.3 Biomass cultivation input parameters.

region <i>g</i>	CY_g (t/d·km ²)	BCD_g^{max} (km ² /km ^{2†})	AD_g (km ² /km ^{2‡})	$UPCb_g$ (€/t)	region <i>g</i>	CY_g (t/d·km ²)	BCD_g^{max} (km ² /km ^{2†})	AD_g (km ² /km ^{2‡})	$UPCb_g$ (€/t)
1	1.9	0.00	0.10	145.6	31	3	0.44	0.70	130.2
2	1.9	0.00	0.10	145.6	32	2.7	0.50	0.65	131.3
3	1.9	0.00	0.10	145.6	33	2.9	0.54	0.75	130.5
4	2.0	0.00	0.10	141.6	34	2.4	0.00	0.10	135.1
5	2.2	0.05	0.10	137.2	35	3.1	0.22	0.38	130.2
6	2.3	0.00	0.10	136.2	36	2.3	0.23	0.42	135.3
7	2.2	0.07	0.15	137.1	37	1.7	0.23	0.58	152.8
8	1.2	0.00	0.20	195.2	38	2.6	0.21	0.39	132.3
9	1.4	0.01	0.20	174.4	39	3.2	0.19	0.67	130.3
10	2.1	0.18	0.20	141.3	40	3.1	0.24	0.89	130.2
11	2.9	0.56	0.25	130.4	41	2.9	0.27	0.73	130.5
12	2.9	0.55	0.10	130.4	42	2.4	0.46	0.81	134.0
13	1.8	0.00	0.10	151.3	43	2.4	0.46	0.73	133.8
14	2.1	0.04	0.10	140.0	44	2.3	0.17	0.29	135.5
15	2.5	0.12	0.15	132.7	45	2	0.14	0.28	142.7
16	2.4	0.12	0.25	134.7	46	1.8	0.10	0.13	151.4
17	4.0	0.15	0.25	134.8	47	2.2	0.10	0.15	138.4
18	2.8	0.19	0.20	130.8	48	2.9	0.05	0.15	130.4
19	1.4	0.08	0.20	170.1	49	2.9	0.07	0.50	130.6
20	2.5	0.25	0.32	133.1	50	2.7	0.11	0.60	131.7
21	2.5	0.39	0.45	133.4	51	2.3	0.17	0.72	135.8
22	2.9	0.56	0.74	130.4	52	2.2	0.20	0.75	138.6
23	2.7	0.37	0.33	131.1	53	0	0.00	0.20	195.2
24	3.4	0.24	0.10	130.7	54	0.5	0.01	0.10	197.3
25	3.0	0.34	0.43	130.3	55	1.8	0.02	0.15	151.3
26	2.7	0.45	0.80	131.5	56	2.8	0.08	0.15	131.1
27	3.1	0.31	0.72	130.2	57	2.5	0.08	0.20	133.0
28	3.7	0.32	0.88	132.0	58	2	0.06	0.25	142.4
29	3.3	0.28	0.60	130.4	59	2	0.06	0.40	142.4
30	2.6	0.31	0.50	131.8	60	3	1.00	1.00	114.6

†ratio between km² of corn crops and km² of total arable land

‡ratio between km² of arable land and km² of regional surface

Appendix B

Secondary Distribution Model

The mathematical formulation of the secondary distribution model used to evaluate the biofuel demand is reported here. The objective function to be minimised is given by the transport operating costs TOC .

Transport operating cost (TOC)

$$TOC = GC + MC + LC + FC \quad (B.1)$$

$$FC = \sum_{d,g} FP \cdot 2 \cdot DD_{d,g} \cdot \frac{Q_{d,g}}{FD \cdot TCap} \quad (B.2)$$

$$LC = \sum_{d,g} DW \cdot \left(\frac{Q_{d,g}}{TCap} \cdot \left(\frac{2 \cdot DD_{d,g}}{SP} + LTU \right) \right) \quad (B.3)$$

$$MC = \sum_{d,g} ME \cdot \left(\frac{2 \cdot DD_{d,g} \cdot Q_{d,g}}{TCap} \right) \quad (B.4)$$

$$GC = \sum_{d,g} GE \cdot \left(\frac{Q_{d,g}}{TMA \cdot TCap} \cdot \left(\frac{2 \cdot DD_{d,g}}{SP} + LTU \right) \right) \quad (B.5)$$

Constraints

$$Q_{d,g} = Z_{d,g} \cdot DEM_g \quad \forall g, d \quad (B.6)$$

$$THR_d^{\max} \geq \sum_g Q_{d,g} \quad \forall d \quad (B.7)$$

$$\sum_d X_{d,g} \leq 1 \quad \forall g \quad (B.8)$$

$$DEMT_d = \sum_g Q_{d,g} \quad \forall d \quad (B.9)$$

Appendix C

Secondary Response Curves

Firstly, the DDGS protein content (DDGS-PC) dependence on nitrogen application has been derived by simply multiplying $PC(N)$ by a conversion factor defined as follows: the standard protein content of DDGS has been divided by the related wheat grain protein content so as to obtain a constant conversion factor of $3.97 \text{ \%}_{\text{grain PC}}/\text{\%}_{\text{DDGS PC}}$ (this value is confirmed by confidential information). Now the soy-meal replacement factor has been estimated by comparing the relative protein content of the two products as indicated by CONCAWE (2003). Figure C.1 shows the curve as estimated and Table C.1 reports the polynomial relation coefficients related to Equation (7.25).

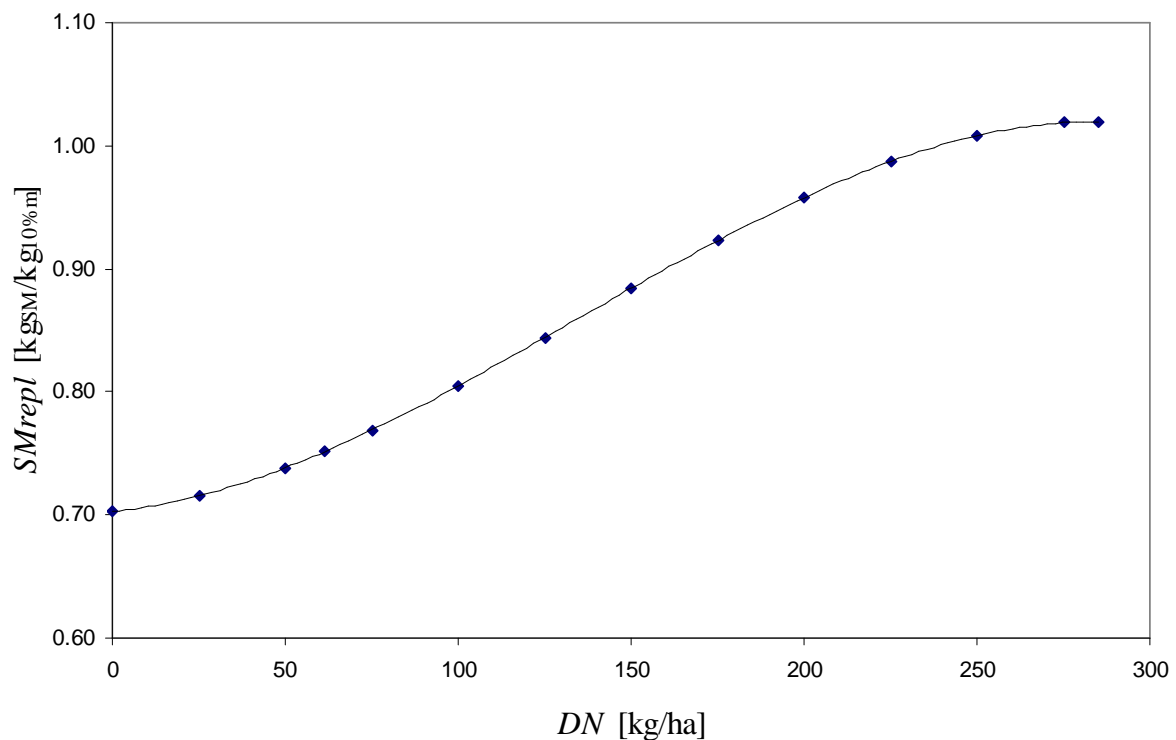


Figure C.1 Secondary response curves for wheat: soy-meal replacement factor.

Table C.1 Response curves polynomial coefficients for soy-meal replacement factor.

	A	B	C	D
SMrepl	-2.2×10^{-7}	9.37×10^{-6}	2.45×10^{-4}	0.703

It is important to highlight that the DDGS quantities are always expressed accounting for a 10% of moisture following its standard characteristics. Accordingly, the DDGS yield (*DDGSY*) has been derived from the relation indicated by Berry *et al.* (2008) and adapted to the moisture content: this relation represents the DDGS yield as a function of protein content and is formulated as follows:

$$DDGSY(t_{DDGS10\%m} / t_{DM}) = 1.11 \cdot (295 + PC(g / 100g) \cdot (7.2 \cdot 0.789)) \quad (C.1)$$

Figure C.2 depicts the response curve related to DDGS yield and Table C.2 the polynomial coefficients of Equation (C.1).

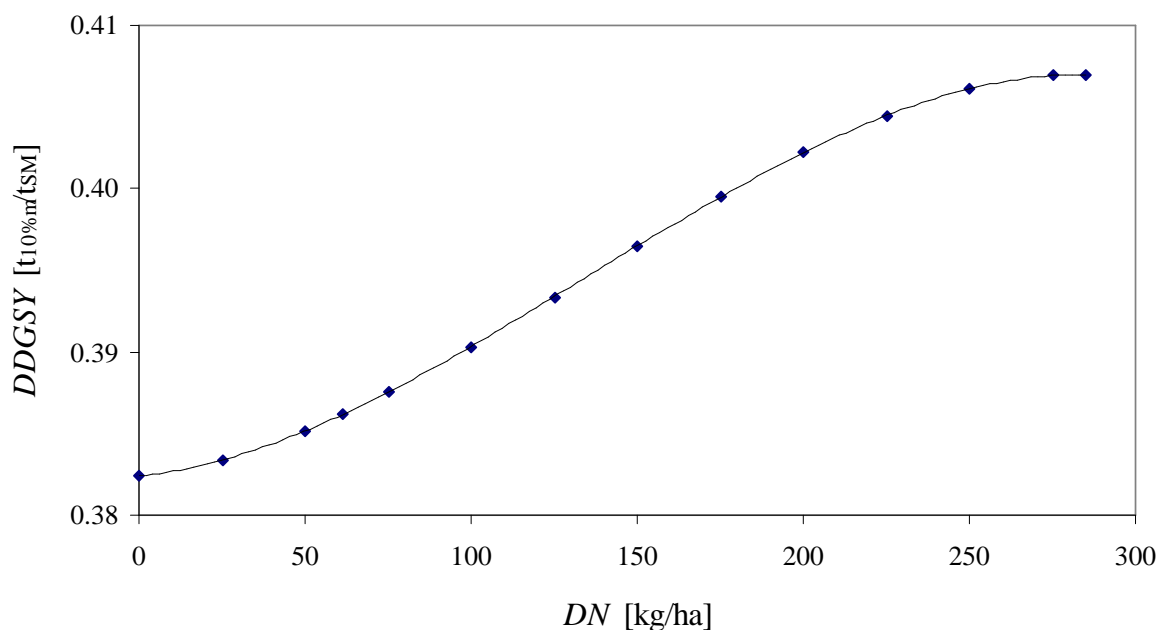


Figure C.2 Secondary response curves for wheat: DDGS yield.

Table C.2 Response curves polynomial coefficients for DDGS yield.

	A	B	C	D
DDGSY	-2.0×10^{-9}	8.0×10^{-7}	2.0×10^{-5}	0.382

Appendix D

Response Curves for Corn

The wheat primary response curves depicted in Chapter 7 (Figure 7.1) and the secondary ones derived in Appendix C (Figure C.1 and C.2) have been adapted to corn cultivation by harnessing the limited data retrieved in literature.

With concerns to corn grain yield (*GY*), data reported by Grignani et al. (2007) evidenced a pretty similar trend between the two different cereal cultivations. In particular, the corn yield data can be thoroughly fitted through an upward translation of the wheat-*GY* curve (see Figure 7.1) by a constant bias of about 3.3 t/ha. This allows obtaining the corn-*GY* response curve depicted in Figure D.1.

The corn grain protein content (*PC*) dependence on nitrogen dosage has been obtained with the same procedure by using literature data from Ibrahim and Kandil (2007). Accordingly, the wheat-curve translation quota results equal to 0.66 percentage units. The resulting corn-*PC* curve is shown in Figure D.1.

The procedure to derive the ethanol yield (*EY*) response for corn crops needed some further simplifications and assumptions, and is listed below:

- 1 corn grain starch content (*SC*) varies as it varies the wheat one, thus *SC* dependence on *PC* for wheat is assumed to equal to the one for corn;
- 2 *EY* is a function of grain starch content and it does not depend on the cereal species.

Once the corn grain *PC* dependence on nitrogen dosage is known and assuming the wheat specific relations, $SC = f(PC)$ and $EY = f(SC)$, equal to the corn ones, the *EY* dependence on nitrogen application can be derived by assuming a standard composition for corn grain (providing an average content of 75% of starch and 8.9% of protein) and hence fixing the resulting *PC* (*SC*) punctual value. Accordingly, we obtain the *EY* response curve shown in Figure D.1.

Now, given the fundamental relations just defined the secondary response curves can be derived by applying the procedure reported in Appendix C. The DDGS yield (*DDGSY*) has been derived from the relation indicated by Berry *et al.* (2008) and adapted to corn cultivation through specific data retrieved in Arosa et al. (2008). Figure D.2 describe the secondary response curve for corn cultivation.

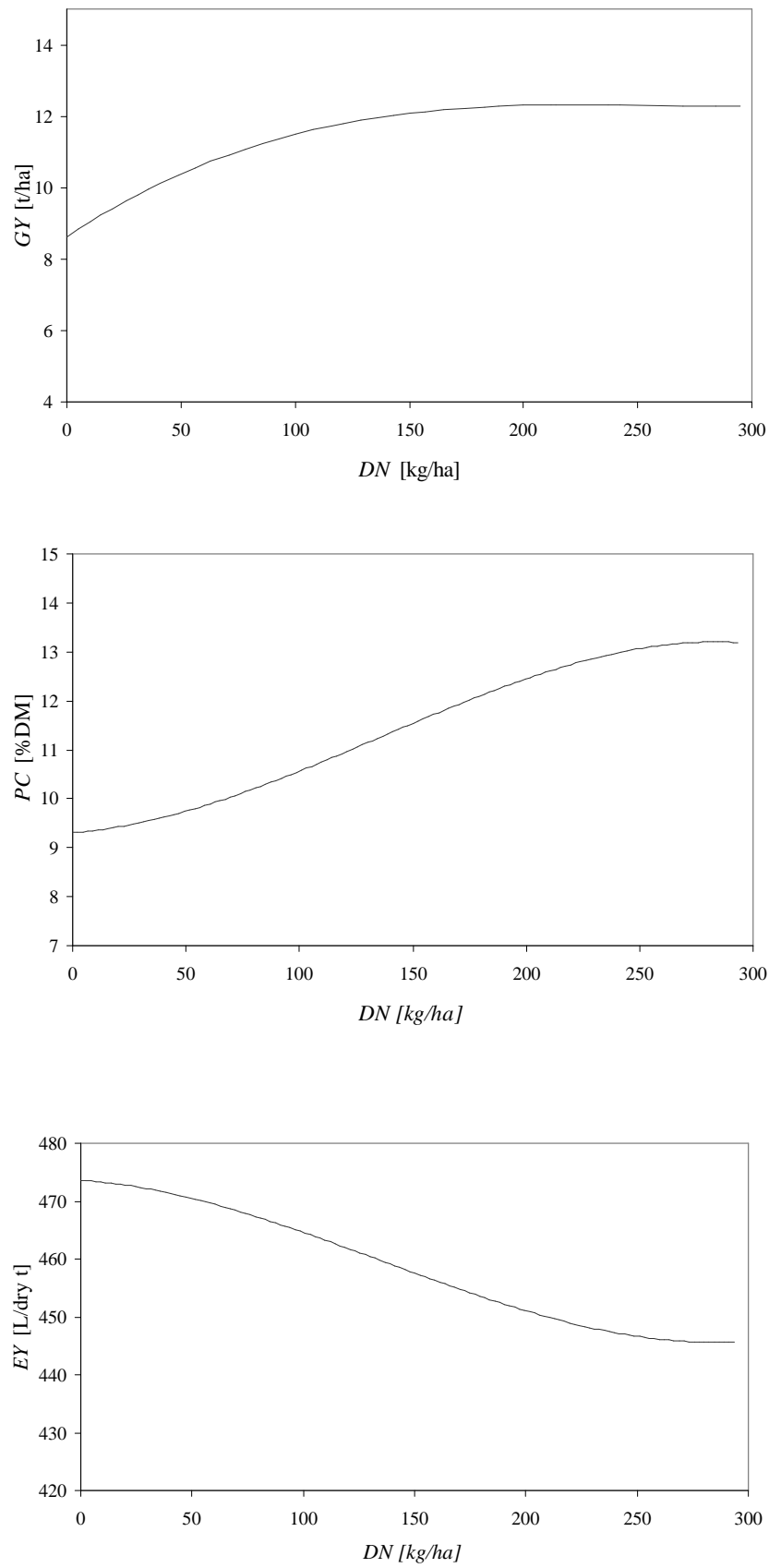


Figure D.1 Response curves as adapted for corn cultivation.

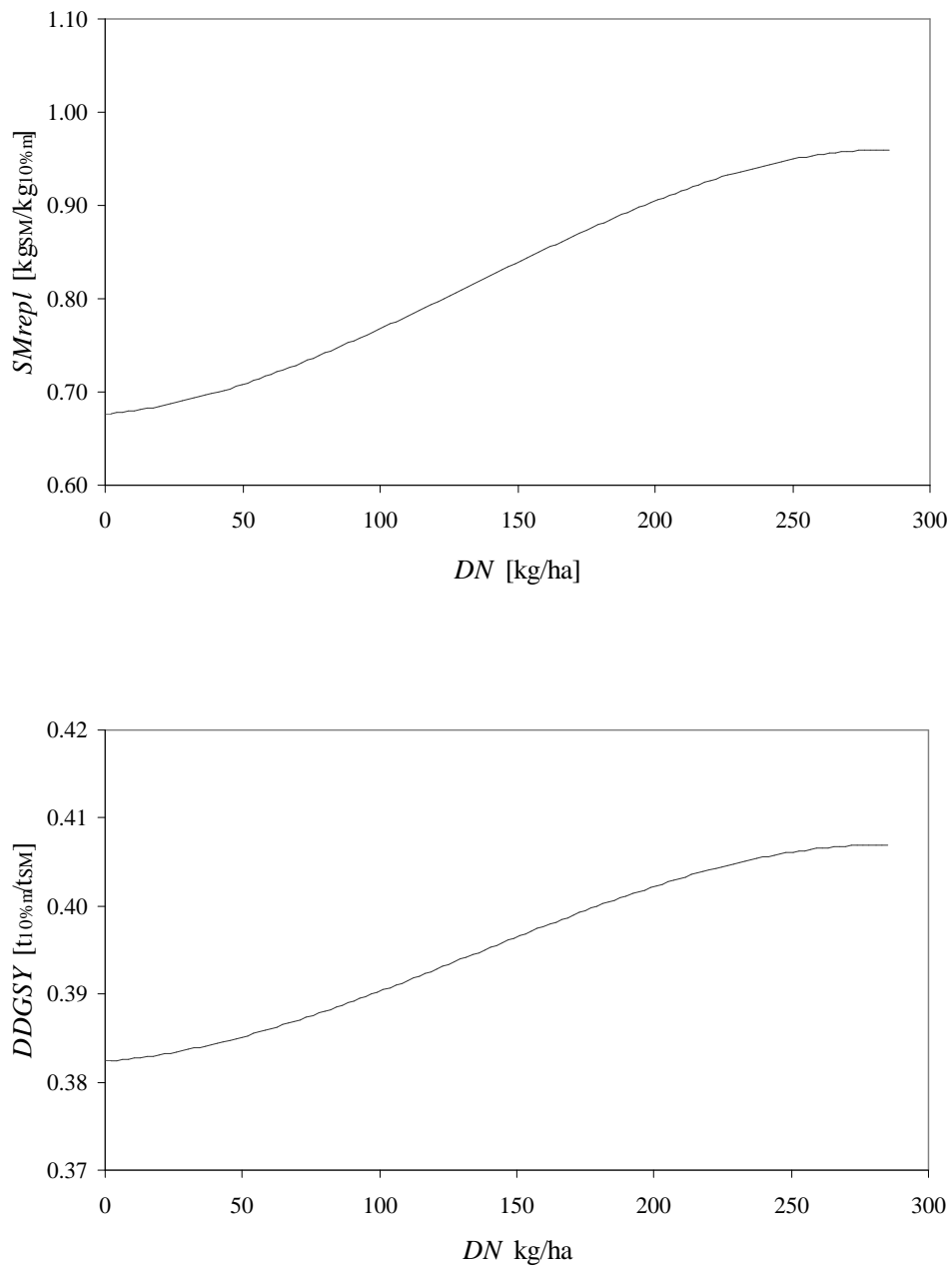


Figure D.2 Secondary response curves for corn cultivation.

Finally, the whole set of response curves here drawn for corn cultivation has to be discretised according to the mathematical formulation outlined in Chapter 7. Hence, the response curves take the discrete form represented by the step lines of Figure D.3 and D.4.

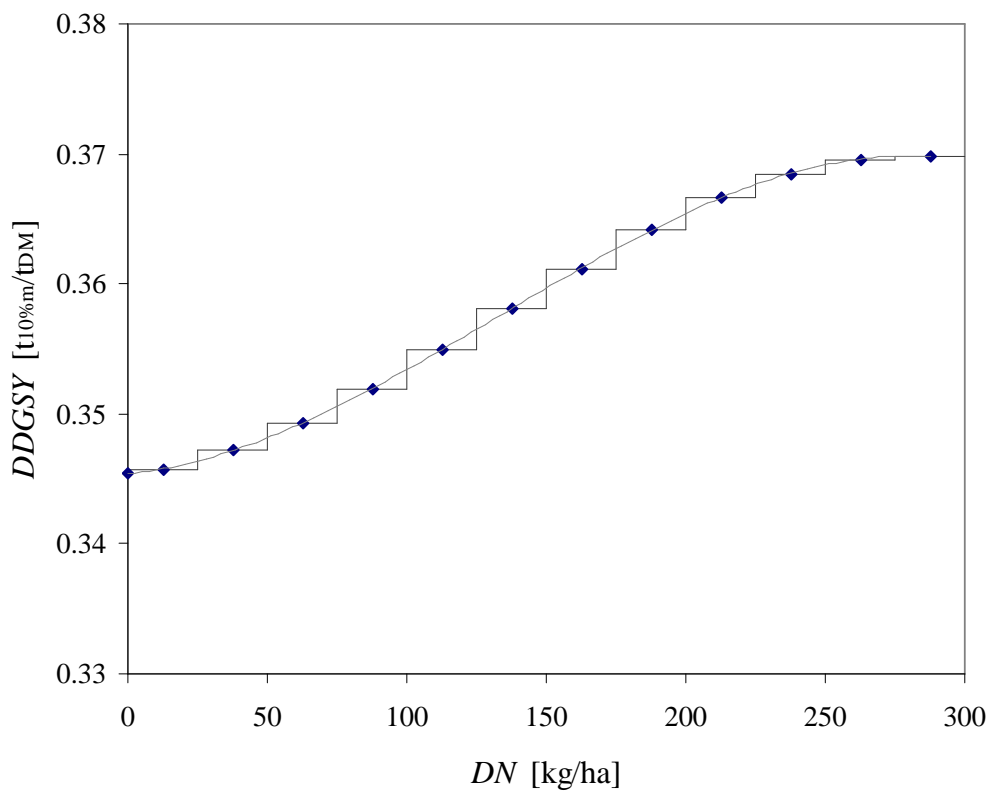
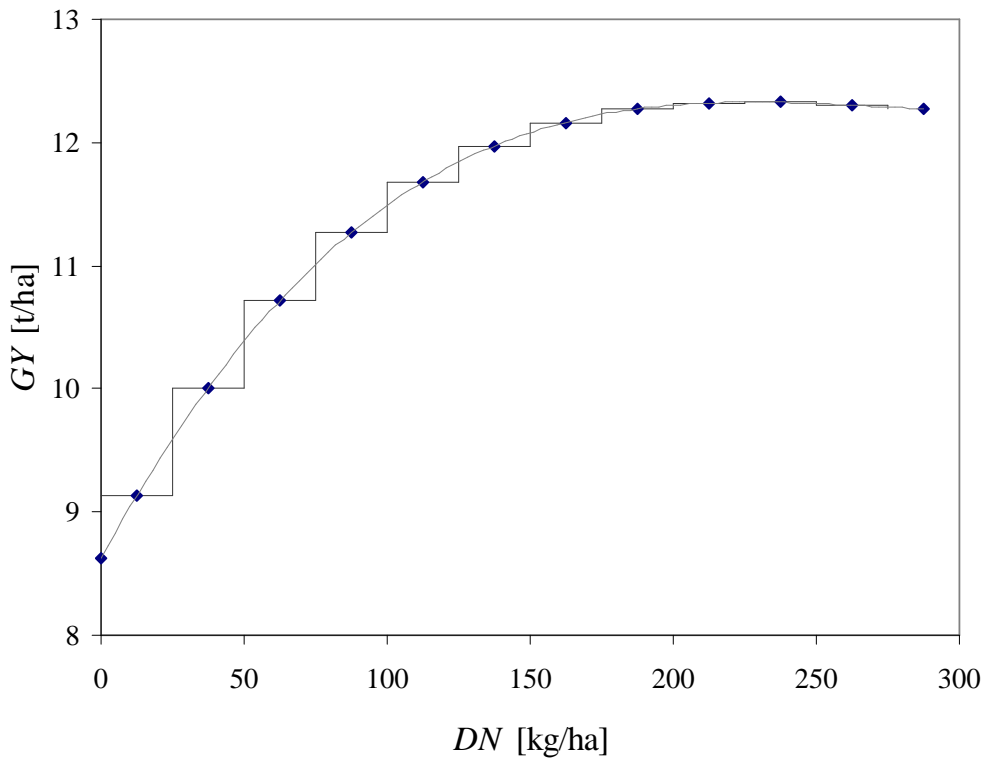


Figure D.3 Response curves discretisation (a).

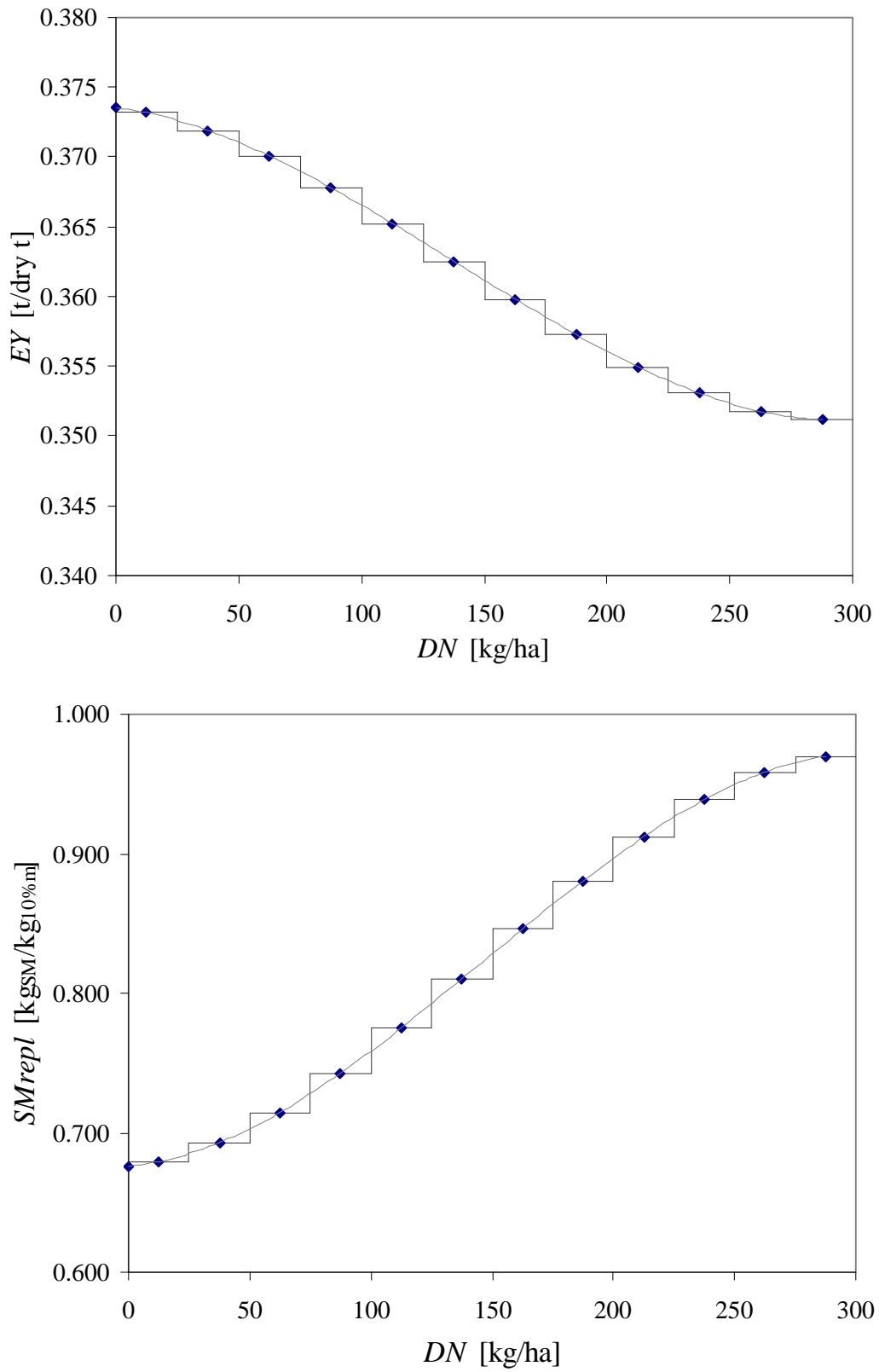


Figure D.4 Response curves discretisation (b).

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